INVESTIGATION OF WATER-WASTE ROCK INTERACTIONS RELATED ENVIRONMENTAL EFFECTS IN ÇELTİKÇİ COAL FIELD, ANKARA - TURKEY

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ABSTRACT

INVESTIGATION OF WATER-WASTE ROCK INTERACTIONS RELATED ENVIRONMENTAL EFFECTS IN ÇELTİKÇİ COAL FIELD, ANKARA - TURKEY

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The purpose of this research is to investigate the water-rock interactions related acid rock drainage potential, leachate chemistry and related processes under test conditions using potential waste rock samples (Bostantepe I, Lower Çavuşlar II and Upper Çavuşlar III) of Çeltikçi formation coal deposit and to predict the drainage leachate chemistry under atmospheric given pile conditions. Mineralogic, static (acid base accounting, net acid generation) test, short-term leach test and long-term kinetic test data are collected for the investigation. The samples include silicate, oxide and hydroxide types of minerals in addition to clay, carbonate, sulphate and sulphide minerals. The ARD potentials of test samples are in the order of I>II>III and do not have acid rock drainage potential in short and long terms. Low-high metal release could occur according to the short term and kinetic leach tests. Relatively high concentrations of As, Mo and SO_4 are detected. Hydrogeochemical modeling results based on prefeasibility pile assumptions and no remediation implementations suggest that pile leachates could be in acidic character under closed CO_2 equilibrium conditions and in basic character in equilibrium with atmospheric CO_2 conditions. The maximum environmental quality limits of Al, As, Fe, Pb, V in all simulated leachates and Cd/Cr/Zn parameters in some simulated leachates for the closed CO_2 equilibrium conditions and As, Si, V in all simulated leachates and Cd/Pb/Zn parameters in some simulated leachates for the atmospheric CO_2 conditions are exceeded. Gradual conditions between the closed CO_2 and the open to atmospheric CO_2 cases would probably be developed under the field conditions. Sensitivity analyses indicate that concentrations show in general slight tendency to decrease when the infiltration amount increase, the number of rainy days decrease and the SI criteria decrease.

Keywords: Çeltikçi coal field, Acid rock drainage, static, kinetic, leach tests

ÖZ

ÇELTİKÇİ KÖMÜR SAHASI PASA KAYAÇLARININ KAYAÇ-SU TEPKİMELERİNE BAĞLI ÇEVRESEL ETKİLERİNİN ARAŞTIRILMASI, ANKARA - TÜRKİYE

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Bu araştırmanın amacı, Çeltikçi formasyonu kömür yatağına ait potansiyel pasa kayaç örneklerini (Bostantepe I, Aşağı Çavuşlar II ve Yukarı Çavuşlar III) kullanarak, su-kayaç etkileşimlerine bağlı asit kaya drenaj potansiyeli, sızıntı suyu kimyası ve ilgili prosesleri test koşullarında incelemek ve atmosferik pasa koşullarında drenaj sızıntı suyu kimyasını tahmin etmektir. Araştırma için mineralojik, statik (asit baz muhasebesi, net asit üretimi) test, kısa süreli sızıntı testi ve uzun süreli kinetik testi verileri toplanmıştır. Örneklerde kil, karbonat, sülfat ve sülfit minerallerinin yanı sıra silikat, oksit ve hidroksit mineralleri gözlenmiştir. Test numuneleri ARD potansiyelinin I> II> III diziniminde olduğu belirlenmiş ve ayrıca numunelerin kısa ve uzun vadede asit kaya drenajı potansiyeline sahip olmadıkları sonucuna varılmıştır. Kısa süreli ve kinetik sızıntı testlerine göre düşük-yüksek konsantrasyonlarda metal salınımı meydana gelebilir. Nispeten yüksek As, Mo ve SO_4 konsantrasyonları gözlenmiştir. Ön fizibilite pasa varsayımları ve iyileştirme uygulaması yapılmayacağı varsayımlarına dayalı hidrojeokimyasal modelleme sonuçları; pasa sızıntı suyunun CO_2 değişimine kapalı system koşullarında asidik karakterde ve atmosferik CO_2 koşullarında ise bazik karakterde olacağına işaret etmektedir. Sistem karbondioksit değişimine kapalı olduğunda Al, As, Fe, Pb, V konsantrasyonları tüm durumlarda ve Cd/Cr/Zn konsantrasyonları bazı durumlarda ve atmosferik CO_2 koşullarında ise As, Si, V konsantrasyonları tüm durumlarda ve Cd/Pb/Zn konsantrasyonları bazı durumlarda maksimum çevresel kalite limitlerinden fazla olabilir. Saha koşullarında muhtemelen kademeli açık-kapalı CO_2 koşulları gelişecektir. Duyarlılık analizlerine göre, infiltrasyon miktarı arttığında, yağmurlu gün sayısı azaldığında ve SI kriterleri azaldığında konsantrasyonlar genel olarak az da olsa azalma eğilimi gösterecektir.

Anahtar Kelimeler: Çeltikçi kömür sahası, Asit kaya drenajı, statik test, liç test, kinetik test

TO MY BELOVED FAMILY

FROM THEIR MIRROR…

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CHAPTER 1

INTRODUCTION

When rocks are taken out of their natural locations due to various activities (e.g. mining, tunneling, construction, etc.) and are piled as a waste under atmospheric conditions, they are subjected to chemical weathering, hence, alteration processes mainly occurring due to precipitation water-rock interactions. Such alterations are also controlled by the characteristics of the new environment and rocks (e.g., amount of water, duration of interaction, mineralogy, grain size, oxidation state, etc.). The water-rock interactions could introduce highly concentrated leachates, which could be acidic as well depending on mainly mineralogical characteristics, to the discharge environment. These drainage waters could cause environmental problems if necessary measures are not taken into consideration and are not implemented. Potentials of such environmental impacts could be assessed by hydrogeochemical prediction studies.

Çeltikçi basin rock units, located 50 km northwest of Ankara province (Figure 1.1), include coal deposits which are planned to be mined. Mining activities would produce waste rocks which will be piled in the area. Therefore, water-rock interactions for the waste rocks are needed to be evaluated and related potential impacts should be assessed.

Water-rock interactions related drainage water ion concentrations are generally determined/predicted by applying either theoretical or empirical modelling approaches. The theoretical approach is based on mineral-water reactions related thermochemical calculations (e.g., Allison et al., 1990, Parkhust and Appelo, 1999). However, especially due to solid-solution including mineral presence in the rocks, these type of models, in general, are used to study pure mineral-water interactions

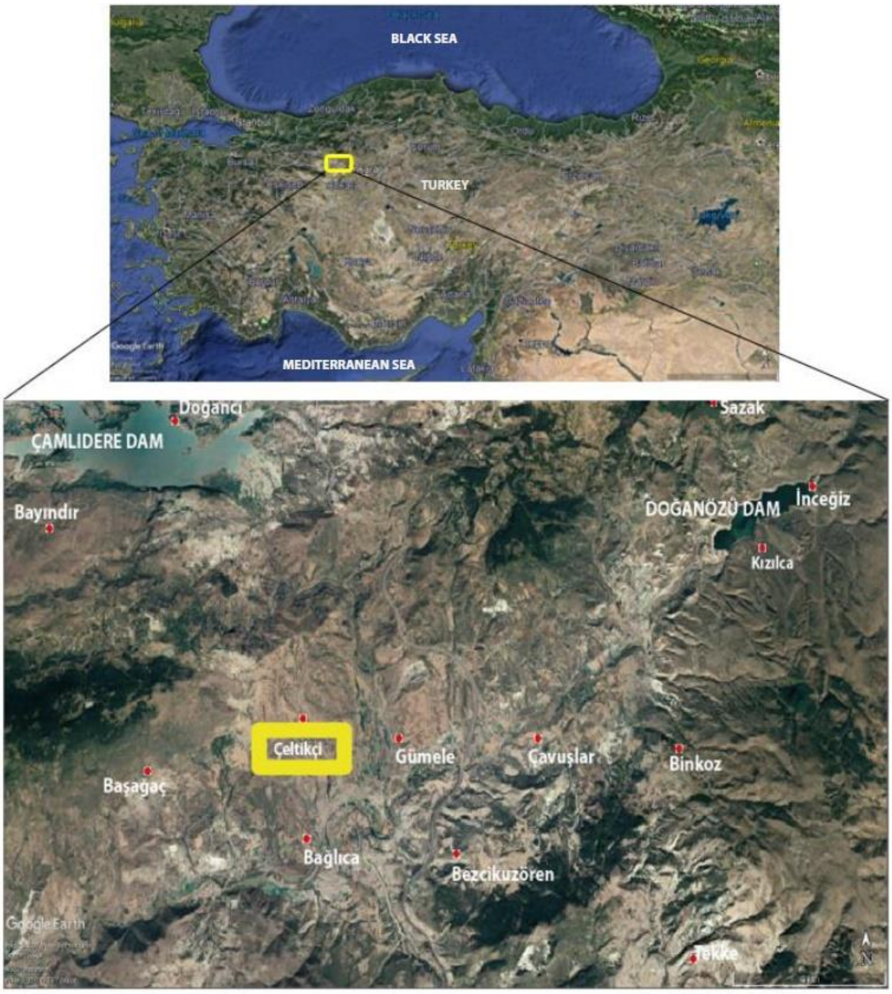


Figure 1.1. Image of the study area.

for the prediction of the drainage water chemistry. In other words, predictions of these models might not be satisfactory for natural materials unless all the solid solution properties of the minerals in the rocks are known. On the other hand, in the empirical approach, site specific kinetic test concentration results from different areas are compiled and are fitted to equations using statistical methods (e.g. Morrin and Hutt, 2001). The results of such models should be subjected to thermodynamic restrictions to finalize the drainage chemistry. Application of empirical models suggest that satisfactory predictions could be achieved depending on how close the site characteristics to those of the compiled database.

The empirical approach related models are very few and their applicability is limited to metallic mine waste rocks-water interactions because of their database restrictions. Mainly due to the lack of enough data from different areas, such models do not exist for evaluations of non-metallic ore (e.g., coal) waste rocks-water interactions. Although coal deposit waste rocks produce non-acid leachates in general, metal leaching does present. In this study, site specific data are collected from potential waste rocks of Çeltikçi coal deposit to determine potential drainage chemistry and to produce data for the development of such empirical models to apply coal fields in future.

1.1 Purpose and Objectives

The purpose of this research is to investigate the water-rock interactions related acid rock drainage potential, leachate chemistry and related processes under test conditions using potential waste rocks of Çeltikçi formation coal deposit and to predict the drainage leachate chemistry under atmospheric given pile conditions.

Mineralogic, static (acid base accounting, net acid generation) test, short-term leach test and long-term kinetic test data collected for the investigation. In order to reach the purpose, the following objectives are aimed to be accomplished.

(1) To determine bulk rock concentration anomalies.
(2) To determine neutralizing and acid producing minerals in the rocks.
(3) To estimate acid rock drainage potentials of the rocks.
(4) To determine short term (easily dissolvable) water-rock interactions related leachate concentrations under test conditions.
(5) To determine long term water-rock interactions related leachate concentrations under test conditions.
(6) To estimate potential drainage leachate concentrations of the possible waste rock pile.

CHAPTER 2

LITERATURE REVIEW

2.1 Acid Rock Drainage

Acid rock drainage (ARD), is the outflow of acidic water especially from mining operations including waste rock, tailings, and exposed surfaces in open pits and underground workings. Investigations of water-rock interactions are based on the evaluations of Acid Base Accounting (ABA), Net Acid Generation (NAG), short-term shake flask leach (SFL) and kinetic test results (EPA, 1994, MEND, 2009, GARD, 2014). These tests are used to evaluate the possible acid rock drainage potentials and metal release amounts. The MEND (2009) is considered as a pioneering guidebook for the ARD characterization in addition to the GARD (2014) guide.

Different neutralization potential (NP) and acid potential (AP) determination methodologies are available (e.g., Sobek et al, 1978; Lawrence and Wang, 1997; AMIRA, 2002). In standard ABA, AP is determined by total sulphur (%S) content that accepts all the sulphur is present as pyrite and the quantity of acid-consuming minerals is estimated by adding a known excess of acid to sample to measure the amount of acid consumed. On the other hand, in the modified ABA test, AP is determined by sulphide-sulphur (%S-S-2) content.

Variety of ARD and metal release related studied have been carried out for different mine sites in recent years (Capanema and Ciminelli, 2003; Benzaazoua et al., 2004; Weber et al., 2006; Méndez-Ortiz et al., 2007; Gautama and Kusuma, 2008; Hakkou et al., 2008; Plante et at., 2010; Campaner et al., 2014; Bouzahzah et al., 2014; Banerjee, 2014; Shoja and Salari, 2015; Gahardi and Bonotto, 2016; Qureshi and

Öhlander, 2016; Yucel and Baba, 2016; Battioui et al., 2016; Singh et al., 2017; Elghali et al., 2018).

Different chemical modeling approaches which could be grouped as empirical and theoretical, exist for the drainage chemistry predictions. Systematic empirical modeling studies have been performed by Morin and co-workers (Morin and Hutt, 1993, 1994, 2001; Morin, 1994; Morin et al., 1995; 2001). As a result, the Empirical Drainage Chemistry Models (EDCM) based on the concentration best fit relations, established using compiled kinetic test results from different metallic mine sites, are established (Morin et al., 2001). Comparisons of the predicted-observed ion concentrations from different mine sites suggest that although from different mine sites, similar models (similar concentration best fit relations) are produced. These empirical models are generally used to predict drainage chemistry for the mine sites which have lithological similarities to those of the database.

On the other hand, theoretical modeling is based on equilibrium thermodynamics approaches to the water-rock interactions. In these studies, different models such as MINTEQA (Allison et al., 1990) and PHREEQC (Parkhust and Appelo, 1999) with different databases such as WATEQ4F (Ball and Nordstrom, 1991), LLNL (Johnson et al., 1992) have been developed.

In addition to the concentration modeling, the drainage chemistry predictions require coupling of the porous media fluid flow modeling of the system (waste rock piles, open-pit areas, heap leach areas, etc.). The porous media fluid modeling approaches could also be grouped as empirical and theoretical. As to the theoretical approach, mostly the numerical solution based variety of porous media fluid flow modeling are available based on finite difference and finite element methodologies (McDonald and Harbaugh, 1988; Trefry & Muffels, 2007), which are not a subject of this study. Since mine-rock piles have rather complex hydrogeologic systems due to heterogeneities of the waste rocks and of hydraulic conductivities, a simplistic empirical model based on general knowledge and available data could be used to obtain rough estimates of the seepage chemistry through time rather than accurate predictions based on detailed simulations of their internal processes as suggested by Morin and Hutt (1994). The major factors, that should mainly be considered in a simplistic empirical model are detailed by Morin and Hutt (1994) as geochemical production rates from the kinetic tests, infiltration of water, elapsed time between infiltration events, residence time of water within a pile (generally assumed to be equal to the elapsed time) and percentage of rock surface flushed by the water flow.

The remediation of the ARD is as important as its characterization. Numerous strategies have been proposed to control ARD (e.g., Kleinmann, 1990; Johnson and Hallberg, 2005). These strategies could be grouped as chemical and biological efforts. Some major strategies include the followings: (a) addition of lime/limestone or fly ash for neutralization (Sahoo et al., 2013; Skoussen et al., 2018) processes, (b) application of permeable reactive barriers (either physico-chemical or bacterial), which includes subsurface insert of reactive materials through which a dissolved contaminant can move as it flows (Ayala-Parra et al., 2016). The remediation processes are not a subject of this study.

2.2 Çeltikçi Coal Basin

The earliest work for the coal potential in the area is conducted by MTA geologist Becker (1957a, 1957b) who recognized the coal at 38 outcrops and made descriptions of these coal seams. The area is later studied in more detail again by MTA geologists (Akyol, 1968 and Turgut, 1978) who provided certain details and prepared geological map at 1/25.000 scale. MTA started a drilling program in the region for the coal exploration. Çeltikçi coal deposit is planned to be exploited for termal power plant operation by AMM company at present. Pre-operation works are currently underway.

The major recent geological studies in the project area in detail were carried out by AMM (Asia Minor Mining) company (Rojay, 2013; AMM, 2014, 2015). The hydrochemical studies related partly to the subjects of this thesis work include studies of Yazıcıgil et al. (2014, 2015). The ARD related single static test study was performed by Gladwell et al. (2014).

The baseline hydrogeology of the area was characterized by Yazıcıgil et al. (2014). Development of groundwater flow model, dewatering system design and possible effects on groundwater for Çeltikçi coal basin were the main subjects of Yazıcıgil et al. (2015) studies. With the contribution of this study, Kahraman (2014) conducted a thesis study about hydrogeological characterization and investigation of the Çeltikçi coal basin. In these studies, it is concluded that there are three main aquifers in the study area. Stratigraphically from top to bottom, the first one is Quaternary aged alluvium deposits, the second one is Bezci-Aktepe-Kocalar unconfined aquifer, and the third one is Volcanic-Çavuşlar aquifer. Open pit dewatering system designs were simulated using groundwater flow models. It is estimated that groundwater levels could be decreased to desired levels at the earlier mine operation period but the levels could not be decreased to desired target values toward the end of operation.

Static test (whole rock, ABA, SFL) results of both coal and Çeltikçi formation rocks were evaluated for the investigation of ARD potentials by Gladwell et al. (2014). These results collected using fifty-six core samples from nine drill cores were also re-evaluated in this work in related chapters. No kinetic test has been carried out for the rocks so far.

Varlı and Yilmaz (2018) worked on surface water-groundwater interactions in the area by using thermal sensing and in-stream measurements. They concluded that the Kirmir stream channel areas can be seperated into three different sections as 1) the downstream section where the stream is gaining, 2) the upstream section where the stream is loosing and 3) the middle section where stream exhibits both gaining and losing seasonal variability.

CHAPTER 3

HYDROCHEMISTRY OF ÇELTİKÇİ FORMATION GROUNDWATER

The geological map and the generalized columnar section of the study area are shown in Figure 4.1 and **Hata! Başvuru kaynağı bulunamadı.**, respectively. The units outcropping in the area are stratigraphically lined from bottom to top as basic volcanics, Çeltikçi formation sedimentary units, Plio-Quaternary sedimentary units and Quaternary alluvium.

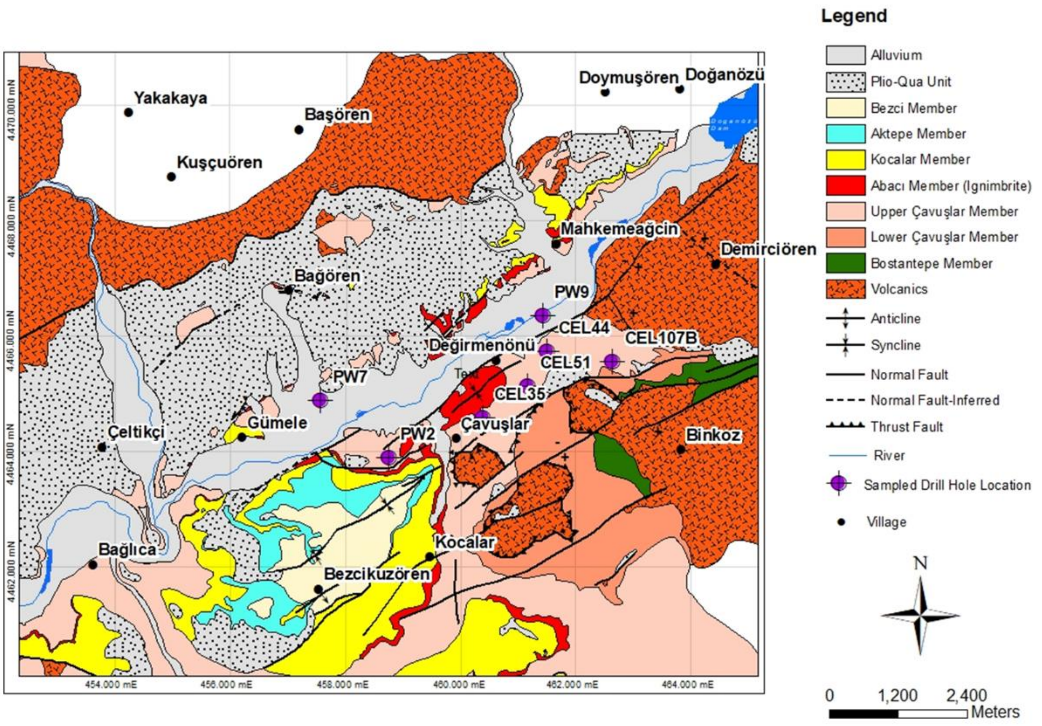


Figure 3.1. The geological map of the study area (AMM, 2015)

All Miocene units having conformable relationship in the area are named as Çeltikçi formation by AMM (2015). All mappable units within this formation are classified as members and divided into seven. These members stratigraphically from bottom to top are called as; Bostantepe, Lower Çavuşlar, Upper Çavuşlar, Abacı, Kocalar, Aktepe and Bezci. The coal levels are located at the base of the Upper Çavuşlar member. These levels have not been considered as a separate member by AMM (2015) in terms of mappability, therefore are not shown in the geological map.

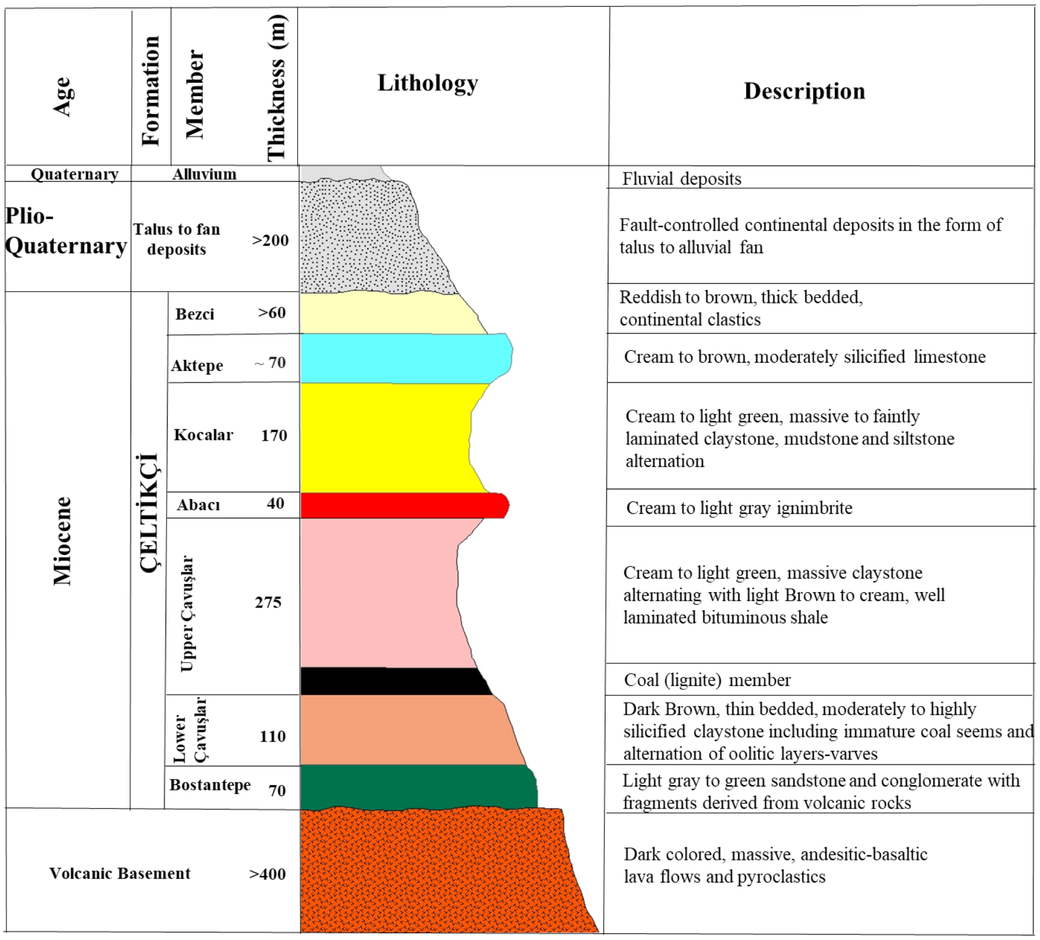


Figure 3.2. Generalized columnar section of the area (AMM, 2015)

In order to present hydrochemical characteristics and quality of groundwaters under natural conditions in the Çeltikçi formation units of Bostantepe member, Lower Çavuşlar member and Upper Çavuşlar member, whose rock samples are used for the tests performed in this work, water quality data of Yazıcıgil et al. (2015) collected from the wells representing groundwaters of these units are evaluated. The water quality data are given in Appendix-F. The locations of the wells are shown in Figure

3.1. CEL107B well filtrates Bostantepe (BT) units (represented by Sample I in this work); CEL35, CEL44 and CEL51 wells filtrate Lower Çavuşlar (LC) units (represented by Sample II in this work) and PW2, PW7 and PW9 wells filtrate Upper Çavuşlar (UC) units (represented by Sample III in this work). PW7 and PW9 wells additionally filtrate alluvium unit as well. Among the UC wells, PW2 well filtering low hydraulic conductivity (1.84X10^{-8} m/s) possessing claystone unit is not actually a representative well for the UC units. However, it is included here to show the extent of some possible deviations.

Average values of electrical conductivity (EC), pH, oxidation-reduction potential (ORP) and dissolved oxygen (DO) measured by Yazıcıgil et al. (2015) in the well waters are listed in Table 3.1 and the unit based averages are shown in Figure 3.3 where PW2 is not included into the unit-based average.

Table 3.1. Field parameter measurements in the wells (Yazıcıgil et al., 2015).

Average	**EC (μS/cm)25C**	**pH**	**ORP (mv)**	**DO (mg/l)**	**Lithology**
PW2*	2011	9.35	-20	3.33	Upper Çavuşlar
PW7	770	7.6	105	8.20	Al + Upper Çavuşler
PW9	412	8.04	7	6.93	Al + Upper Çavuşler
CEL35	878	8.14	-57	3.26	Lower Çavuşlar
CEL44	729	9.24***		9.20	Lower Çavuşlar
CEL51	1027	9.4***		7.30	Lower Çavuşlar
CEL100**	856	7.98	-32	2.16	Lower Çavuşlar
CEL104**	1050	7.51	-42	2.34	Lower Çavuşlar
CEL107A**	1006	7.88	-26	2.30	Lower Çavuşlar
CEL107B**	747	8.01	-17	2.82	Bostantepe

* Very Low Hydraulic Conductivity, **No lab anaylses, *** Possible drilling mud effect

The unit based average electric conductivity (specific conductivity) values are ordered as Lower Çavuşlar (924 μS/cm) > Bostantepe (747 μS/cm) > Upper Çavuşlar (591 μS/cm) groundwaters. Very high EC value in PW2 well water filtered from claystone is related to the longer water-rock reaction time due to low hydraulic conductivity.

All groundwater samples are in basic character in Table 3.1. The unit based average pH values increasing from upper to the lower units are 7.82, 7.88 and 8.01 in the UC (excluding PW2), LC (excluding CEL44 and CEL51) and BT groundwaters, respectively in Figure 3.3.

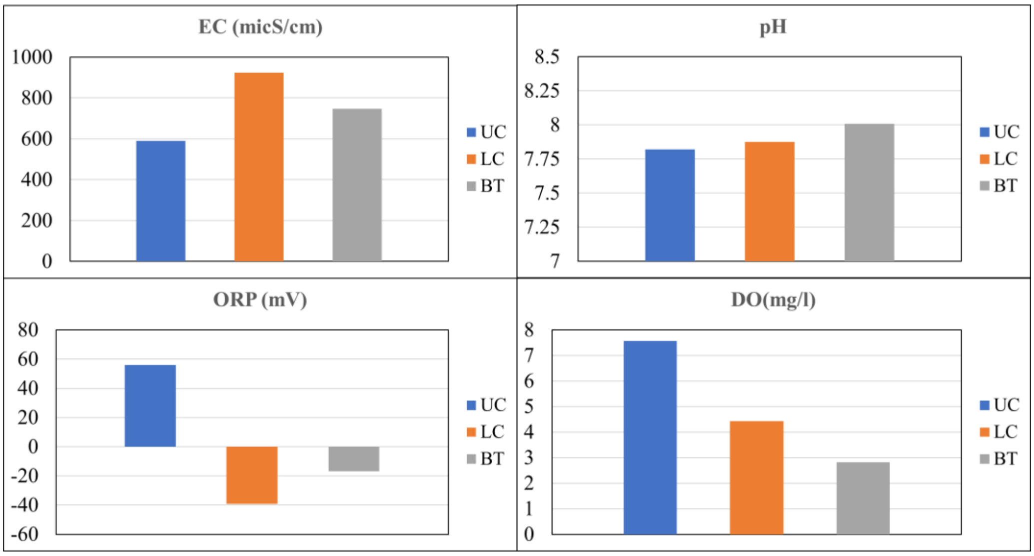


Figure 3.3. Lithology-based average values of pH, EC, DO and ORP in groundwaters.

The unit based dissolved oxygen values in the groundwaters (7.57 mg/l, 4.43 mg/l and 2.82 mg/l in UC, LC and BT, respectively) decrease from upper to the lower units. Relatively high DO value of the UC groundwater is probably reflecting partly alluvium unit groundwater effect.

The ORP values are in reducing character in relatively deeply circulating groundwaters of BT and LC units. The unit based average values of 56 mV, -39 mV and -17 mV are determined in UC, LC and BT groundwaters, respectively.

Major ion concentration shown in Figure 3.4. The Upper Çavuşlar well waters (PW7 and PW9) are in Mix-HCO_3 type facies and probably partly reflecting the alluvium groundwater effect. PW2 water is in Na-Cl facies and as mentioned earlier this different facies is related to the lower hydraulic conductivity of the unit where PW2 is filtered. The Lower Çavuşlar groundwater (CEL35, CEL44 and CEL51) on the other hand is in Mg-HCO_3 facies. There is no available data for Bostantepe groundwater.

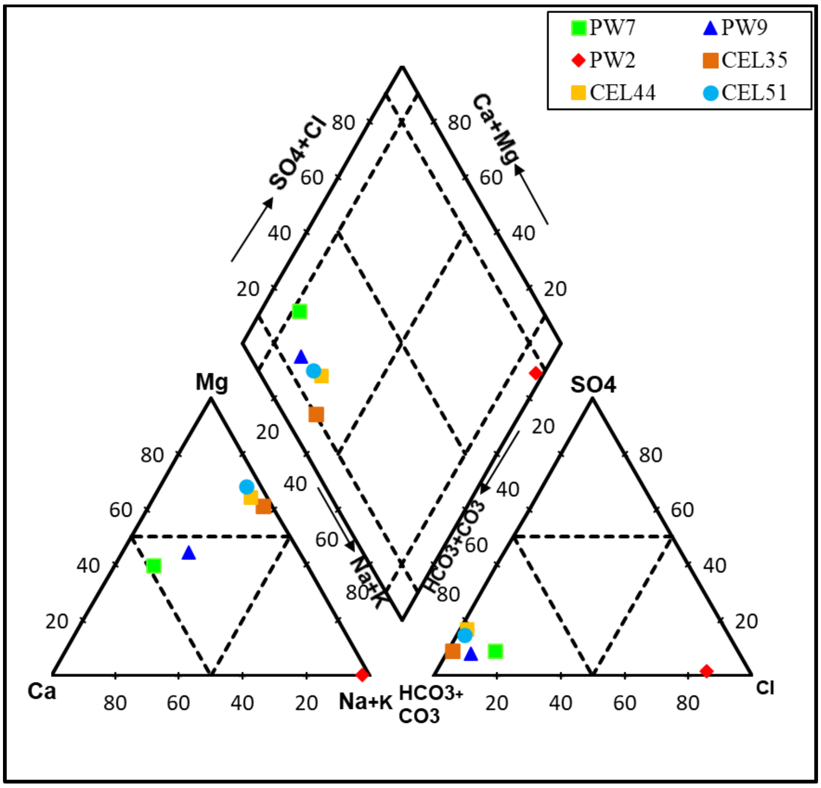


Figure 3.4. Piper diagram showing groundwater facies of Çeltikci formation.

The distributions of the trace elements which have greater concentrations than the detection limits in the sampled waters are shown in Figure 3.5. In general, the concentrations are higher in Lower Çavuşlar groundwater. In order to provide means of comparison with the later ARD related leachate concentrations, the distribution of metal concentrations in the Ficklin graph is also plotted (Figure 3.5) where detection limit concentrations are taken as zero. According to the graph, all groundwater concentrations fall into the near neutral-low metal area although three samples plot close to the near neutral-high metal boundary.

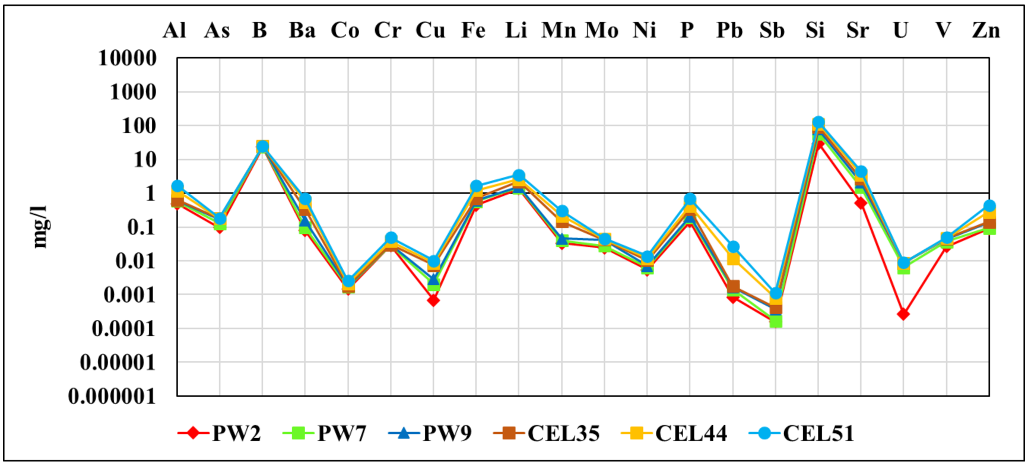


Figure 3.5. Trace element concentrations of the groundwater samples.

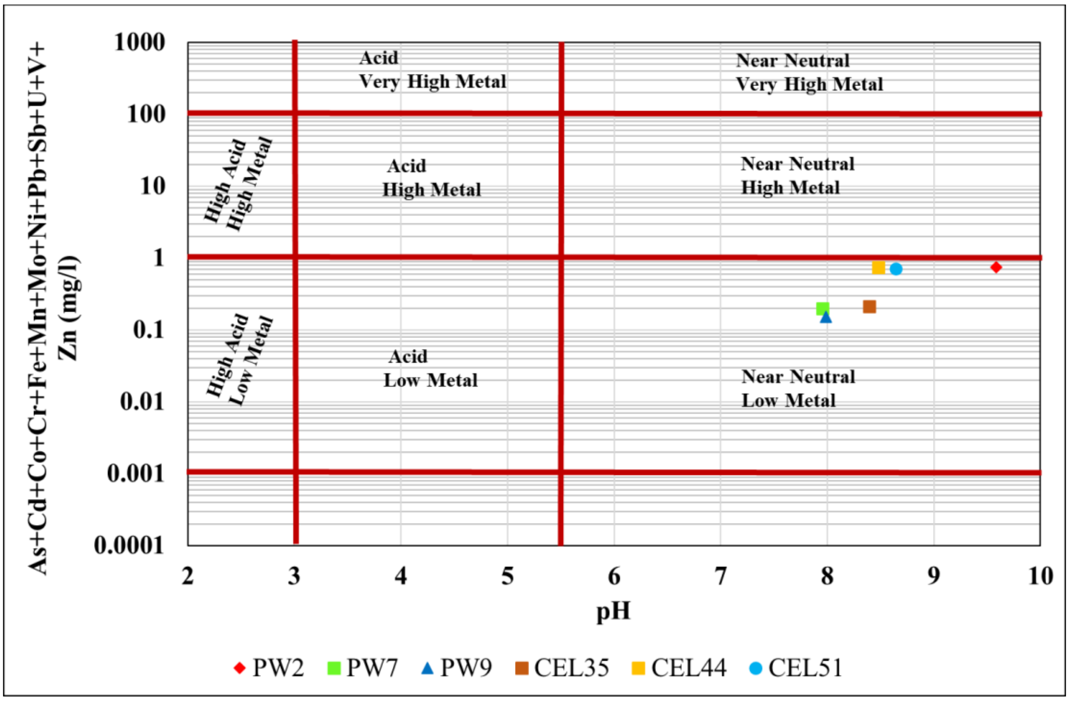


Figure 3.6. Groundwater concentrations in Ficklin leachate categorization diagram.

3.1 Groundwater Quality

In oder to compare the groundwater quality results with those of waste rock leachates that will be determined/estimated in this study, the leachate quality evaluation criteria of (a) limits for the surface water classification (SWC) and maximum environmental quality (MEQ) for rivers of MFW (2016) and (b) waste categorization (WC) limits of MEF (2010) are used to determine the quality of groundwaters. The results are given in Table 3.2. Groundwater quality according to the surface water quality limits and waste categorization criteria.

Table 3.2. Groundwater quality according to the surface water quality limits and waste categorization criteria.

Sample Name	**SWQR (MFW,2016)**	**MEQ (MFW,2016)**	**WC (MEF, 2010)**
PW2	Class IV- COD,EC,N(Kjel),pH	Al, As, B, Fe, Si	Non-Hazardous - As, Cl
PW7	Class II- DO,EC,N-NO3,o-PO4	Al, Fe, Si	Inert
PW9	Class II- DO,EC,o-PO4	Al, Si	Inert
CEL35	Class II- DO,EC,N(Kjel),o-PO4,P(t)	Cu, Si	Inert
CEL44	Class II- EC,N(Kjel),o-PO4,P(t)	Al, Fe, Si	Inert
CEL51	Class III- o-PO4,P(t)	Al, Fe, Pb, Si	Inert

According to the waste categorization limits, all groundwater samples are in “Inert” class except that of PW2 which is classified as Non-Hazardous class due to high As and Cl concentrations. According to the surface water classification, PW7 and PW9 waters filtered from Upper Çavuşlar unit are classified as Class II (Slightly Contaminated) due to high DO, EC, o-PO_4, and N-NO_3 concentrations. Unlike these groundwater samples, PW2 also filtered from Upper Çavuşlar unit is classified as Class IV (Highly Contaminated) due to high COD (Chemical Oxygen Demand), EC, N(Kjel), and pH values. On the other hand, among the groundwaters filtered from Lower Çavuşlar unit, only CEL51 is classified as Class III (Contaminated) due to high o-PO_4 and P(t) values. The others, CEL35 and CEL44 waters are classified as Class II due to relatively high EC, N(Kjel), o-PO_4, P(t), and DO values. In addition, the concentration of Si is higher than the maximum environmental quality limits in all groundwater samples. Besides Si, concentrations of Al and Fe in PW7 water; Al in PW9 water; Al, As, B and Fe in PW2 water; Cu in CEL35 water; Al and Fe in CEL44 water and Al, Fe and Pb in CEL51 water are higher than the maximum environmental quality limits.

CHAPTER 4

METHODOLOGY

In this study, mineralogic, static, shake-flask leach and column kinetic tests were performed using drilling core rock samples representing potential waste rocks of Çeltikçi coal mine field. The collected data are used to determine the water-rock interactions related acid rock drainage potential, leachate concentrations and related processes under test conditions and potential drainage water chemistry that could seep from waste rock pile(s). Major steps of the research methodology are given in detail below. Methodology of the hydrogeochemical modeling of the pile seepage quality is provided in the Chapter 10.

4.1 Sample Selection and Preparation

Three rock samples used for the research were obtained from the drilling cores in the Çeltikçi - Kızılcahamam area. Due to the limited project budget, the number of samples were kept to three samples. The sample locations are shown in Figure 4.1. The unit descriptions of the samples used in the tests are summarized from AMM (2015) given below from old to young.

- Sample I is a fine, medium-grained clastic sedimentary rock (sandstone). Volcanic and sedimentary fragments lie in a sandy-clayey matrix. It was taken from Bostantepe member, which is underlain by volcanic breccia levels.
- Sample II is a tuff and bituminous shale mixture. Lower Çavuşlar member from which this sample was taken, consists of oolitic limestone and thin immature coal layers alternating with sediment levels of tuff and chert.

- Sample III is mudstone. Upper Çavuşlar member from which this sample was taken, consists of cream-white-light green mudstones containing sandstones, tuffs and well laminated bituminous shale levels.

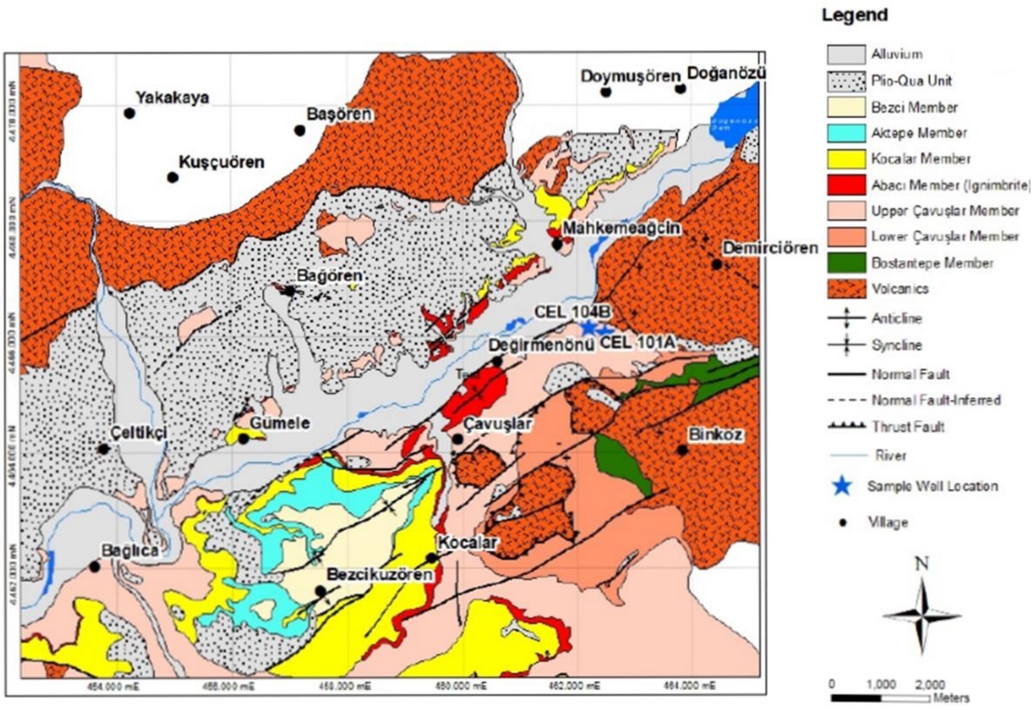


Figure 4.1. Locations of sampled drill holes on the geological map of the area (AMM, 2015).

The sampling information is listed in Table 4.1 Potential waste rocks are taken into consideration for the determination of the sampling location and depth. Expertise of the company expolaration geologists is used for the selection. Due to both the limited project budget and temporary piling of coal in the mining operations, coal ore was not sampled.

For the preparation of samples as test materials, initially each core sample was crushed to a grain size of <10 mm using a jaw crusher. Then, 1 kg of II.1 and II.2 samples obtained using the quartering method for each and mixed to obtain Sample II. Using the similar procedure, samples III.1 and III.2 were mixed to obtain Sample III.

Table 4.1. Test sample information.

Sample Name	Well Number	Latitude	Longitude	Depth (m)	Explanations
I	CEL 101 A	462212	4466162	117.20-117.60	Bostantepe Member (Below coal zone, above volcanic breccia)
II	CEL 101 A			65.10-65.60	Lower Çavuşlar (Below coal zone)
	CEL 101 A	462212	4466162	65.60-65.90	Lower Çavuşlar, Bituminous shale (Below coal zone)
				67.80-67.90	Lower Çavuşlar, Tuff (Below coal zone)
III	CEL 104 B	462497	4466056	11.00-11.40	Upper Çavuşlar (Above coal zone)
	CEL 101 A	462212	4466162	18.70-19.10	Upper Çavuşlar (Above coal zone)

Samples I, II and III then were used to prepare 1kg kinetic test sample with the quartering method for each and placed into the column apparatus after the sieve analyses. After separating 250 grams of each remaining sample with the quartering method for the shake-flask leach tests, the grain size of the remaining samples was reduced to < 2 mm by grinding. The ground samples were used for static tests and XRD analyses.

4.2 Determination of Mineralogical Properties of the Samples

The constituents that react with water in rocks are minerals during water-rock interactions. Therefore, one of the most important factors that determines chemistry of the leachate formed as a result of the reaction is the mineralogical properties of the interacting rock. Mineralogical characteristics of the test samples (I, II and III) were determined by XRD analyses in the Geological Engineering Department of Middle East Technical University.

Sample II and III were subjected to random measurements only but in addition to random measurements, Sample I was also analyzed further after treatment (air dried, ethylene glycolated, at 400 °C and at 550 °C). Due to the swelling problem encountered with this sample during kinetic test, it was thought that clay minerals were present. The XRD peaks are evaluated using MDI Jade 6 Software (MDI, 2019) but further evaluation with charts (Moore and Reynolds, 1997) was required for Sample I peaks due to its clay content.

The following information mostly summarized from MEND (2009) is used to interpret whether a detected mineral has acid producting or neutralizing effect in the solution.

Iron-sulphur minerals produce acid upon oxidation.

Example: $FeS_2 + 3.5O_2 + H_2O \rightarrow Fe^{2+} + \mathbf{2H^+} + 2SO_4^{2-}$

As, Mo, Sb, Se - sulphur minerals in general produce acid due to their compound formation characteristics after dissolution.

Example: (Molybdenite) $MoS_2 + 9/2O_2 + 3H_2O \rightarrow MoO_4^{2-} + \mathbf{6H^+} + 2SO_4^{2-}$

Ag, Cd, Co, Cu, Ni, Pb and Zn - sulphur minerals do not produce acid if they are in free metal cation form after oxidation.

Example: (Sphalerite) $ZnS + 2O_2 = Zn^{2+} + SO_4^{2-}$

Usually Ag, Cd, Co, Ni and Zn meet this criterion. But if they are in the form of compounds (especially Cu and Pb), they can produce acid upon dissolution.

Example: (Chalcopyrite) $CuFeS_2 + 17/4O_2 + 5/2H_2O \rightarrow Fe(OH)_3 + Cu^{2+} + \mathbf{2H^+} + 2SO_4^{2-}$

As to *sulphate minerals*, complete metal hydroxide and ion compound/ exchange /precipitation forming *acidic cation* (Al^{3+}, Cu^{2+}, Fe^{2+}, Fe^{3+}, Pb^{2+}, Zn^{2+}) hydroxy sulphate minerals can produce acid after dissolution.

Example: (Melanterite) $FeSO_4.7H_2O + (1/4)O_2 \rightarrow Fe(OH)_3 + SO_4^{2-} + (9/2)H_2O + \mathbf{2H^+}$

If *base cation* (e.g. Na, K) is present in the mineral and if it forms cation hydroxides or ion compounds/exchange/precipitation upon dissolution, acid can be produced.

Example: (K-jarosite) $KFe_3(SO_4)_2(OH)_6 + 3H_2O \rightarrow K^+ + 3Fe(OH)_3 + 2SO_4^{2-} + \mathbf{3H^+}$

As a general rule, metal (hydro) oxide formation would produce additional acid. If cations do not produce ionic compounds (present as free cations) acid production does not occur.

Example: (Melanterite) $FeSO_4.7H_2O + (1/4)O_2 \rightarrow Fe^{3+} + SO_4^{2-} + (13/2)H_2O + OH^-$

Ca and Mg *carbonate minerals* are neutralizing in oxidized environments. The neutralization capacity of Fe solid solution including carbonate minerals decreases as Fe content increases in the solid solution. The neutralization effect of Fe and Mn carbonates depends on oxygen amount of the environment. Neutralization producing Fe and Mn carbonates upon initial oxidation, would produce acid due to hydrolysis later as oxidation continue.

Example:

$FeCO_3 + 2H+ \rightarrow Fe^{2+} + H_2CO_3$ low oxygen environment-acid consumption.

$Fe^{2+} + 5/2H_2O + 1/4O_2 \rightarrow Fe(OH)_3 + \mathbf{2H^+}$ high oxygen environment-acid production.

Combining two conditions: $FeCO_3 + ¼O_2 + 2½H2O = Fe(OH)_3 + H^+ + HCO_3^-$ indicates no change at the end result in terms of acidity/neutralization effects. Therefore, Fe and Mn carbonate minerals contribution to neutralization is possible only under low oxidizing (anaerobic) conditions. In general, acidic cation (Al^{3+}, Cu^{2+}, Fe^{2+}, Fe^{3+}, Pb^{2+}, Zn^{2+}) bearing carbonate minerals can possibly contribution to neutralization is possible only under low oxidizing (anaerobic) environments.

4.3 Determination of Acid Rock Drainage Potential of the Samples

The acid rock drainage (ARD) potential of rocks is determined using the acid base accounting (ABA) and the net acid generation (NAG) static tests (Sobek et al., 1978; Amira, 2002; MEND, 2009). These tests were carried out on the samples having grain size of < 2 mm at the Encon Laboratory Inc., Ankara. ARD potentials of test samples (I, II, and III) are evaluated using data obtained from modified ABA (Sobek et al., 1982) tests (total sulphur, sulphide-sulphur, sulphate-sulphur, paste pH, neutralization potential and inorganic carbon) and NAG tests (NAG pH, NAG values at pH of 4.5 and 7). Since sulphide values of the samples are less than 1% and there are relatively low metal concentrations, instead of sequential, single NAG tests were performed.

Acid potential estimation:

Static tests generate data to estimate the total acid production potential and the total neutralizing potential of a sample. The acid potential (AP) in the static tests is calculated generally using sulphide amount of the sample using the following formula:

$$AP_{\text{Sulphide}}(\text{kgCaCO3/ton}) = \%S_{\text{Sulphide}} * 31.25$$

This is actual kg amount of $CaCO_3$ required to neutralize 1 ton material. The calculation procedure is based on the following reaction relationships:

(Pyrite) $FeS_2 + (15/4)\, O_2 + (7/2)\, H_2O \rightarrow Fe(OH)_3 + 2\, SO_4^{2-} + 4H^+$

(Calcite) $CaCO_3 + 2H^+ \rightarrow Ca^{2+} + H_2O + CO_2$

In pyrite reaction: 1 mole sulphide-sulphur produces 2 moles H^+ and
In calcite reaction: 1 mole calcite neutralizes 2 moles H^+.

(1 molecular weight of calcite / 1 molecular weight of sulphur in pyrite) * % to kg/ton conversion factor = [(1*100) / (1*32)]*10 = 31.25 kgCaCO3/ton

Cu and Pb sulphur minerals similarly also produce 2 moles H^+.

If there is acid generating base cation including sulphate minerals such as Na-, K Jarosite:

$$AP_{\text{sulphate}}\,(\text{kgCaCO3/ton}) = \%SO_4 * 23.438.$$

Based on the following reaction relationships:

(K-jarosite) $KFe_3(SO_4)_2(OH)_6 + 3H_2O \rightarrow K^+ + 3\ Fe(OH)_3 + 2SO_4^{2-} + 3H^+$

(Calcite) $1\ CaCO_3 + 2H^+ \rightarrow Ca^{2+} + H_2O + CO_2$

In jarosite reaction: 4 mole sulphate produces 6 moles H^+ and
In calcite reaction: 3 mole calcite neutralizes 6 moles H^+.

(3 molecular weight of calcite / 4 molecular weight of sulphur in jarosite) * % to kg/ton conversion factor = [(3*100) / (4*32)]*10 = 23.438 kgCaCO3/ton

If there is acid generating sulphate minerals without base cations such as melanterite:

$AP_{Sulphate}$ (kgCaCO3/ton) = $\%S_{Sulphate}$ * 31.25

Based on the following reaction relationships:

(Melanterite) $FeSO_4\ 7H_2O + (1/4)O_2 \rightarrow Fe(OH)_3 + SO_4^{2-} + (9/2)H_2O + 2H^+$

(Calcite) $CaCO_3 + 2H^+ \rightarrow Ca^{2+} + H_2O + CO_2$

In melanterite reaction: 1 mole sulphate produces 2 moles H^+ and
In calcite reaction: 1 mole calcite neutralizes 2 moles H^+.

ARD evaluation:

The neutralizing potential (NP) is measured either by back titration of acidified sample or directly by acid titration. Net neutralizing potential (NNP) is estimated by subtracting AP value from that of NP. The negative NNP value is interpreted that the rock has a potential of acid production. The positive value indicates low risk of acid production. However, a small positive value does not necessarily indicate that the rock would not produce acid. It is difficult to determine whether the acid production potential exists if the NNP value is between -20 and +20 (kg CaCO3/ton). Therefore, NP to AP ratio is also used in the estimation. Previous application results show that if the ratio is greater than 3:1, acid production risk is low (MEND, 2009). The ratios between 3:1 and 1:1 reflect uncertain conditions. The kinetic test is recommended

(MEND, 2009) under these circumstances. If the ratio is 1:1 or less, it indicates that the sample would most probably produce acid.

If the final NAG pH value of the sample is greater than 4.5, it is interpreted that rock has low or none acid production potential (AMIRA, 2002).

The other two evaluation criteria used are the paste pH and sulphide percentage values of the samples. It is generally assumed that the samples with paste pH values greater than 5.5 and sulphide percentages less than 0.3 would not generate acid rock drainage (MEND, 2009).

The carbonate NP (CNP) calculations are also made to determine the short-term neutralization potential (before neutralization production by aluminosilicate minerals) of the samples to reduce possible acid generation. The CNP is calculated using the inorganic carbon content with the following formula;

$$\text{CNP (kg CaCO}_3\text{/t)} = \%TIC * \frac{M_{CaCO_3}}{M_C} * \frac{1000\frac{kg}{t}}{100\%} = \%TIC * \frac{100.08}{12.011} * 10$$

<u>Sample classification</u>:

The test samples are classified as non-acid generating waste (NAGW), possibly acid generating waste (PAGW) and acid generating waste (AGW) using ABA test results according to the internationally applied following criteria:

NPR > 3 → NAGW ; 1<NPR<3 → PAGW ; NPR < 3 → AGW

In addition, static tests are evaluated based on waste rock classification criteria of MEU (2015). According to the “Mine Waste Regulation”, considering only sulphide content and NPR values the waste (the test samples) is classified as follows:

* Sulphide <0.1wt% → “inert”

* 0.1 <Sulphide<1 wt% uncertain condition, but if NPR>3 → “inert”

* 0.1 <Sulphide<1 wt% uncertain condition, but if NPR<3 → "non-hazardous/hazardous"

* Sulphide >1 wt% "non-hazardous/hazardous".

Non-hazardous/hazardous determinations require further evaluation of short term and kinetic test leachate characteristics.

4.4 Determination of Short-term Leachate Concentrations

The short-term leachate concentrations of the samples are determined by shake flask leach tests (MEND, 2009) in METU Geological Engineering Department. The test for each sample was carried out using the prepared test material that composed of 250 g sample having a grain size of <6.35 mm (MEND, 2009) and 750 ml deionized water (3:1 ratio) in a bottle. Shaking for 24 hours at 200 rpm was applied. Relatively high agitation (close to the maximum of gentle shaking interval) is adapted to increase leaching rates. Photographs form the test are shown in Figure 4.2.

Figure 4.2. Shake flask leach test photographs.

After termination of the test, the solutions were separated from the sediments by centrifuging (30 minutes at 2300 rpm) and electrical conductivity (EC) and pH measurements were carried out. Approximately 100 ml of each sample solution is preserved by acidifying with 60% ultrapure HNO_3 (MERCK KGaA) after filtration with 0.45-micron filter for metal analysis. A bottle of filtered-acidified test solution for metal analyses and a bottle of unfiltered-unacidified test solution for anion analyses from each sample test were sent to Encon Laboratory Inc. in order to determine concentrations of chloride, sulphate, alkalinity and dissolved metals (Al , As, B, Ba, Be, Bi, Ca, Cd, Co, Cr, Cu, Fe, Hg, K, Li, Mg, Mn, Mo, Na, Ni, P, Pb, Se, Sb, Si, Sn, Sr, Ti, U, V, Zn, Zr). Ion chromatography and Inductively Coupled Plasma – Mass Spectrometer (ICP-MS) methods were used in the laboratory for the analyses of anions and cations, respectively.

Leachate concentration quality of samples were determined using (a) surface water classification (SWC) and maximum environmental quality (MEQ) standards for rivers of MFW (2016) (Table 4.2) and (b) waste categorization (WC) limits of MEF (2010) (Table 4.2).

4.5 Sample Preparation for Column Kinetic Tests

The grain size distribution of the rock material to be tested in the column is an important factor affecting the water-rock reactions. The larger the surface area (smaller the grain size) of the rock, greater the water-rock reaction would be. Although there is no pre-established standard for the grain size used in the column tests, the main idea is that the test material size should represent the actual waste material size resulting from mining activities as much as possible. The important point for the evaluation of test results is, though to have the information of grain size distribution of the test material rather than its representativeness with respect to a pile material.

Table 4.2. Quality limits of MFW (2016) on the left, and MEF (2010) on the right.

Parameter (mg/l)	Class I / Max-EQS (Rivers&Lakes)	Class II	Class III	Class IV
Ag	0.0015			
Al	0.027			
As	0.053			
B	1.472			
Ba	0.68			
Be	0.0039			
BOD	< 4	8	20	> 20
Br	0.046			
Cd	< 0.00045	0.0006	0.0009	> 0.0015
CN	0.006			
Co	0.0026			
COD	< 25	50	70	> 70
Color	< 25	50	300	> 300
Cr, t	0.142			
Cu	0.0031			
DO (mg O2/L)	> 8	6	3	< 3
EC (µS/cm)	< 400	1000	3000	> 3000
F	≤ 1	1.5	2	> 2
Fe	0.101			
Mn	≤ 0.1	0.5	3	> 3
Ni	0.034			
N, Kjeldahl, t	< 0.5	1.5	5	>5
N-NH4	< 0.2	1	2	>2
N-NO3	< 3	10	20	> 20
Oil & Grease	< 0.2	0.3	0.5	> 0.5
o-PO4	< 0.05	0.16	0.65	> 0.65
P, t	< 0.08	0.2	0.8	> 0.8
Pb	0.014			
pH	6.0-9.0	6.0-9.0	6.0-9.0	6.0-9.0
S-2	≤ 0.002	0.005	0.01	> 0.01
Sb	0.103			
Se	≤ 0.01	0.015	0.02	> 0.02
Si	1.83			
Sn	0.013			
Ti	0.042			
V	0.097			
Zn	0.231			

Parameter (mg/l)	Inert	Non Hazardous	Hazardous	Very Hazardous
As	< 0.05	0.2	2.5	> 2.5
Ba	< 2	10	30	> 30
Cd	< 0.004	0.1	0.5	> 0.5
Cl	< 80	1500	2500	> 2500
Cr, t	< 0.05	1	7	>7
Cu	< 0.2	5	10	>10
F	<1	15	50	>50
Hg	< 0.001	0.02	0.2	> 0.2
Mo	< 0.05	1	3	> 3
Ni	< 0.04	1	4	> 4
Pb	< 0.05	1	5	> 5
Sb	<0.006	0.07	0.5	> 0.5
Se	< 0.01	0.05	0.7	> 0.7
SO4	< 100	2000	5000	> 5000
Zn	< 0.4	5	20	> 20

The grain size distribution of each 1 kg kinetic test sample having grain size of <10 mm (MEND, 2009), is determined with sieve analyses. The densities of the sampled rocks were also determined using the core samples in order to estimate the surface area of the kinetic test samples. All sample preparation was carried out in Geological Engineering Department at METU.

4.6 Determination of Column Kinetic Test Concentrations

Column kinetic tests were carried out for 13 weeks for Sample I and for 16 weeks for samples II and III excluding Week 0 in the METU Geological Engineering Department by using the plexiglass column apparatus.

A cross-sectional schematic view of the column test apparatus and a photograph taken during the test are shown in Figure 4.3. The upper column (sample chamber; inside diameter: 11 cm, height: 22.5 cm) including a plexiglass disc (thickness: 1 cm, diameter: 11 cm, porosity: 0.38) at the base is attached to the lower column (leachate collection chamber; inside diameter: 11 cm, height: 3.5 cm) having a plexiglass plate (with 7 mm hole at the center) at the base before the dry sample placement. A silicon

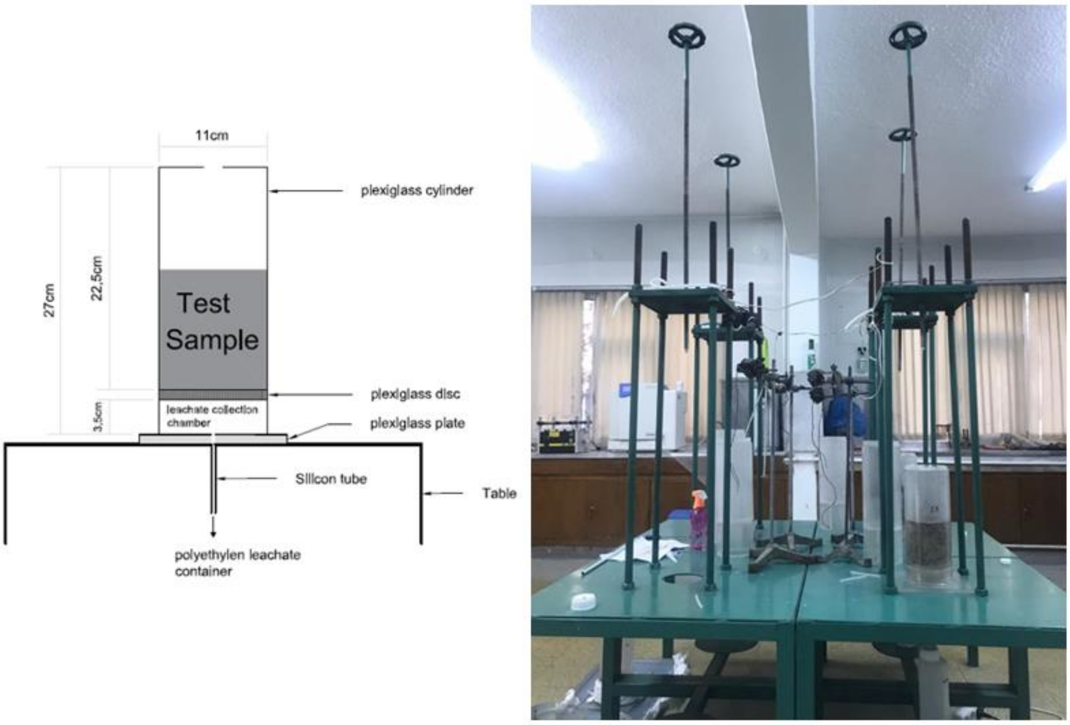


Figure 4.3. The schematic view of column test equipment and photograph taken during the test on the right.

tube (diameter: 7 mm) is placed between the hole of the plate and a polyethylene solution collection bottle rest at the shelf below the test table in order to transfer the leachate from the collection chamber. A transparent silicon is used for sealing the connection interfaces (between the plexiglass disc and the upper column inside wall, between the outside walls of two columns and between the base plate and lower column outside wall) to prevent possible solution leakage. The top of the upper column is kept closed with a plexiglass disc having holes of 3 cm and 1.5 cm in dimeter during test period.

In the beginning of the test, the sample in each column was saturated with a measured amount of deionized water and the drained leachate (Week 0) was collected for chemical analyses. Afterwards, 4.5 days of dry period and 2.5 days of wet period weekly cycle, which was determined by reducing the number of annual wet and dry days (determined using the daily precipitation data of 2013-2015 at Kızılcahamam meteorology station) was adapted. This does not mean that each cycle represents actual annual period. In the wet period, each column was irrigated with about 750 mm of deionized water over 2.5 days using a peristaltic pump. The amount of water added, and the room temperature were recorded daily. The drained water (leachate) from the bottom of the column was weekly collected in a polyethylene container.

Following collection of the leachate in a weekly cycle for each column, including Week 0; leachate volume, electrical conductivity and pH values are measured. The weekly amount of leachate collected averages about 695 ml. Approximately 100 ml of each collected leachate is preserved by acidifying with 60% ultrapure HNO3 (MERCK KGaA) after filtration with 0.45-micron filter for metal analysis. Sample I leachates were centrifuged before filtration due to high sediment content throughout the test period. The centrifuge residues were replaced back to the sample chamber. However, due to the centrifuge instrument malfunction, leachates of Week 3 and the following cycles were centrifuged in the laboratory where chemical analysis were done. Hence the centrifuge residues (total of about 45 gr) were not replaced back to the Sample I chamber. Although this amount was very small, it still was taken into consideration on a weekly basis during kinetic concentration ratio calculations of the sample. A bottle of filtered-acidified test solution for metal analyses and a bottle of unfiltered-unacidified test solution for anion analyses from each sample at the end of each weekly cycle were sent to Encon Laboratory Inc. in the same or the following day after collection in order to determine concentrations of chloride, sulphate, alkalinity and dissolved metals (Al , As, B, Ba, Be, Bi, Ca, Cd, Co, Cr, Cu, Fe, Hg, K, Li, Mg, Mn, Mo, Na, Ni, P, Pb, Se, Sb, Si, Sn, Sr, Ti, U, V, Zn, Zr). Ion chromatography and ICP-MS methods were used in the laboratory for the analyses of anions and cations, respectively. A total of 49 kinetic test leachate (including 1 duplicate) drain was analyzed.

Moreover, a series of quality control measurements were carried out during the column tests for the accuracy and precision evaluation of pH and EC values.

As different from initial plans: (a) although test period is planned for 15 weeks for each sample, Sample I test is terminated at the end of Week 13 due to seepage droplets development between the upper and lower column interface. On the other hand, the test periods of Sample II and III are extended to Week 16. (b) Leachate drainage was ceased after Week 1 from Sample I column due to clogging of the porous disc caused by very high clay content of the sample. As a result, the sample became saturated in irrigation days (wet period) and added water accumulated at the top of the sample. After every irrigation, the slurry (sample + solution at the top) was mechanically mixed for a short period of time in order to ensure interaction of the added water with the sample. The leachate at the end of a cycle is collected from the upper column with a pump after allowing enough sedimentation time. (c) Due to pandemic measures, days of Week 10 and Week 11 cycles were changed to 6 days and 8 days, respectively considering dry-wet days.

CHAPTER 5

ROCK GEOCHEMISTRY

Rock chemistry evaluations provide initial information about potential ions which could have high concentration in leachates upon water-rock reactions. Whole rock chemical analyses were not done for the test samples but there are enough data from the previous study of Gladwell and others (2014) for evaluations of the waste rock chemistry in Çeltikçi coal mine area. The data and sampling location information are given in Appendix-A. The database includes rock analyses from Upper Çavuşlar member above the coal zone (10 rock analyses) and below the main coal zone (20 rock analyses).

Whole rock concentrations from above and below the main coal zone are compared with those of Upper crustal average (Rudnick and Gao, 2003). The averages of the calculated ratios are listed in Table 5.1 and all values are shown in Figure 5.1. As it can be seen both in the table and the figure, regardless whether the rocks are from above or below the coal zone, they exhibit similar anomalies except for Cd and Zn. Concentrations of As, Ca, Cd, Li, Mg, Mo, S and Sr in the rocks are higher than those of the Upper crust. However, these high concentrations do not necessarily mean that they would leach from the rocks upon water-rock interactions. Leachate characteristics of the rocks will further be evaluated using results of short-term and long-term leach tests.

Table 5.1. Average of the ratios of rock sample concentrations to those of the Upper crustal average.

ppm	Above the Coal Zone(U)	Below the Coal Zone (B)	ppm	Above the Coal Zone(U)	Below the Coal Zone (B)
Ag	0.00	0.00	**Ni**	0.17	0.13
Al	0.22	0.13	**P**	0.52	0.62
As	7.50	3.95	**Pb**	0.37	0.22
Au	0.00	0.00	**Rb**	0.49	0.30
Ba	0.23	0.20	**S**	7.49	6.72
Be	0.24	0.24	**Sb**	0.34	0.29
Bi	0.53	0.47	**Sc**	0.12	0.09
Ca	4.26	5.21	**Se**	0.00	0.00
Cd	0.89	1.58	**Si**	0.51	0.42
Ce	0.21	0.13	**Sn**	0.17	0.09
Co	0.17	0.11	**Sr**	1.73	1.87
Cr	0.66	0.51	**Ta**	0.26	0.14
Fe	0.25	0.24	**Th**	0.52	0.16
Hf	0.12	0.08	**Ti**	0.16	0.10
K	0.46	0.15	**Tl**	0.46	0.40
La	0.22	0.14	**U**	0.92	0.50
Li	8.04	3.96	**V**	0.20	0.31
Mg	5.27	5.46	**W**	0.13	0.11
Mn	0.54	0.91	**Y**	0.18	0.11
Mo	4.95	4.35	**Zn**	1.09	0.84
Na	0.16	0.11	**Zr**	0.11	0.06
Nb	0.22	0.09			

Yellow color represents the concentrations higher than those of the upper crustal averages of Rudnick and Gao (2003).

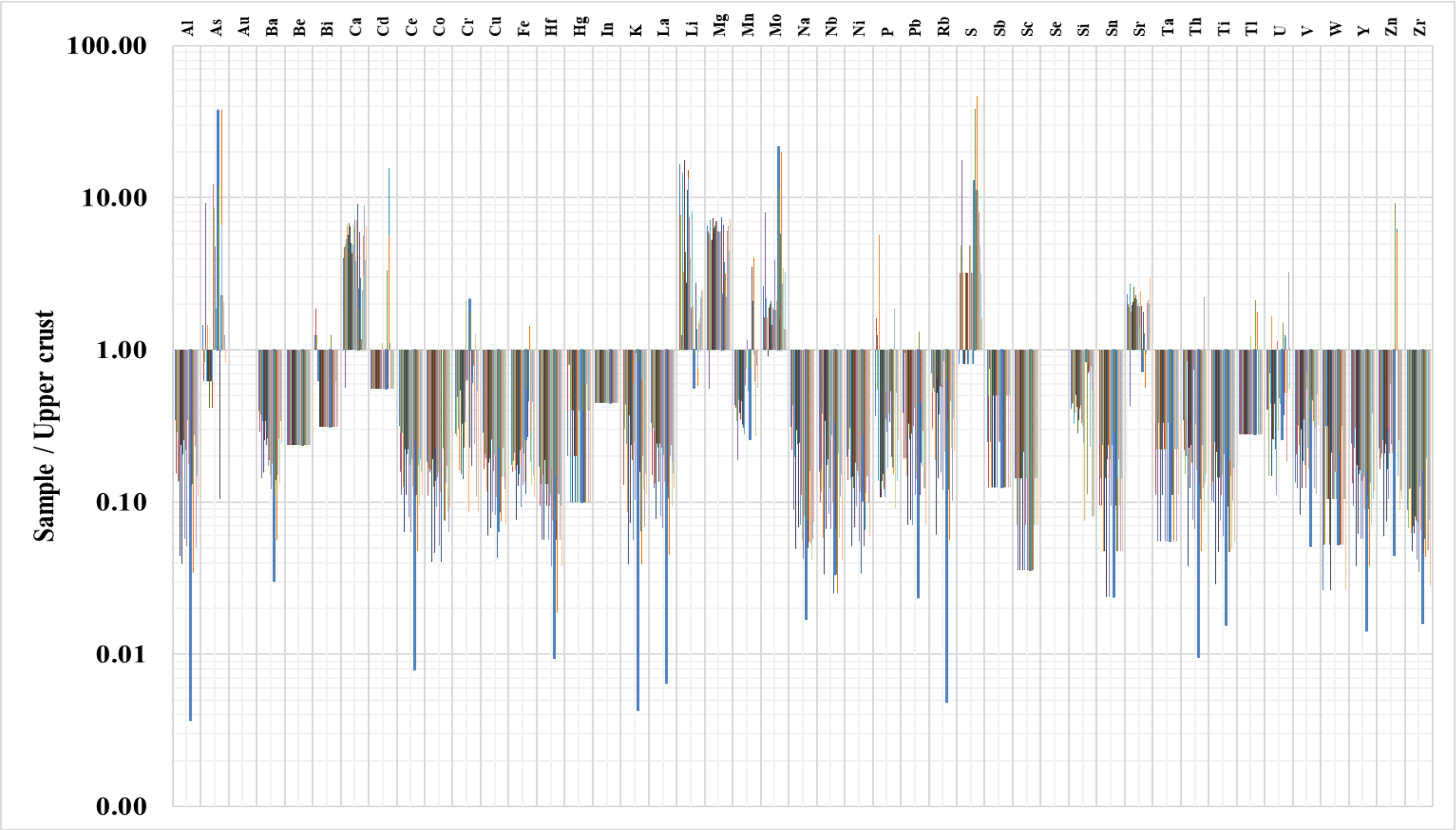


Figure 5.1. The ratios of all rock sample concentrations to those of the Upper crustal averages of Rudnick and Gao (2003).

CHAPTER 6

MINERALOGY

SAMPLE I:

The XRD peaks of Sample I are shown in Figure 6.1 and the determined minerals are listed in Table 6.1 from the possibility of the most abundant to least abundant. Montmorillonite, nontronite, volkonskonite, illite, as clay minerals; surite as a carbonate mineral; margarite, feldspar as silicate minerals; polyhalite as a sulphate mineral and one unnamed mineral exist in the sample.

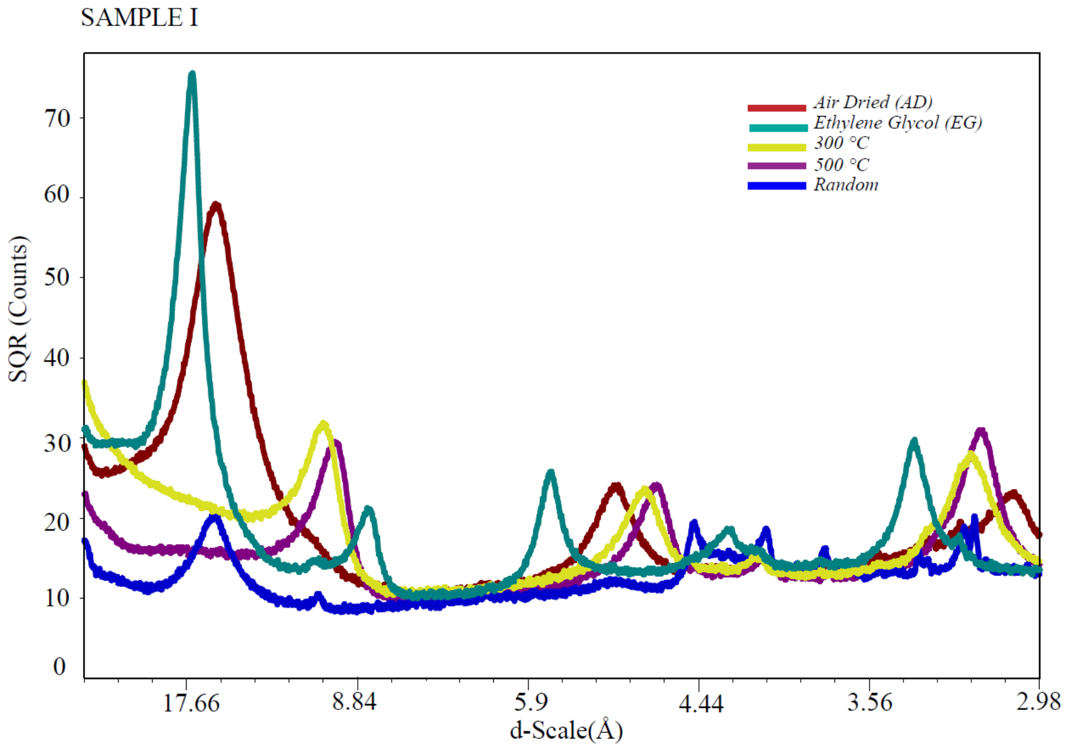


Figure 6.1. Unoriented, and heat & acid treated XRD results of Sample I.

Table 6.1. XRD results of the Sample I.

Sample I		
Mineral Name	Chemical Formula	Mineral group
Montmorillonite	$(Na, Ca)_{0.33} (Al\,Mg)_2 (Si_4O_{10}) (OH)_2\, nH_2O$	Clay
Nontronite	$Na_{0.3}Fe_2((Si,Al)_4O_{10})(OH)_2 \cdot nH_2O$	Clay
Volkonskonite	$Ca_{0.3}(Cr,Mg,Fe)_2((Si,Al)_4O_{10})(OH)_2 \cdot 4H_2O$	Clay
Surite	$(Pb,Cu)_3(Al,Fe^{2+},Mg)_2((Si,Al)_4O_{10})(CO_3)_2(OH)_2$	Carbonate
Margarite	$CaAl_2(Al_2Si_2)O_{10}(OH)_2$	Silicate
Illite	$K_{0.65}Al_{2.0}[Al_{0.65}Si_{3.35}O_{10}](OH)_2$	Clay
Albite	$Na(AlSi_3O_8)$	Silicate
Anorthite	$Ca(Al_2Si_2O_8)$	Silicate
Albite (Ca-rich)	$Ca(AlSi_3O_8)$	Silicate
Polyhalite	$K_2Ca_2Mg(SO_4)_4 \cdot 2H_2O$	Sulphate
Unnamed Mineral	$MgAsO_4.H_2O$	

Although sulphide concentration is measured in ABA tests, any sulphur mineral which could possibly cause acid generation was not identified in the XRD analyses. Therefore, it is interpreted that the sample contains sulphur mineral with amounts less than the XRD detection limit (about 2-5%). Polyhalite is not the type of sulphate mineral that could produce acidity either. The determined carbonate mineral (surite) neutralization capacity is probably very limited under aerobic conditions. The low neutralization potential determined from ABA tests for this sample is related to aluminosilicates and hydroxides as will be discussed in the next chapter. However, calcite mineral was also reported in petrographic analyses of these member rocks (AMM, 2014).

Mineralogic content, in addition to commonly present major elements, includes As, Cr, Cu and Pb trace elements that could create environmental problems if released. Because there is not any available rock analysis from Bostantepe member, comparison between mineral content and the rock chemistry cannot be performed.

Sample II:

The XRD peaks of Sample II are shown in Figure 6.2 and the determined minerals are listed in Table 6.2 from the possibility of the most abundant to least abundant one. According to the peaks, dolomite, magnesite, ankerite as carbonate minerals; quartz as a silicate mineral and teallite as a sulphur mineral exist in this sample. No sulphate mineral was detected although in small amounts sulphate concentration is measured in ABA tests. Therefore, it is interpreted that the sample contains sulphate mineral with amounts less than the XRD detection limit (about 2-5%).

Table 6.2. XRD results of Sample II.

Sample II		
Mineral Name	Chemical Formula	Mineral group
Dolomite	$CaMg(CO_3)_2$	Carbonate
Quartz	SiO_2	Silicate
Magnesite	$MgCO_3$	Carbonate
Ankerite	$Ca(Fe^{2+},Mg,Mn)(CO_3)_2$	Carbonate
Teallite	$PbSnS_2$	Sulphur

Among the carbonate minerals, dolomite has a neutralization capacity that would be active very early. Indeed, neutralization potential of this sample is high in the ABA test results. Ankerite, on the other hand, has the neutralization capacity in only anaerobic conditions. Otherwise, it has no effect on the neutralization. Teallite is the only sulphur mineral that could create acidity. However, acid generation potential of this mineral is relatively low as indicated by lower acid potential (AP) value in the ABA test probably due to presence in low amount of the mineral in the sample. Teallite mineral contains Pb and Sn heavy metals which should be taken into consideration for possible environmental problems. But trace element comparison with whole rock analyses suggests that Pb and Sn heavy metals including teallite must be in very small amount in the sample.

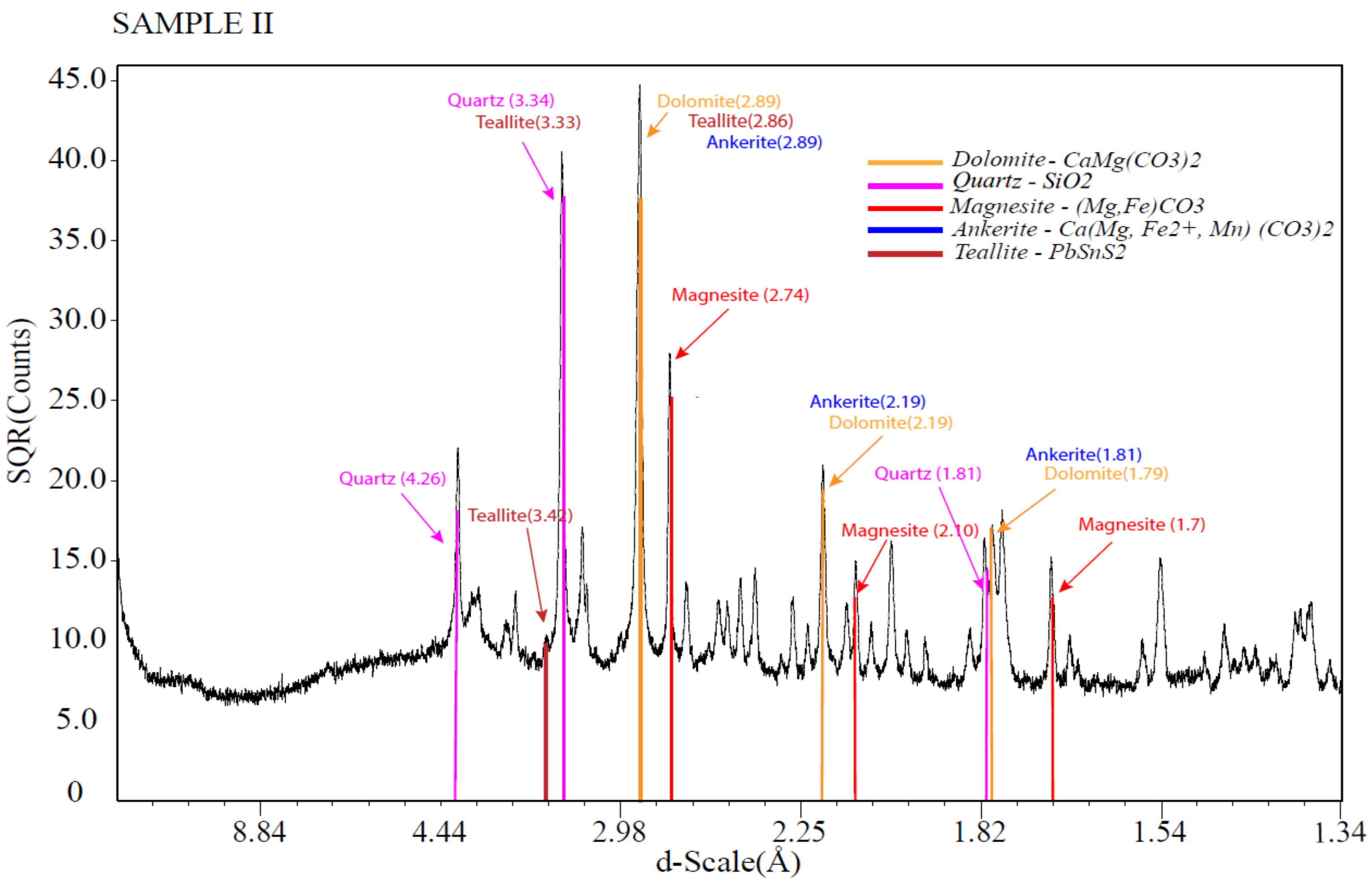


Figure 6.2. XRD peaks of the Sample II.

Sample III:

The XRD peaks of Sample III are shown in Figure 6.3 and the determined minerals are listed in Table 6.3 from the possibility of the most abundant to least abundant one.

Table 6.3. XRD results of Sample III.

Sample III		
Mineral Name	Chemical Formula	Mineral Group
Dolomite	$CaMg(CO_3)_2$	Carbonate
Minrecordite	$CaZn(CO_3)_2$	Carbonate
Sanidine	$K(AlSi_3O_8)$	Silicate
Teallite	$PbSnS_2$	Sulphur
Hodgkinsonite	$Mn^{2+}Zn_2(SiO_4)(OH)_2$	Silicate
Lanarkite	$Pb_2(SO_4)O$	Sulphate
Haradaite	$(Ba,Sr)VSi_2O_7$	Silicate
Wilhelmkleinite	$ZnFe^{3+}_2(AsO_4)_2(OH)_2$	Phosphate
Quartz	SiO_2	Silicate
Argentopyrite	$AgFe_2S_3$	Sulphur

According to the peaks, dolomite and minrecordite as carbonate minerals; teallite and argentopyrite as sulphur minerals; sanidine, hodgkinsonite, haradaite and quartz as silicate minerals; lanarkite as a sulphate mineral; and wilhelmkleinite as a hydroxide mineral exist in the sample. Although the peaks of some minerals are overlying each other, they are included into the output due to heavy metals in their chemical formulas.

Among the carbonate minerals, dolomite has a neutralization capacity that would be active very early. The neutralization potential of this sample is relatively high in the ABA test results. Minrecordite, on the other hand, has the neutralization capacity in relatively anaerobic conditions because released Zn after the dissolution could produce acid due to hydrolyzation upon oxidation in the solution. Lanarkite sulphate

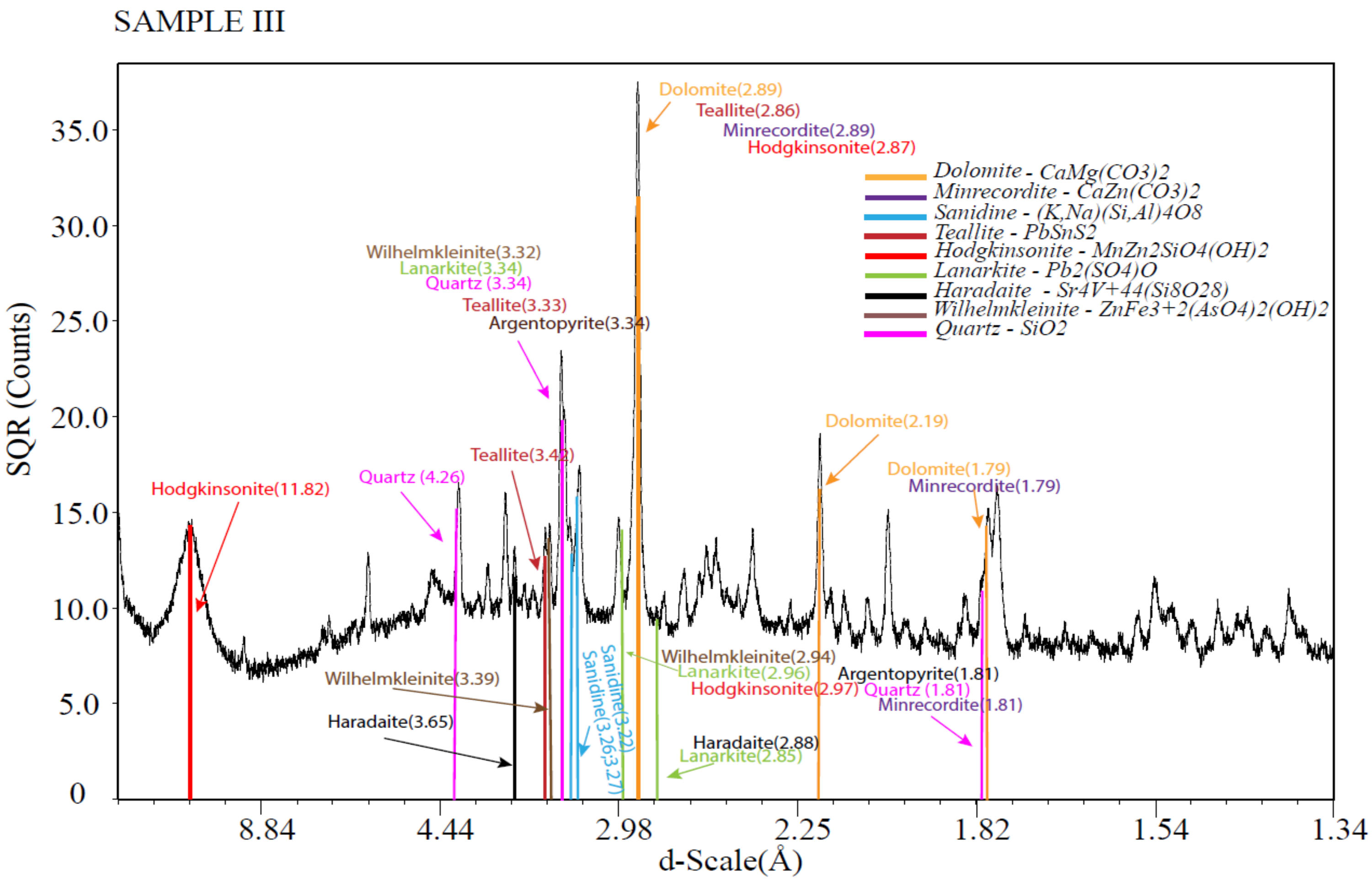


Figure 6.3. XRD peaks of the Sample III.

mineral could produce acid in addition to sulphur minerals. Although teallite and argentopyrite sulphur minerals are detected in the sample, these minerals as well as lanarkite mineral must be in small amounts because acid generation potential of this sample is found to be low in ABA test results.

In addition to commonly present elements, some minerals contain heavy metals that may cause environmental problems highlighted in the table. These are As, Pb, Sn, V and Zn elements. However, trace element comparison with whole rock analyses suggests that minerals including these elements with the exception of As, must be in small amounts in the samples.

CHAPTER 7

STATIC TESTS

The parameters and related measurements of the static tests (Paste pH, sulphur, Carbon, NAG pH, NAG at pH 4.5 and 7) are listed in Table 7.1.

Table 7.1. Static test measurements.

Sample Name	I	II	III
Modified ABA			
Sample Weight(g)	2.0031	2.0061	2.0027
Fizz Rate	2	4	4
Fizz Rate	Weak	Strong	Strong
1.0 N HCl (0 h) Volume (mL)	2.00	3.00	3.00
1.0 N HCl (2 h) Volume(mL)	1.00	2.00	2.00
HCI (Normality)	1.0	1.0	1.0
pH 22 hours later	2.12	2.25	2.28
Needed volume of 1.0M HCl to reach 2.0-2.5	0.0	4.65	8
pH of 125 ml Sample	2.25	5.21	4.84
NaOH Normality	1.0	1.0	1.0
Needed volume of 0.1M NaOH to have 8.3 pH	0.90	3.25	4.50
NP (kg CaCO3/t sample)	52.42	159.5	212.2
Paste pH			
Paste pH (1:1 ratio)	7.56	8.75	8.19
Paste pH (1:2 ratio)	7.40	8.70	8.17
Sulphur			
Total Sulphur (%S)	0.774	0.273	0.328
HCl Acid Insoluble Sulphur (%S)	0.546	0.239	0.281
Acid Soluble Sulphate Sulphur (%SO4-S)	0.228	0.034	0.047
HNO3 Insoluble Sulphur	0.103	0.107	0.13
Sulphide-Sulphur (%S-2-S)	0.443	0.132	0.151
Carbon			
Total Carbon %	0.85	9.30	6.60
Organic Carbon %	0.19	1.40	1.44
Total Inorganic Carbon %(TIC)	0.66	7.90	5.16
NAG			
Sample Name	I	II	III
Sample Weight(g)	2.5055	2.5068	0.5023
Final pH	5.14	5.53	5.71
EC	883	691	888
NaOH Normality	0.1	0.1	0.1
NaOH Volume	0	0	0
NaOH Volume	6.2	6.65	5.2
NAG (kg H2SO4/t) (pH 4.5)	0	0	0
NAG (kg H2SO4/t) (pH 7.0)	12.13	13.00	50.73

Paste pH values in general reflect the pH values of short term (operation period) leachates. The paste pH values of the samples I, II and III are measured as 7.56, 8.75 and 8.19 for 1:1 ratio (solid/liquid) case and 7.40, 8.70 and 8.17 for 1:2 ratio case. Therefore, the values indicate that acid production should not expected in the short term leachates. However, it should be kept in mind that the acid generation capacity of the samples cannot be determined solely based on paste pH tests as it is explained in the following sections.

7.1 Modified Acid Base Accounting Tests

The measured values of neutralization potential (NP) and NAG Final pH, and calculated values of acid potential (AP), net neutralization potential (NNP), neutralization potential ratio (NPR) together with resulting waste categorization are listed in Table 7.2.

Table 7.2. Static test evaluation results.

SAMPLE NO	AP (kg CaCO3/t)	Net NP(NP-AP) (kg CaCO3/t)	NP/AP (NPR)	NAG Final pH	Sulphide -S Result	NPR Result	NAG Result	NNP Result
I	13.75	38.67	3.81	5.14	Uncertain	NAGW	NAGW	NAGW
II	4.06	155.45	39.26	5.53	Uncertain	NAGW	NAGW	NAGW
III	4.69	207.52	45.27	5.71	Uncertain	NAGW	NAGW	NAGW

In addition to sulphur minerals, acid producing any significant sulphate mineral was not detected in the mineralogic analyses. Therefore, the acid potentials (AP) of the samples are calculated using sulphide concentrations based on the assumption that 1 mole sulphur would produce 2 moles H^+ as in the case of pyrite, Cu and Pb sulphur minerals. After completion of the sulphide-based AP evaluations, in order to simulate probable worst scenario, sulphate concentrations were also added to the AP calculations and the results are further evaluated. According to the sulphide-based calculations, the test samples include very low AP values in general, in kg CaCO3/t unit: Sample I (Bostantepe member sandstone); 13.8, Sample II (lower Çeltikçi member tuff, bituminous shale); 4.1 and Sample III (upper Çeltikçi member mudstone with sandstone, tuff and coal levels); 4.7.

The NP values are 52.4, 159.5 and 212.2 in kg CaCO3/t for samples I, II and III, respectively. Relatively high NP values are mainly related to the presence of dolomite minerals as determined in the XRD analyses and also indicate the contributions of aluminosilicates and in some samples, hydroxide and oxide minerals. The AP and NP distribution of the samples is shown in Figure 7.1.

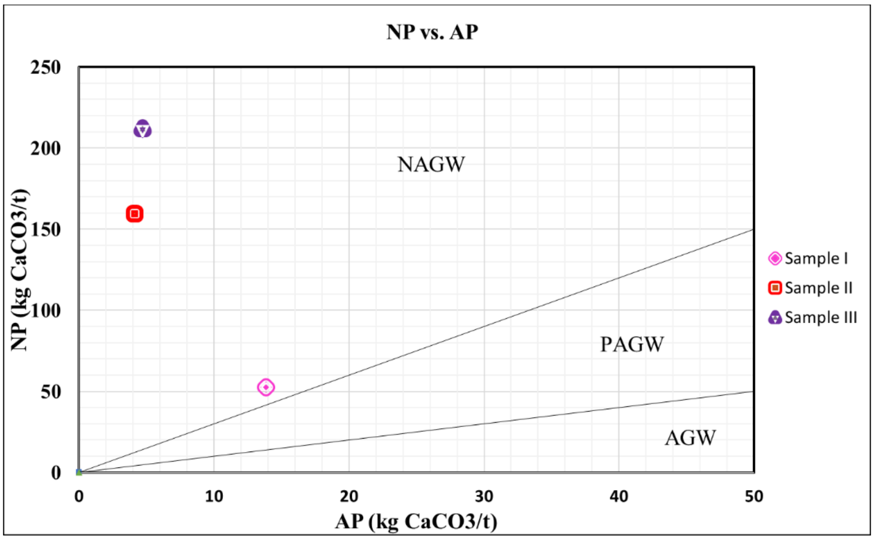


Figure 7.1. AP and NP distribution. Lines represent the limits of NP/AP values (1<NP/AP<3).

The carbonate NP calculations were also made to determine the short-term neutralization potential (before neutralization production by aluminosilicate minerals) of the samples to reduce possible acid generation. CNP values are calculated as 55, 658, 430 in kg CaCO3/t for the samples I, II and III, respectively.

When compared with total NP values, although Sample I includes a similar CNP value, the CNP values of the others are greater. These results suggest that either enough acid addition during NP measurements was not done (it as confirmed by the laboratory that performed in the analysis) or determined inorganic carbon do not produce alkalinity. Latter possibility may be caused by 1) the presence of non-carbonate carbon (e.g. organic matter, graphite) content in the samples and/or 2) the presence of significant amounts of Fe-Mn carbonate minerals. Sample content and XRD studies suggest that high CNP values are mainly as a result of the existence of non-carbonate carbon content, in addition to only anaerobic environment neutralization producing carbonate minerals. Therefore, it is not possible to determine how much of total NP values are related to the neutralizing carbonate minerals and hence, whether the neutralization potential would be operative in short term (operation period) or not considering CNP values.

The calculated NNP values are 38.7, 155.5 and 207.5 in kg CaCO3/t for the samples I, II and III, respectively. Since all NNP values are greater than 20 kg CaCO3/t, the samples are considered as none acid generating waste (NAGW) (Figure 7.2). Previous study data of Gladwell et al. (2014) are also shown in the Figure 7.2. The test samples include relatively low NP values when compared to the previous data. The non-linear relationship between positive NNP and sulphide indicates that NNP values are controlled by varying high NP rather than relatively low AP.

Another important parameter indicating acid rock drainage potential of rocks is NPR. Calculated values are 3.8, 38.7 and 45 for the samples I, II and III, respectively. Since all these values are greater than 3, the samples are considered as NAGW (Figure 7.2). Gladwell et al.(2014) samples which were taken from Upper Çavuşlar member above the coal zone and below the main coal zone, also fall into the none acid generating area in the Figure 7.2.

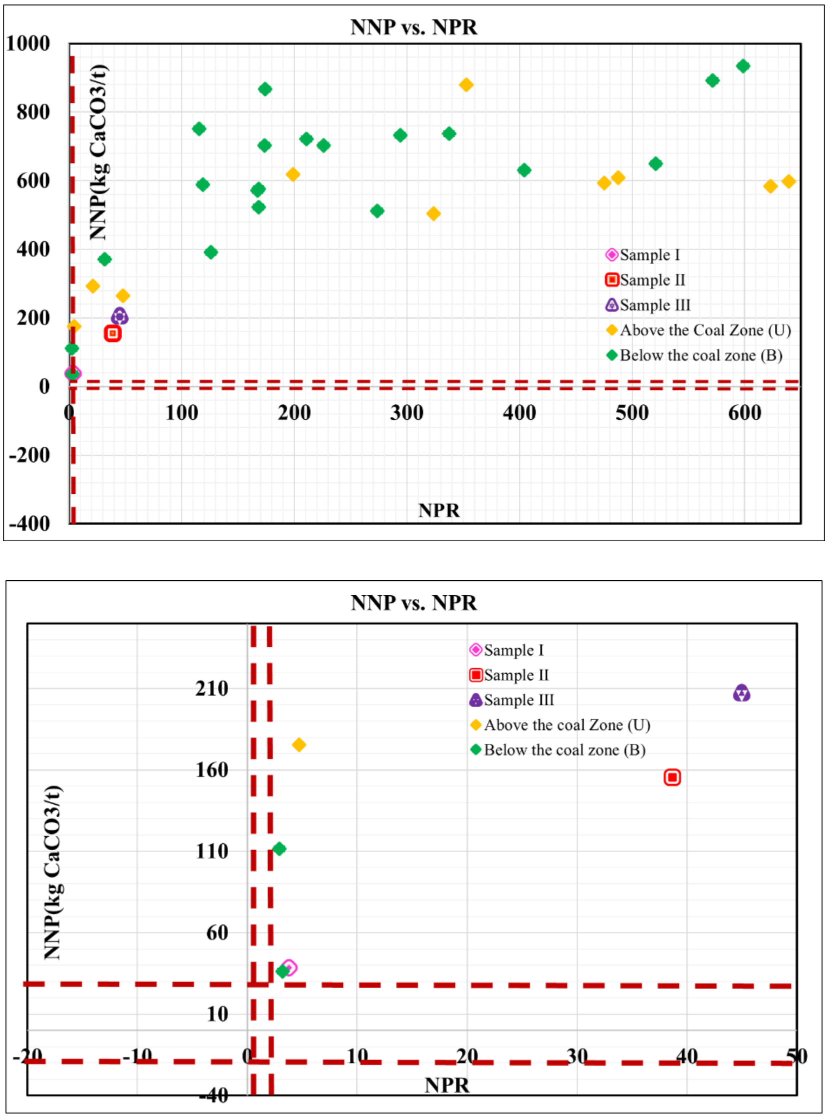


Figure 7.2. NNP vs NPR relationship. Below: Zoomed version of the same graph.

According to MEU (2015) mine waste classification sulphide criteria only, all test samples having > 0.1% sulphide content are in non-inert waste (non-hazardous/hazardous) class. But when the second criteria (NPR > 3) for samples with %0.1< sulphide <1% (in the samples I, II and III; %0.44, %0.13 and %0.15, respectively) is used, test samples could be considered inert waste (provided that concentration release is low upon water-rock interaction) indicating none or very low acid production property. Indeed, NNP values of the samples are high as well.

7.2 Net Acid Generation Tests

The net acid generation (NAG) static tests based on oxidation of sulphur minerals with hydrogen peroxide, were used for the long-term acid generation potential determinations. If the final NAG pH value of the sample is greater than 4.5, it is interpreted that rock has low or none acid production potential. The NAG pH values of the samples I, II and III are 5.14, 5.53 and 5.71, respectively, indicating that the samples do not have acid producing potential in long term period. When NAG pH values are considered, it is possible to conclude that the test samples (falling in non-inert waste class due to only sulphide MEU (2015) criteria but considered inert when NPR criteria is applied) do not bear acid production potential.

NAG (pH 4.5) potential, which indicates acid production generally caused by Fe, Al and H ions, is less than the detection limits. However, NAG (pH 7.0) potential, which indicates acid production caused by soluble hydroxide metals (e.g. Cu, Zn), is measured greater than the detection limit value in the samples as (kg $CaCO_3$/t) 12.4, 13.3 and 51.8 for the samples I, II and III, respectively. These values indicate possibility (being higher in Sample III) of hydroxides related pH buffering and possible metal release upon increasing oxidation in the leachates.

Electrical conductivity (EC) values of NAG solutions do not show linear relationship with sulphide content (Figure 7.3) and were measured as, in µS/cm, 883, 691, and 888 for the samples I, II and III, respectively. These values indicate moderate dissolved metal concentrations in the long term. Therefore, possible metal release would be at low to moderate total concentrations as also indicated by low NAG (pH 7) values.

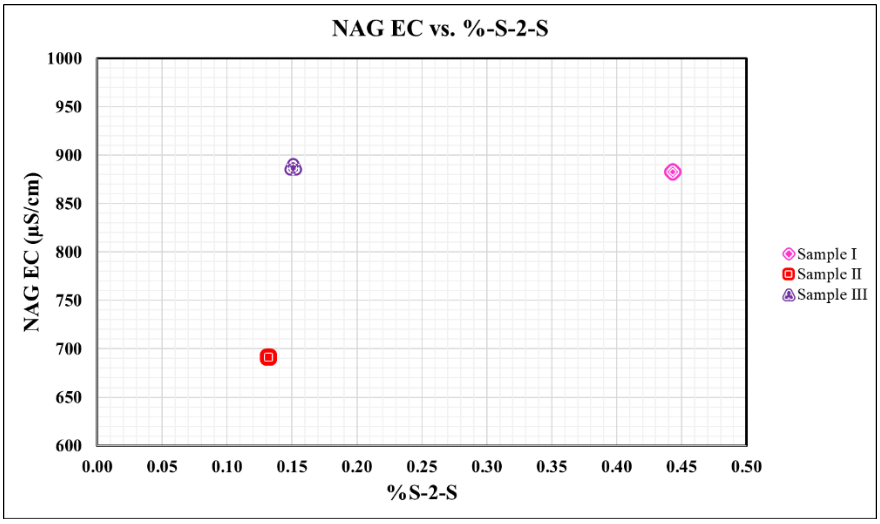
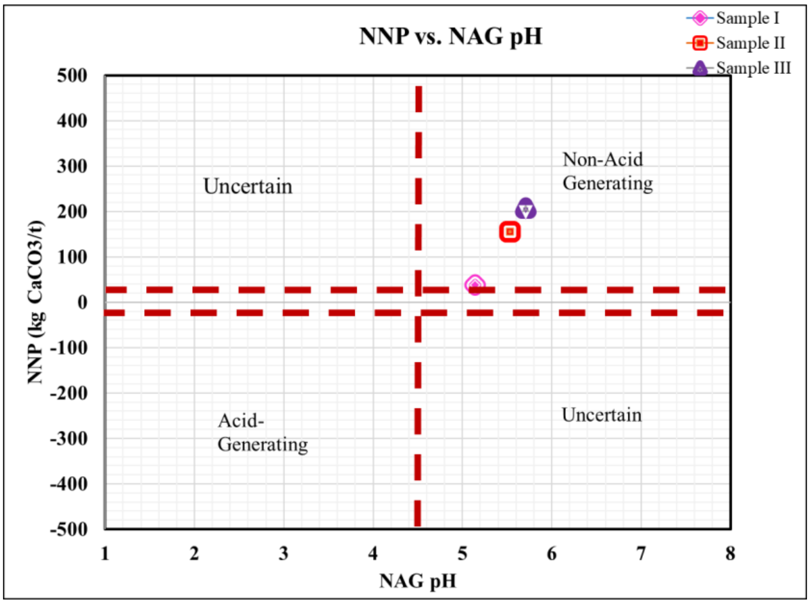


Figure 7.3. Relationship between NAG test EC and Sulphide%-Sulphur.

7.3 Static Test Results Summary

In summary, static test (paste pH, ABA, NAG) evaluation results indicate that: The test samples I, II and III exhibiting ARD potential in the order of I>II>III (controlled by high neutralization potential rather than low acid potential) do not have acid rock drainage potential in short or long term and any acid production will be neutralized by the minerals in the rocks (Figure 7.4). However, lack of ARD potential should not be interpreted as none ion release occurrence. NAG (pH 7) potential values indicate hydroxides related pH buffering and possible low-intermediate total concentration metal release upon excessive oxidation increase in the leachates. The metal release processes will further be evaluated using short-term and long-term leach tests. Ignoring leachate chemical characteristics, the samples could be classified as inert wastes according to MEU (2015) static test criteria.



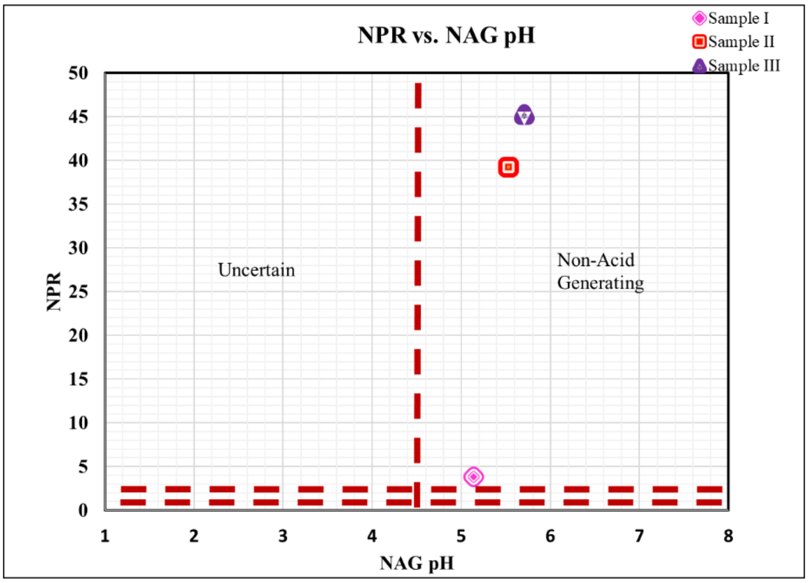


Figure 7.4. Summary graph of static tests. Above: NNP vs. NAG pH; Below: NPR vs. NAG pH.

The ABA evaluations as suggested by the mineralogy are based on the assumption that AP is related to sulphur mineralogy of the samples. Although no significant acid producing sulphate mineral was determined in the samples, for the first worst scenario case, sulphate concentrations were added to the AP calculation procedure and the results were re-evaluated. In the calculations, for Sample I; AP multiplication coefficient of 23.44 was used due to base cation including sulphate mineral (polyhalite; which is actually none-acid-producing sulphate mineral), for Sample III; 31.25 was used due to acid cation including sulphate mineral (lanarkite) and for Sample II; no sulphate mineral is detected but due to similar formation properties to Sample III, 31.25 was used. Furthermore, for the second worst scenario, insoluble sulphur concentrations (assuming representing sulphide) were added to the measured sulphide concentrations in the AP calculations. The calculated AP, NNP, and NPR values under given worst scenario conditions are listed in Table 7.3.

Table 7.3. AP, NP, NNP and NPR values determined by Sum of Sulphur-S-2 & Sulphur-SO4 concentrations and Sulphur-S-2 & insoluble S

SAMPLE NO	**% S-2-S; % SO4-S**	**AP (kg CaCO3/t)**	**NNP (kg CaCO3/t)**	**NPR**	**SAMPLE NO**	**%S-2-S + Insoluble S**	**AP (kg CaCO3/t)**	**NNP (kg CaCO3/t)**	**NPR**
I	0.443;0.228	19.19	33.23	2.73	I	0.55	17.06	35.36	3.07
II	0.132; 0.034	5.19	154.32	30.75	II	0.24	7.47	152.04	21.36
III	0.151; 0.047	6.19	206.02	34.30	III	0.28	8.78	203.43	24.17

In the scenarios results, sulphide concentrations are less than 1% and NPR values are greater than 3 with the exception of Sample I (NPR =2.7) in the first scenario. But it should be kept in mind that NAG test pH value of Sample I is relatively high and the scenarios represent very extreme conditions. These evaluations indicate that even under worst possible scenario, only sulphide related previous results (before worse scenarios) would not change.

CHAPTER 8

SHAKE FLASK LEACH TESTS

The shake flask leach test is an effective indicator of waste pile short term hydro-geochemistry. From the leach test data, leaching concentrations of the elements, pH and electrical conductivity could be obtained. The test results are listed in Table 8.1.

Table 8.1. Shake flask leachate test results.

Parameter / Sample	**Detection**	**I-F**	**II-F**	**III-F**
EC µS/cm at 25°C	<0.001	1000	493.2	438.6
pH	<0.1	9.49	9.35	8.61
Alkalinity	<3	211	213.4	9.5
Cl	<1.5	7	<1.5	4
SO4	<10	339	49	99.706
Al	<0.01	<0.01	<0.01	<0.01
As	<0.001	0.0953	0.0362	0.04318
B	<0.01	<0.01	<0.01	<0.01
Ba	<0.01	0.05738	0.03976	0.03545
Be	<0.001	<0.001	<0.001	<0.001
Bi	<0.040	<0.040	<0.040	<0.040
Ca	<1	45.22	29.29	7.753
Cd	<0.0005	0.00176	<0.0005	0.00067
Co	<0.0005	0.00274	<0.0005	0.00079
Cr, t	<0.001	0.02577	<0.001	<0.001
Cu	<0.001	<0.001	<0.001	<0.001
Fe	<0.01	<0.01	<0.01	<0.01
Hg	<0.0001	<0.0001	<0.0001	<0.0001
K	<1	23.5	11	13.5
Li	<0.01	0.04514	0.74461	0.70073
Mg	<1	16.4	52.5	28
Mn	<0.01	0.0134	<0.01	<0.01
Mo	<0.001	0.89984	0.23106	0.59882
Na	<1	21.2	52.5	26.6
Ni	<0.01	<0.01	<0.01	<0.01
P	<0.040	<0.040	<0.040	<0.040
Pb	<0.0005	0.01804	0.00226	0.00417
Sb	<0.0005	0.00223	0.00114	0.00719
Se	<0.01	<0.01	<0.01	<0.01
Si	<0.04	21.07	18.44	10.04
Sn	<0.001	<0.001	<0.001	<0.001
Sr	<0.01	1.03074	0.71193	0.71696
Ti	<0.01	<0.01	<0.01	<0.01
U	<0.005	2.93039	0.5263	1.03667
V	<0.001	0.0018	0.0364	0.0119
Zn	<0.01	0.02078	<0.01	<0.01
Zr	<0.040	<0.040	<0.040	<0.040
*Unit (mg/l)				

pH and EC values are evaluated based on relative values (by comparing values among samples) rather than absolute ones due to the nature of the test because relatively high solid/liquid (1/3) ratios are used. Hence,pH and EC values are not good absolute value indicators of the real conditions. Test leach pH and EC values are in the order of Bostantepe (I)>Lower Çavuşlar (II)>Upper Çavuşlar (III) and all results are basic which indicates that EC values reflect basic environment ion release conditions pH and electrical conductivity values is shown in Figure 8.1. Previous test results (see Appendix-B) with the same solid/liquid ratio of Gladwell et. al (2014) are also plotted in the figure. It should be pointed out that Bostantepe member (Sample I) rocks were not sampled in the previous study.

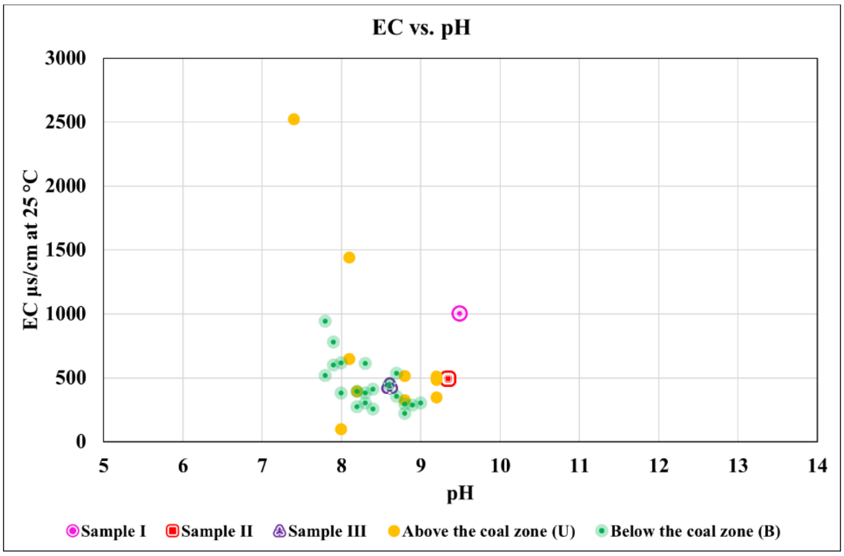


Figure 8.1. EC and pH plot of this study and the previous study results (taken from Gladwell et al., 2014)

The relative order of sample leachate pH values is the same as that of groundwaters, but it is not compatible with the static test results. Although static test results provide information mainly for the long term, the incompatibility are investigated for possible reasons. Since NPR value of Sample I is lower than those of the others, it is expected that its leachate should relatively be the most acidic one but it is not. The highest pH value of Sample I leachate could be explained by the presence of Fe, Mn carbonate minerals. As explained earlier, such minerals introduce neutralization at earlier stages of water-rock interaction but then produce acid due to hydrolysis effects at later stages. Therefore, it is possible that the pH value of Sample I reflects results of the earlier (carbonate release) stage reactions. Mineralogical analyses indicate that surite mineral which could produce such effects is present in Sample I. These types of minerals are not necessarily subject to the same reaction rate, but Sample II and III also contain such minerals. Another explanation for the highest pH value of Sample I leachate could be related to the montmorillonite content of its sample. As it will also be discussed in the kinetic test section, montmorillonite is not stable under alkaline conditions, subject to hydrolysis and Na and H^+ exchange increases solution pH (Kaufhold et al., 2008). As a result, sulphide oxidation related acid production in Sample I leachate must have been much lower than the alkali production of the montmorillonite related reaction. Contrary to the static test indications, (NPR value of III is higher than that of II), pH value of Sample II leachate is greater than that of Sample III as well. This could be explained by the earlier stage reaction effects of the detected ankerite (Fe, Mn carbonate) and possibly iron bearing magnesite mineral in Sample II. Such effects related minrecordite (Ca, Zn carbonate) detected in Sample III is probably present in relatively small amounts as below detection limit concentrations of Zn suggested (Table 8.1). Yet another explanation could the different rates of sulphide mineral oxidation/carbonate mineral dissolution in the samples due to the nature of the minerals present, remembering that static test results provide information for the long-term results.

According to the major ion concentrations, facies types of the leachates: Sample I leachate is Mix-SO_4 type; Sample II leachate is Mg-HCO_3 type (compatible with that of groundwater) and Sample III leachate is Mg-SO_4 type (Figure 8.2). Relatively high sulphate concentrations of Samples I and III, in addition to the sulphide oxidation could be related to the dissolution of sulphate minerals (e.g. polyhalite, lanarkite) as they were determined in the XRD analyses of these samples but not in

Sample II. Relatively high amounts of Mg in the leachates of II and III are probably related to the presence of dolomite mineral as it was determined in the XRD analyses.

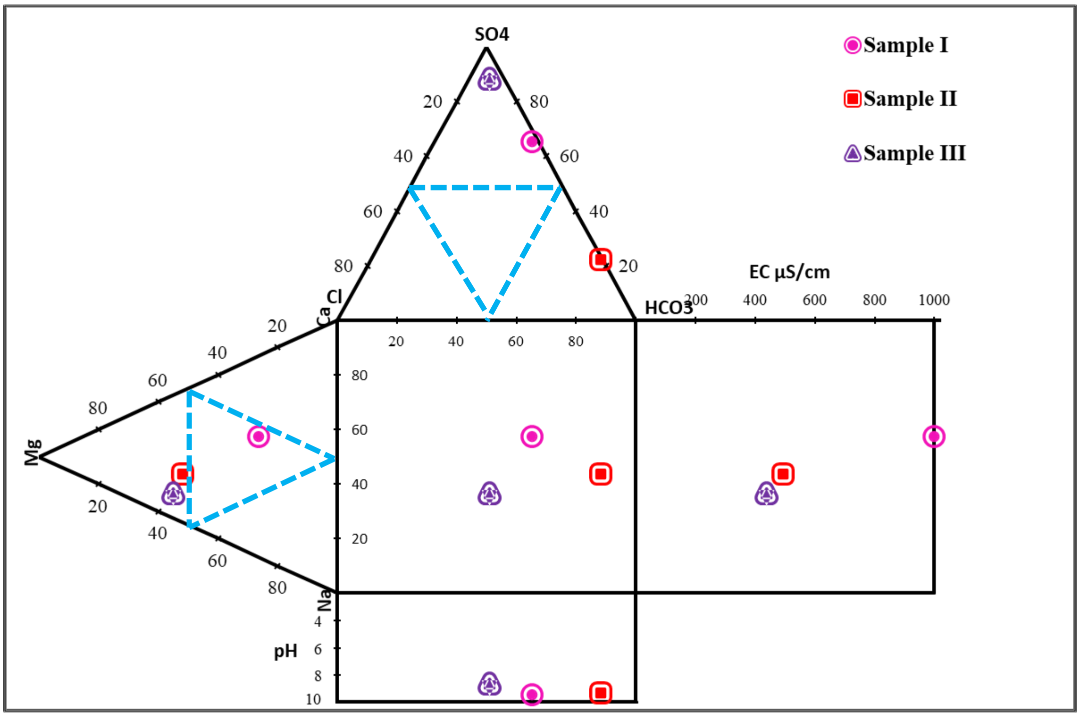


Figure 8.2. Durov diagram of samples for facies analyses.

The test results indicate that concentrations of Al, B, Be, Bi, Cu, Fe, Hg, Ni, P, Se, Sn, Ti and Zr are lower than the detection limits and the concentrations of alkalinity, Ca, K, Mg, Na, Si, SO_4, Cl, As, Ba, Li, Mo, Pb, Sb, Sr, U and V are higher than the detection limits in all sample leachates. Additionally, the leachates include above detection limit values of Cd, Co, Cr, Mn and Zn in Sample I and Cd and Co in Sample III. The sample leachates are in neutral pH-low metal category (similar to the groundwater composition) according to Ficklin graph (Figure 8.3), where Sample I composition plot close to the low-high metal boundary.

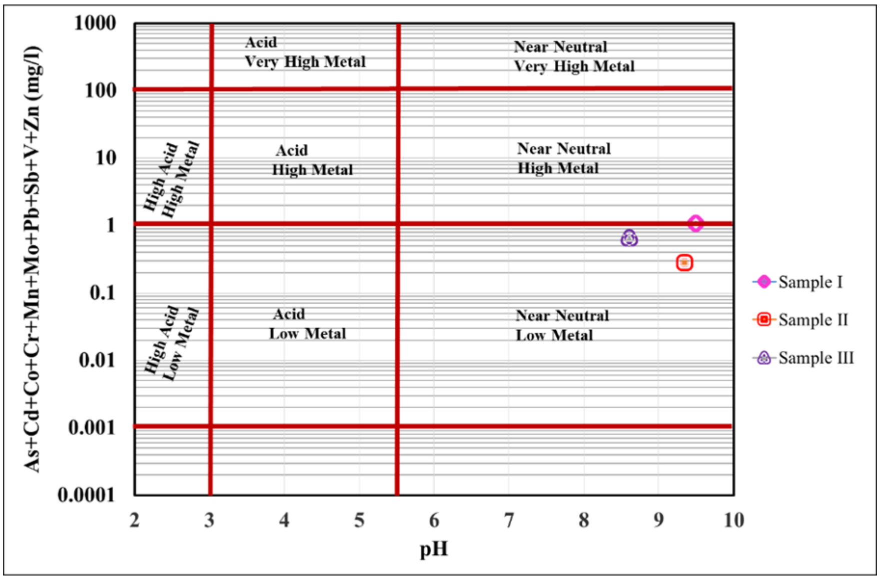


Figure 8.3. Leachate categorization in Ficklin diagram based on pH and trace metal ion content.

In order to evaluate the leachate qualities, quality limits (a) for the surface water classification (SWC) and maximum environmental quality (MEQ) for rivers of MFW (2016) and (b) waste categorization (WC) limits of MEF (2010) are used as explained in the related methodology section(4.4) and the results are given in Table 8.2. According to the waste categorization limits, the test samples are in “Non-hazardous” class. The parameters causing this class with relatively high concentrations are given in Table 8.2.

Table 8.2. Classification of short-term leach test results according to surface water and waste categorization limits.

Sample No	SWC (MFW, 2016)	MEQ (MFW, 2016)	WC (MEF, 2010)
I	Class IV - pH	As, Cd(IV), Co, Si, Pb	Non-Hazardous; As, Mo, SO4
II	Class IV - pH	Si	Non-Hazardous; Mo
III	Class II - EC	Cd(III), Si	Non-Hazardous; Mo, Sb

According to surface water classification, Sample I and Sample II were classified as Class IV (highly contaminated) due to the high pH values and Sample III was classified as Class II (slightly contaminated) due to relatively higher EC value. If pH parameter was neglected, Sample I and Sample II also could be classified as Class II (slightly contaminated) according to the EC values. Moreover, according to surface water maximum environmental quality, As, Co, Si, Cd, and Pb concentration for Sample I; Si concentration for Sample II; Si and Cd concentration for Sample III exist above the limit standard. Previous study results(Gladwell et al.(2014)) (provided in Appendix-B) are similar to those of this work, As, Mo and SO4 concentrations are higher according to the waste categorization limits. Surface water quality evaluations are also similar indicating high As, Co, Si concentrations. Although does not necessarily has to be competitive, high concentrations of trace metal ions (As, Cd, Li, Mo, and Sr) detected in the whole rock analyses as greater than those of the average Upper crust are also high in the leachates. Groundwater includes high Al, As, Fe, Pb, Si concentrations

These shake flask leach test results indicate that low-high concentration metal release could occur from the test samples in short term (easily dissolvable) period under saturated test conditions. However, to determine whether such metal releases in short and long terms under field waste pile conditions would occur and if occur in what amounts, require water-rock reaction based hydrogeochemical modelling using kinetic test results. The model works will be presented in Chapter 10.

CHAPTER 9

KINETIC TESTS

9.1 Grain Size Distributions and Surface Areas of Test Samples

Densities and sieve analyses results measured in kinetic test samples are listed in Table 9.1. The densities of the test samples are in the order of II> I> III. The grain size analyses curves are shown in Figure 9.1. The grain size distribution of the samples is in the order of II <III <I.

Table 9.1. Results of density and sieve analyses.

Sample No		Density(g/cm3)	
I	I	2.46	2.46
II	II.1	2.11	2.51
	II.2	2.91	
III	III.1	1.64	2.01
	III.2	2.37	

Range (mm)	Size (mm)	I (g)	II (g)	III(g)
>6.35	6.35	304	75.6	270.2
5.66-6.35	5.66	97.1	84.4	178.5
4.76-5.66	4.76	60.7	107.3	134.5
4.00-4.76	4	61.9	143.1	135.2
2.83-4.00	2.83	81.4	222	170.7
2.00-2.83	2	54.1	135	121.8
1.68-2.00	1.68	37.5	98.9	80.1
1.19-1.68	1.19	47.9	115.6	96.4
1.00-1.19	1	23.6	46.5	39.9
<1	0	218.4	458.2	283.1
Total		986.6	1486.6	1510.4

Surface area calculations (MDAG, 2020) based on the grain size distribution and sample density indicate that surface area of Samples I, II and III are 1.54 m^2 / kg, 2.07 m^2 / kg, and 1.82 m^2 / kg, respectively. As it is expected, the reverse of the grain size distribution, the surface areas of the samples are in the order of II> III> I.

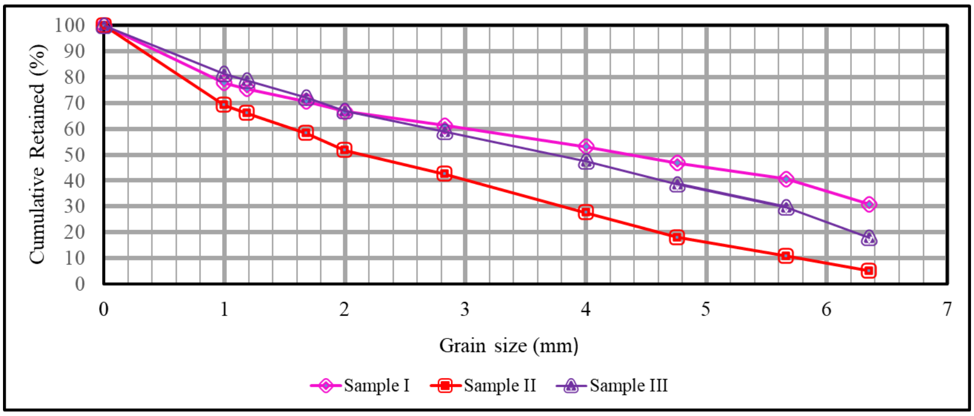


Figure 9.1. Grain size analyses of samples.

9.2 Quality Control

Quality control measurements were carried out during kinetic test runs to determine the accuracy and repeatability of the pH values and repeatability of the EC values. These measurements indicate that accuracy error of the pH values were very low (0.09 %). The repeatability for pH and EC values includes errors of about 2 % (+/- 0.15 pH unit) and 0.13 % (+/- 0.55 µS/cm), respectively.

In addition to these measurements, the kinetic leachate test solution of Sample II was separated into two different solutions (duplicate) and were sent to the laboratory in the 16th week. The estimated percent average deviations (average deviation *100/average) associated with the parameters, which have concentrations above the detection limit values, are listed in Table 9.2 as percent errors. These parameters are alkalinity, As, Ca, Li, Mg, Mo, Pb, Si, Sr and V.

Table 9.2. Duplicate sample percent deviation error of the parameters in kinetic test.

Parameter	Alkalinity	As	Ca	Li	Mg	Mo	Pb	Si	Sr	V
%Error	10.3	2.1	1.5	5.1	0.2	3.1	55.6	1.8	0.5	1.0

Lead parameter includes higher error than normally acceptable error of 30 % for these types of tests. The error is partially related to the very low concentrations measured (0.0044 mg/l, 0.0013 mg/l). But in any case, this possible error will be taken into consideration during lead parameter related evaluations.

9.3 Test Results

Room temperature values measured during the kinetic test are listed in Table 9.3 and distribution of the values are shown in Figure 9.2. The room temperature values were

Table 9.3. Room temperature values during the kinetic test.

Time	T (°C)
17.02.2020 10:30	28
18.02.2020 10:46	27.5
19.02.2020 15:46	28.2
20.02.2020 13:35	29.2
21.02.2020 15:25	29.6
24.02.2020 10:52	29.8
25.02.2020 09:52	30
26.02.2020 16:59	30.6
27.02.2020 15:20	30.8
28.02.2020 13:50	30.8
29.02.2020 13:52	30.8
3.03.2020 15:25	31.1
4.03.2020 16:32	32
5.03.2020 15:15	32
6.03.2020 15:15	31.6
9.03.2020 11:35	31.6
10.03.2020 10:12	31.1
11.03.2020 10:33	30.2
12.03.2020 14:03	30
13.03.2020 14:45	29.8
16.03.2020 10:32	29.3
17.03.2020 11:55	28.8
18.03.2020 10:45	27
19.03.2020 11:27	26
23.03.2020 10:45	27
24.03.2020 10:07	27.7
25.03.2020 11:09	27.8
26.03.2020 11:05	28
30.03.2020 10:27	26.3
31.03.2020 09:30	26
1.04.2020 12:23	26.1
2.04.2020 11:55	26
6.04.2020 10:45	25
7.04.2020 10:47	25
8.04.2020 10:25	25
9.04.2020 12:11	26
13.04.2020 10:32	25.6
14.04.2020 10:29	25.9
15.04.2020 10:31	26
16.04.2020 12:22	26.9
20.04.2020 13:25	27.2
21.04.2020 10:42	27
22.04.2020 12:29	27.1
27.04.2020 10:41	26
28.04.2020 10:39	26.2
29.04.2020 11:01	26.7
30.04.2020 13:02	27.2
4.05.2020 13:32	26.8
5.05.2020 09:41	26.1
6.05.2020 13:05	26.3
7.05.2020 12:25	26.9
11.05.2020 13:08	26.7
12.05.2020 10:14	26.7
13.05.2020 12:45	27.2
14.05.2020 12:48	28
15.05.2020 16:15	28
20.05.2020 10:57	29.1
21.05.2020 10:25	29.6
22.05.2020 12:24	30
27.05.2020 11:28	26
28.05.2020 10:00	25.2
29.05.2020 11:47	25.2
1.06.2020 11:37	24.1
2.06.2020 12:30	24.2
3.06.2020 12:08	24
4.06.2020 11:38	24.7

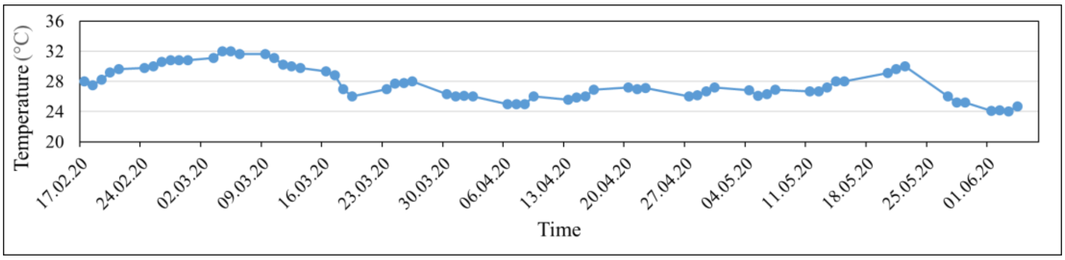


Figure 9.2. Room temperature distribution during the kinetic test.

in range of 24 °C and 32 °C with the average of 28 °C which is slightly higher than that of air temperature in the study area. Considering the characteristic of the kinetic leach test (excessive sample alteration in a short period of time in comparison to natural conditions) and other alteration agents (e.g. wind, abrupt changes of temperatute) which are not simulated in the tests but will be active in the field, the room and field temperature difference is considered acceptable.

The kinetic test related other results of samples are listed in Table 9.4. As it was explained before, the leachate drainage was ceased after the 1st Week from Sample I column due to clogging of the porous disc caused by very high clay content of the sample. Because of it, the sample became saturated in irrigation days (wet period) and added water accumulated at the top of the sample. After the irrigation, the slurry (sample + solution at the top) is mechanically mixed for a short period of time in order to ensure interaction of the added water with the sample. The leachate at the end of a cycle is collected from the upper column with a pump after allowing enough sedimentation time. However, while collecting with the pump, approximately 3 cm height slurry was left in the upper column in order not to collect the sample sediments present in the slurry. The effect of this remaining solution to the concentrations of the following cycle is estimated by considering volume and concentrations of the remaining solution and volume and concentrations of the next cycle solution as explained in Appendix-C. The values of Sample I listed in Table 9.4 are those estimated mixing free values. The mixing effects are in fact negligible as demonstrated in Appendix-C where the original laboratory measurements are also provided.

Table 9.4. Kinetic test results

Sample No	Starting date	Week	Added Volume of Water	Collected Volume of Water	Decreased Sample Amount	T °C	pH	EC	Alkalinity	Cl	SO4
Detection							**<0.1**	**<0.1**	**<3**	**<1.5**	**<10**
Unit (mg/l)			**ml**	**ml**	**g**			**µS/cm**	**mg/l**	**mg/l**	**mg/l**
I-0	13.02.2020	0	1700	640			7.76	732.0	88	7	247.64
II-0			1400	1070		21.6	7.27	232.1	70.7	<1.5	33.92
III-0			1600	1070		21.3	7.09	346.0	73.8	1.95	87.00
I-1	20.02.2020	1	900	700		25.8	7.66	1473.0	76.2	6.65	498.53
II-1			800	745		22.3	7.72	366.8	70.1	<1.5	122.26
III-1			800	747		22.8	7.32	573.0	63.0	3.95	236.24
I-2	27.02.2020	2	750	532.5		27.7	7.92	479.8	84.4	7.9	166.55
II-2			750	645		25.1	7.89	275.0	68.8	4	59.57
III-2			750	732		25.2	7.54	404.0	60.0	6	124.70
I-3	5.03.2020	3	750	565	4*	26.7	8.75	657.9	168.6	69.6	149.87
II-3			750	707		26.7	7.72	205.2	66.0	3	31.32
III-3			750	705		26.9	8.40	335.5	63.4	3	87.25
I-4	12.03.2020	4	750	655	4*	24.3	9.04	524.8	102.6	6.7	84.06
II-4			800	782.5		24.5	7.59	189.5	62.6	2	27.01
III-4			800	744		24.6	7.97	298.3	60.0	5	75.93
I-5	19.03.2020	5	750	743	1.47	20.7	9.44	324.3	242.9	<1.5	68.33
II-5			750	712.5		20.3	7.09	148.4	73.4	<1.5	11.45
III-5			750	699		20.4	8.15	250.1	74.8	<1.5	70.72
I-6	26.03.2020	6	750	675	2.55	22.4	8.81	271.9	86.0	<1.5	21.33
II-6			750	725		22.3	7.02	133.2	63.0	<1.5	<10
III-6			750	725		22.3	7.63	232.9	60.2	<1.5	49.69
I-7	2.04.2020	7	750	684	3.11	20.7	8.80	225.5	86.5	<1.5	25.47
II-7			750	733		20.7	6.84	126.1	61.3	<1.5	14.68
III-7			750	730		20.6	7.60	228.3	56.6	<1.5	49.69
I-8	9.04.2020	8	750	676	11	20.5	8.61	191.6	81.9	<1.5	16.35
II-8			750	735		20.4	6.88	122.7	57.8	0.65	<10
III-8			750	732.5		20.3	7.49	198.9	59.2	<1.5	39.76
I-9	16.04.2020	9	750	644	0.13	21.6	8.50	182.4	91.8	<1.5	8.95
II-9			750	718		21.5	6.82	119.0	59.0	<1.5	<10
III-9			750	726		21.3	7.44	183.7	58.5	<1.5	33.57
I-10	22.04.2020	10	720	635	10.5	21.9	8.29	153.6	81.2	<1.5	10.31
II-10			710	665		21.9	6.68	108.8	65.8	1.6	<10
III-10			710	670		21.7	7.24	149.2	58.1	<1.5	26.89
I-11	30.04.2020	11	700	682	1.86	22	8.23	164.5	94.7	<1.5	16.53
II-11			725	690		21.9	6.57	118.8	65.4	<1.5	<10
III-11			725	694		21.7	7.20	165.7	62.3	<1.5	30.15
I-12	7.05.2020	12	700	670	2.54	21.6	8.29	141.2	90.8	<1.5	<10
II-12			725	692		21.5	6.61	119.7	59.9	<1.5	<10
III-12			725	702.5		21.5	7.17	160.2	62.0	<1.5	23.80
I-13	14.05.2020	13	715	681	1.98	22.4	8.23	133.3	69.0	2.4	16.42
II-13			725	686		22.4	6.55	112.3	63.4	2	<10
III-13			725	695		22.3	7.29	151.3	64.6	2.3	22.50
I-14	21.05.2020	14	-	-	-	-	-	-	-	-	-
II-14			750	704.5		24.4	6.81	129.8	70.4	<1.5	<10
III-14			750	690		24.5	8.19	137.1	56	<1.5	22.66
I-15	28.05.2020	15	-	-	-	-	-	-	-	-	-
II-15			750	677.5		20	6.54	106.2	53	<1.5	<10
III-15			750	685		19.9	7.15	129.3	52.4	<1.5	19.73
I-16	4.06.2020	16	-	-	-	-	-	-	-	-	-
II-16			750	695		19.2	6.54	87.3	58.3	<1.5	<10
III-16			750	735		19	7.28	133.9	52.1	1.65	24.614

*Estimated value. nm: Not measured due to insufficient sample solution.

Table 9.4. Cont’d.

Sample No	Starting date	Week	Al	As	B	Ba	Be	Bi	Ca	Cd	Co	Cr. t	Cu
Detection			**<0.01**	**<0.001**	**<0.01**	**<0.01**	**<0.001**	**<0.040**	**<1.00**	**<0.0005**	**<0.0005**	**<0.001**	**<0.001**
Unit (mg/l)			**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**
I-0	13.02.2020	0	0.68555	0.082	<0.01	0.078	<0.001	<0.040	30.95	0.0007	0.0141	0.001	0.015
II-0			<0.01	0.012	<0.01	0.020	<0.001	<0.040	5.78	<0.0005	0.00064	0.00129	0.009
III-0			<0.01	0.028	<0.01	0.035	<0.001	<0.040	7.97	<0.0005	<0.0005	<0.001	0.007
I-1	20.02.2020	1	<0.01	0.104	<0.01	0.080	<0.001	<0.040	56.84	0.004	0.00232	<0.001	<0.001
II-1			0.01811	0.017	<0.01	0.031	<0.001	<0.040	7.48	0.00062	0.00139	<0.001	0.001
III-1			<0.01	0.066	<0.01	0.041	<0.001	<0.040	21.42	0.00271	0.00211	<0.001	<0.001
I-2	27.02.2020	2	0.03473	0.139	<0.01	0.061	<0.001	<0.040	0.00	0.00108	0.00078	<0.001	<0.001
II-2			0.01287	0.021	<0.01	0.021	<0.001	<0.040	4.89	0.00036	0.00127	<0.001	<0.001
III-2			<0.01	0.094	<0.01	0.033	<0.001	<0.040	8.43	0.00162	0.00323	<0.001	<0.001
I-3	5.03.2020	3	0.01398	0.108	<0.01	0.009	<0.001	<0.040	nm	<0.0005	<0.0005	<0.001	0.022
II-3			0.01026	0.024	<0.01	0.016	<0.001	<0.040	nm	<0.0005	<0.0005	<0.01	0.004
III-3			<0.01	0.102	<0.01	0.029	<0.001	<0.040	nm	<0.0005	<0.0005	0.00102	0.004
I-4	12.03.2020	4	0.28589	0.201	<0.01	0.061	<0.001	<0.040	nm	<0.0005	0.00047	0.00316	0.002
II-4			<0.01	0.028	<0.01	0.017	<0.001	<0.040	nm	<0.0005	<0.0005	0.00103	0.004
III-4			<0.01	0.102	<0.01	0.026	<0.001	<0.040	nm	<0.0005	<0.0005	<0.001	0.003
I-5	19.03.2020	5	0.3533	0.093	<0.01	0.028	<0.001	<0.040	2.58	<0.0005	0.00048	0.00055	0.004
II-5			<0.01	0.024	<0.01	0.012	<0.001	<0.040	5.34	<0.0005	<0.0005	<0.001	0.002
III-5			0.02311	0.097	<0.01	0.039	<0.001	<0.040	6.21	<0.0005	0.00064	0.00105	0.013
I-6	26.03.2020	6	0.9176	0.137	<0.01	0.027	<0.001	<0.040	17.80	<0.0005	<0.0005	<0.001	0.003
II-6			0.02372	0.020	<0.01	0.012	<0.001	<0.040	4.45	<0.0005	<0.0005	<0.001	0.001
III-6			0.03863	0.076	<0.01	0.025	<0.001	<0.040	6.04	<0.0005	<0.0005	<0.001	0.001
I-7	2.04.2020	7	0.65681	0.133	<0.01	0.014	<0.001	<0.040	29.44	<0.0005	<0.0005	<0.001	0.002
II-7			0.02599	0.020	<0.01	0.011	<0.001	<0.040	4.98	<0.0005	<0.0005	<0.001	0.001
III-7			0.01653	0.068	<0.01	0.026	<0.001	<0.040	6.56	<0.0005	<0.0005	<0.001	0.001
I-8	9.04.2020	8	1.43763	0.281	<0.01	0.011	<0.001	<0.040	4.54	<0.0005	<0.0005	<0.001	0.002
II-8			0.02621	0.019	<0.01	0.011	<0.001	<0.040	5.37	<0.0005	<0.0005	<0.001	0.001
III-8			0.03537	0.071	<0.01	0.023	<0.001	<0.040	6.16	<0.0005	<0.0005	<0.001	0.001
I-9	16.04.2020	9	0.76418	0.085	<0.01	0.020	<0.001	<0.040	8.20	<0.0005	<0.0005	<0.001	0.003
II-9			0.02387	0.018	<0.01	<0.01	<0.001	<0.040	4.63	<0.0005	<0.0005	<0.001	<0.001
III-9			0.0216	0.071	<0.01	0.020	<0.001	<0.040	6.11	<0.0005	<0.0005	<0.001	<0.001
I-10	22.04.2020	10	2.43357	0.106	<0.01	0.011	<0.001	<0.040	3.62	<0.0005	<0.0005	<0.001	0.002
II-10			0.03364	0.016	<0.01	<0.01	<0.001	<0.040	4.79	<0.0005	<0.0005	<0.001	<0.001
III-10			0.01167	0.059	<0.01	0.016	<0.001	<0.040	4.97	<0.0005	<0.0005	<0.001	<0.001
I-11	30.04.2020	11	1.54133	0.238	<0.01	0.014	<0.001	<0.040	5.11	<0.0005	<0.0005	<0.001	0.002
II-11			0.02961	0.018	<0.01	<0.01	<0.001	<0.040	5.06	<0.0005	<0.0005	<0.001	<0.001
III-11			0.01594	0.068	<0.01	0.020	<0.001	<0.040	5.40	<0.0005	<0.0005	<0.001	<0.001
I-12	7.05.2020	12	10.0423	0.079	<0.01	0.029	<0.001	<0.040	3.51	<0.0005	<0.0005	0.01239	<0.001
II-12			0.02449	0.019	<0.01	<0.01	<0.001	<0.040	7.16	<0.0005	<0.0005	<0.001	<0.001
III-12			0.00325	0.062	<0.01	0.015	<0.001	<0.040	9.93	<0.0005	<0.0005	0.00165	<0.001
I-13	14.05.2020	13	4.23968	0.069	<0.01	0.045	<0.001	<0.040	2.44	<0.0005	<0.0005	0.0067	<0.001
II-13			0.01929	0.017	<0.01	<0.01	<0.001	<0.040	16.51	<0.0005	<0.0005	<0.001	<0.001
III-13			<0.01	0.062	<0.01	0.013	<0.001	<0.040	3.21	<0.0005	<0.0005	<0.001	<0.001
I-14	21.05.2020	14	-	-	-	-	-	-	-	-	-	-	-
II-14			<0.01	0.01474	<0.01	<0.01	<0.001	<0.040	9.009	<0.0005	<0.0005	<0.001	<0.001
III-14			<0.01	0.0452	<0.01	0.01192	<0.001	<0.040	4.727	<0.0005	<0.0005	<0.001	<0.001
I-15	28.05.2020	15	-	-	-	-	-	-	-	-	-	-	-
II-15			<0.01	0.02968	<0.01	<0.01	<0.001	<0.040	4.635	<0.0005	<0.0005	<0.001	<0.001
III-15			<0.01	0.03672	<0.01	0.0131	<0.001	<0.040	4.465	<0.0005	<0.0005	<0.001	<0.001
I-16	4.06.2020	16	-	-	-	-	-	-	-	-	-	-	-
II-16			<0.01	0.01002	<0.01	<0.01	<0.001	<0.040	4.011	<0.0005	<0.0005	<0.001	<0.001
III-16			<0.01	0.0424	<0.01	0.01089	<0.001	<0.040	4.638	<0.0005	<0.0005	<0.001	<0.001

Table 9.4. Cont’d.

Sample No	**Starting date**	**Week**	**Fe**	**Hg**	**K**	**Li**	**Mg**	**Mn**	**Mo**	**Na**	**Ni**	**P**	**Pb**
Detection			**<0.01**	**<0.0001**	**<1.00**	**<0.01**	**<1.00**	**<0.01**	**<0.001**	**<1.00**	**<0.01**	**<0.040**	**<0.0005**
Unit (mg/l)			**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**
I-0	13.02.2020	0	1.140	<0.0001	23.18	0.044	8.35	0.0487	0.88359	10.78	0.01689	<0.040	0.0047
II-0			<0.01	<0.0001	6.36	0.092	22.40	<0.01	0.14754	17.95	0.02701	<0.040	0.00544
III-0			<0.01	<0.0001	9.37	0.262	25.18	<0.01	0.45989	33.28	<0.01	<0.040	0.00061
I-1	20.02.2020	1	<0.01	<0.0001	3.16	0.085	20.24	<0.01	2.8465	20.24	<0.01	<0.040	0.01202
II-1			<0.01	<0.0001	6.30	0.121	32.70	0.02176	0.26813	22.70	<0.01	<0.040	0.02163
III-1			<0.01	<0.0001	6.89	0.379	38.52	<0.01	1.31469	42.62	<0.01	<0.040	0.01472
I-2	27.02.2020	2	<0.01	<0.0001	20.56	0.031	3.73	<0.01	0.454	110.07	<0.01	<0.040	0.00325
II-2			<0.01	<0.0001	4.24	0.104	25.25	0.0173	0.16925	10.97	<0.01	<0.040	0.00159
III-2			<0.01	<0.0001	7.71	0.251	25.81	<0.01	0.69712	33.39	<0.01	<0.040	0.00429
I-3	5.03.2020	3	<0.01	<0.0001	nm	0.038	nm	<0.01	0.60744	nm	<0.01	<0.040	5.4E-05
II-3			0.024	<0.0001	nm	0.091	nm	0.0153	0.1027	nm	<0.01	<0.040	0.01377
III-3			<0.01	<0.0001	nm	0.268	nm	<0.01	0.38272	nm	<0.01	<0.040	0.00793
I-4	12.03.2020	4	0.084	<0.0001	nm	0.046	nm	<0.01	0.66105	nm	<0.01	<0.040	<0.0005
II-4			<0.01	<0.0001	nm	0.088	nm	0.01378	0.06784	nm	<0.01	<0.040	0.00937
III-4			<0.01	<0.0001	nm	0.236	nm	<0.01	0.22222	nm	<0.01	<0.040	0.00273
I-5	19.03.2020	5	0.106	<0.0001	23.88	0.019	9.42	0.00958	0.19752	108.60	<0.01	<0.040	0.00435
II-5			<0.01	<0.0001	2.00	0.065	15.39	0.01234	0.05802	3.48	<0.01	<0.040	0.00279
III-5			0.088	<0.0001	5.70	0.173	18.00	<0.01	0.12515	17.78	<0.01	<0.040	0.0187
I-6	26.03.2020	6	0.102	<0.0001	8.92	0.015	2.78	0.04839	0.20117	37.22	<0.01	<0.040	<0.0005
II-6			0.069	<0.0001	1.47	0.039	14.36	<0.01	0.0323	2.44	<0.01	<0.040	0.00937
III-6			0.096	<0.0001	4.98	0.121	18.87	<0.01	0.07401	19.95	<0.01	<0.040	0.01165
I-7	2.04.2020	7	0.174	<0.0001	8.92	0.014	7.05	0.02824	0.11021	41.93	<0.01	<0.040	<0.0005
II-7			0.085	<0.0001	1.34	0.033	13.00	0.01049	0.02492	2.29	<0.01	<0.040	0.00213
III-7			0.068	<0.0001	4.34	0.110	15.69	<0.01	0.0588	20.42	<0.01	<0.040	0.00536
I-8	9.04.2020	8	8.868	<0.0001	8.44	0.012	2.27	0.0099	0.09534	40.79	<0.01	<0.040	<0.0005
II-8			0.089	<0.0001	1.12	0.028	13.89	<0.01	0.0183	2.24	<0.01	<0.040	0.00735
III-8			0.097	<0.0001	3.87	0.096	14.93	<0.01	0.04734	13.68	<0.01	<0.040	0.0046
I-9	16.04.2020	9	0.286	<0.0001	7.46	0.009	3.13	0.02192	0.06717	33.54	<0.01	<0.040	<0.0005
II-9			0.079	<0.0001	1.09	0.025	12.78	<0.01	0.01587	1.69	<0.01	<0.040	0.00994
III-9			0.075	<0.0001	3.80	0.087	15.22	<0.01	0.04093	1.36	<0.01	<0.040	0.00526
I-10	22.04.2020	10	0.474	<0.0001	6.54	<0.01	2.31	0.01165	0.04043	24.56	<0.01	<0.040	0.00272
II-10			0.074	<0.0001	<1.00	0.022	12.25	<0.01	0.01322	1.33	<0.01	<0.040	0.00205
III-10			0.049	<0.0001	3.02	0.070	13.02	<0.01	0.03404	8.10	<0.01	<0.040	0.00427
I-11	30.04.2020	11	0.419	<0.0001	8.57	0.013	2.41	0.01417	0.06592	35.52	<0.01	<0.040	0.00687
II-11			0.092	<0.0001	<1.00	0.023	13.08	<0.01	0.01512	1.29	<0.01	<0.040	0.00943
III-11			0.060	<0.0001	3.25	0.075	14.48	<0.01	0.03939	8.63	<0.01	<0.040	0.00501
I-12	7.05.2020	12	2.501	<0.0001	4.38	0.012	2.40	0.01658	0.032	9.78	<0.01	<0.040	0.00078
II-12			0.083	<0.0001	<1.00	0.027	5.62	<0.01	0.01343	<1.00	<0.01	<0.040	0.00497
III-12			<0.01	<0.0001	1.10	0.079	5.58	<0.01	0.03465	3.33	<0.01	<0.040	0.02537
I-13	14.05.2020	13	0.276	<0.0001	2.35	0.012	1.09	0.00969	0.03468	8.80	<0.01	<0.040	0.00061
II-13			<0.01	<0.0001	5.56	0.025	5.56	<0.01	0.01137	<1.00	<0.01	<0.040	0.00438
III-13			<0.01	<0.0001	1.07	0.076	5.39	<0.01	0.02919	3.07	<0.01	<0.040	<0.0005
I-14	21.05.2020	14	-	-	-	-	-	-	-	-	-	-	-
II-14			<0.01	<0.0001	<1.00	0.02653	11.13	<0.01	0.01275	<1.00	<0.01	<0.040	<0.0005
III-14			<0.01	<0.0001	2.531	0.06226	10.51	<0.01	0.02874	5.461	<0.01	<0.040	0.00061
I-15	28.05.2020	15	-	-	-	-	-	-	-	-	-	-	-
II-15			0.07959	<0.0001	<1.00	0.02799	10.86	<0.01	0.01175	<1.00	<0.01	<0.040	0.00163
III-15			<0.01	<0.0001	2.235	0.07703	9.935	<0.01	0.02999	4.989	<0.01	<0.040	0.00552
I-16	4.06.2020	16	-	-	-	-	-	-	-	-	-	-	-
II-16			<0.01	<0.0001	<1.00	0.0198	9.01	<0.01	0.00481	<1.00	<0.01	<0.040	0.00441
III-16			<0.01	<0.0001	2.328	0.06428	10.92	<0.01	0.02129	5.215	<0.01	<0.040	0.00292

Table 9.4. Cont'd.

Sample No	Starting date	Week	Sb	Se	Si	Sn	Sr	Ti	U	V	Zn	Zr
Detection			**<0.0005**	**<0.01**	**<0.04**	**<0.001**	**<0.01**	**<0.01**	**<0.0005**	**<0.001**	**<0.01**	**<0.040**
Unit (mg/l)			**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**	**mg/l**
I-0	13.02.2020	0	<0.0005	<0.01	207.7	<0.001	0.70754	<0.01	1.26085	0.0036	0.07047	<0.040
II-0			0.00055	<0.01	4.894	<0.001	0.31682	<0.01	0.32137	0.04981	0.01808	<0.040
III-0			0.00425	0.01161	7.948	<0.001	0.54703	<0.01	0.50051	0.01189	0.01207	<0.040
I-1	20.02.2020	1	0.0005	<0.01	13.66	<0.001	2.61677	<0.01	2.07852	<0.001	0.02536	<0.040
II-1			0.0013	<0.01	8.063	<0.001	0.64858	<0.01	0.27463	0.04917	0.01353	<0.040
III-1			0.00864	0.021	10.54	<0.001	0.8474	<0.01	0.5804	0.02438	0.01504	<0.040
I-2	27.02.2020	2	0.00068	<0.01	12.3393	<0.001	0.23083	<0.01	1.1291	<0.001	<0.01	<0.040
II-2			0.00134	<0.01	9.848	<0.001	0.43761	<0.01	0.14368	0.05766	0.01859	<0.040
III-2			0.00995	0.01207	11.08	<0.001	0.6156	<0.01	0.42634	0.03705	0.01965	<0.040
I-3	5.03.2020	3	0.00298	<0.01	1.25199	<0.001	0.517	<0.01	0	0.00289	0.01133	<0.040
II-3			0.0013	<0.01	0.1667	<0.001	0.42312	<0.01	<0.0005	0.06777	0.01361	<0.040
III-3			0.01009	<0.01	2.505	<0.001	0.54057	<0.01	<0.0005	0.0474	0.00877	<0.040
I-4	12.03.2020	4	0.00111	<0.01	148.23	<0.001	0.96039	<0.01	0.00233	0.00295	0.00907	<0.040
II-4			0.00198	<0.01	2.562	<0.001	0.37363	<0.01	<0.0005	0.06314	0.01252	<0.040
III-4			0.01207	<0.01	1.103	<0.001	0.52229	<0.01	<0.0005	0.04295	<0.01	<0.040
I-5	19.03.2020	5	0.00404	<0.01	0	<0.001	0.24047	<0.01	0.0001	0.00241	0.01891	<0.040
II-5			0.00185	<0.01	17.1	<0.001	0.37675	<0.01	<0.0005	0.05124	0.01234	<0.040
III-5			0.01116	<0.01	19.44	<0.001	0.37449	<0.01	0.00045	0.04067	<0.01	<0.040
I-6	26.03.2020	6	<0.0005	<0.01	5.21378	<0.001	0.32608	<0.01	<0.0005	0.00488	<0.01	<0.040
II-6			<0.0005	<0.01	5.775	<0.001	0.15683	<0.01	<0.0005	0.05076	<0.01	<0.040
III-6			0.00655	<0.01	6.439	<0.001	0.86769	<0.01	<0.0005	0.03766	<0.01	<0.040
I-7	2.04.2020	7	0.001	<0.01	9.78384	<0.001	0.58577	<0.01	<0.0005	0.00576	<0.01	<0.040
II-7			<0.0005	<0.01	4.752	<0.001	0.15387	<0.01	<0.0005	0.04742	<0.01	<0.040
III-7			0.00542	<0.01	4.582	<0.001	0.85869	<0.01	<0.0005	0.03364	<0.01	<0.040
I-8	9.04.2020	8	<0.0005	<0.01	10.7239	<0.001	0.0203	<0.01	<0.0005	0.00783	<0.01	<0.040
II-8			<0.0005	<0.01	4.557	<0.001	0.14531	<0.01	<0.0005	0.04402	<0.01	<0.040
III-8			0.00547	<0.01	4.324	<0.001	1.1247	<0.01	<0.0005	0.03387	<0.01	<0.040
I-9	16.04.2020	9	<0.0005	<0.01	11.8577	<0.001	0.1063	<0.01	<0.0005	0.00661	<0.01	<0.040
II-9			<0.0005	<0.01	3.996	<0.001	0.14297	<0.01	<0.0005	0.04348	<0.01	<0.040
III-9			0.00535	<0.01	5.008	<0.001	0.64076	<0.01	<0.0005	0.03619	<0.01	<0.040
I-10	22.04.2020	10	<0.0005	<0.01	14.722	<0.001	0.07375	<0.01	<0.0005	0.00924	<0.01	<0.040
II-10			<0.0005	<0.01	4.241	<0.001	0.12995	<0.01	<0.0005	0.03976	<0.01	<0.040
III-10			0.00421	<0.01	4.385	<0.001	1.36163	<0.01	<0.0005	0.03228	<0.01	<0.040
I-11	30.04.2020	11	<0.0005	<0.01	7.83332	<0.001	0.11106	<0.01	<0.0005	0.0063	<0.01	<0.040
II-11			<0.0005	<0.01	3.271	<0.001	0.14527	<0.01	<0.0005	0.04206	<0.01	<0.040
III-11			0.0051	<0.01	6.424	<0.001	0.65022	<0.01	<0.0005	0.03535	<0.01	<0.040
I-12	7.05.2020	12	0.00053	<0.01	36.0288	<0.001	0.16178	<0.01	<0.0005	0.01866	<0.01	<0.040
II-12			<0.0005	<0.01	10.01	<0.001	0.17799	<0.01	<0.0005	0.04296	<0.01	<0.040
III-12			0.00551	<0.01	8.979	<0.001	0.22446	<0.01	<0.0005	0.03233	<0.01	<0.040
I-13	14.05.2020	13	0.00062	<0.01	23.2825	<0.001	0.10867	<0.01	<0.0005	0.01097	<0.01	<0.040
II-13			<0.0005	<0.01	4.303	<0.001	0.17073	<0.01	<0.0005	0.03887	<0.01	<0.040
III-13			0.00545	<0.01	4.69	<0.001	0.21259	<0.01	<0.0005	0.03291	<0.01	<0.040
I-14	21.05.2020	14	-	-	-	-	-	-	-	-	-	-
II-14			<0.0005	<0.01	4.092	<0.001	0.16747	<0.01	<0.0005	0.15964	<0.01	<0.040
III-14			0.00433	<0.01	3.182	<0.001	0.19121	<0.01	<0.0005	0.10503	<0.01	<0.040
I-15	28.05.2020	15	-	-	-	-	-	-	-	-	-	-
II-15			0.00051	<0.01	151.1	<0.001	0.1681	<0.01	<0.0005	0.03318	<0.01	<0.040
III-15			0.0041	<0.01	129.8	<0.001	0.20894	<0.01	<0.0005	0.02421	<0.01	<0.040
I-16	4.06.2020	16	-	-	-	-	-	-	-	-	-	-
II-16			<0.0005	<0.01	132.9	<0.001	0.12403	<0.01	<0.0005	0.03002	<0.01	<0.040
III-16			0.00389	<0.01	134.6	<0.001	0.19247	<0.01	<0.0005	0.02354	<0.01	<0.040

pH Evaluation:

The column test leachate pH values of each sample and pH percent differences calculated from the difference between deionized irrigation water (pH=7) and drained leachate are shown in Figure 9.3.

pH values of all sample leachates are basic in character except the values of sample II after the 6th week and the values are in the order of Bostantepe (I) > Upper Çavuşlar (III) > Lower Çavuşlar (II) sequence. Changing trends are similar after the 5th week. The pH value ranges are 7.66-9.43; 6.54-7.89 and 7.09-8.40 for Sample I, Sample II and Sample III, respectively. The values show a continuous increasing trend for all samples in the early weeks (0-5th week for sample I, 0-2nd week for sample II and 0-3rd week; for sample III) and afterwards, generally decreasing trends are observed except the 5th and the 14th weeks of samples II and III and the 16th week of Sample III (Figure 9.3a).

Value differences between the measured pH and the irrigation water (deionized water) pH reflect the mineral-rock reactions related pH changes which occurred as 9.4-34.9% increase in Sample I leachates; 1.3-12.7% increase and 1.7-6.6% decrease in Sample II leachates; and 1.3-20% increase in Sample III leachates with respect to the irrigation water pH (Figure 9.3b). The reasons behind these changes in the pH values are related to the oxidation of sulphide minerals, dissolution of the neutralizing minerals and related chemical processes in leachates.

Acid generation potentials of the Sample II and Sample III having similar AP values as indicated by the static test results, are controlled by the neutralization reactions. Early weeks pH increasing in leachates of Sample II and Sample III indicates the dissolution of short-term neutralization introducing carbonate minerals (specifically dolomite). Higher pH values of Sample II leachates with respect to those of Sample III in the first two weeks are probably related to the dissolution of other carbonate minerals (magnesite and ankerite) present in Sample II in addition to dolomite reflecting the earlier stage neutralization effects of Fe-Mn carbonate minerals.

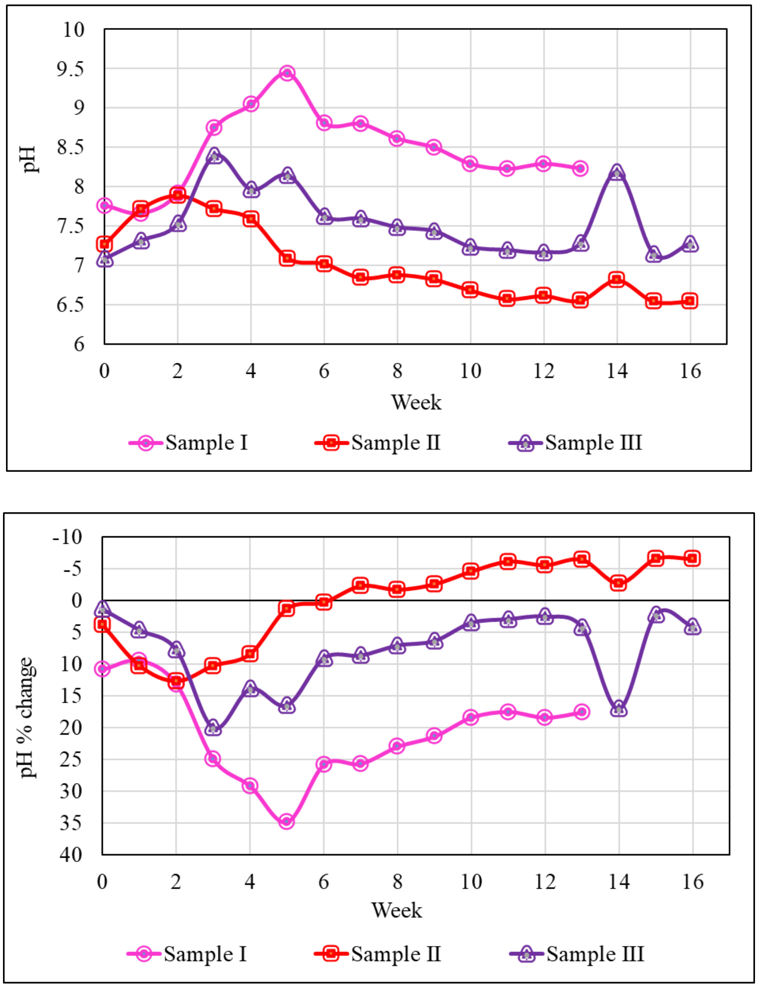


Figure 9.3. Kinetic test pH values (above) and percentage changes with respect to the irrigation water pH (below).

After early weeks, pH values of the sample II and sample III were decreased gradually. Considering that NNP is controlled by neutralizing minerals rather than sulphide minerals as indicated by ABA test results, this could be explained by ceasing of short-term neutralizing carbonate minerals related reactions. Oxidation of sulphide minerals were probably also slowed down during this phase as indicated by the decreasing sulphate concentrations hence values are still basic and sharp pH decrease was not observed. Nevertheless, in Sample II leachates, acid producing mineral reactions (sulphide oxidation and metal hydroxide formation) must have been at greater rates than those of neutralizing minerals after the 6th week, as a result, pH values decreased to acidic values. Lower pH values of Sample II with respect to those of Sample III are consistent with the static test ABA results (NPR value of Sample II is lower that of Sample III). Silicate minerals related relatively long-term neutralizing reactions are suggested by mineralogy for Sample III but not for Sample II.

According to the static test results, Sample I leachates should have included relatively lower pH values than those of Sample II and III but they are not. This could be explained by either insufficient sulphide oxidation under water saturated conditions or lack of sulphide minerals as suggested by XRD analyses. However, AP value of Sample I is higher than those of the others (suggesting sulphide mineral presence) and pH of this sample showed relative decrease in the 1st week then increased under the saturated conditions. This could be interpreted as an indication of the saturated test condition related control. The increasing pH trend of Sample I up to the 5th week could be related to the dissolution of carbonate minerals (calcite and partially surite) and continuation of the increase with respect to the irrigation water pH at decreasing rates afterwards, could be explained by the exhaustion of oxidized sample parts and ceasing of short-term neutralizing carbonate minerals related reactions together with late stage acid producing reactions of surite. But lack of direct observation of calcite in the sample requires substitutional/further reasoning. In fact, saturated conditions related montmorillonite reactions could explain the observed pH trend as well. As introduced in the earlier sections, montmorillonite mineral is not stable under alkaline conditions, subject to hydrolysis and Na and H^+ exchange increases solution pH (Kaufhold et al., 2008). Therefore, the increasing pH trend up to the 5th week could be related to the such clay reactions (contributed also by surite mineral dissolution) and continuation of the increase with respect to the irrigation water pH at decreasing rates afterwards, could be explained by the metal hydroxide formations under such basic conditions in addition to ceasing of montmorillonite related control together with late stage acid producing reactions of surite. In any case, sulphide oxidation or other processes (metal hydroxide formation) related acid production in Sample I leachates under saturated conditions were much lower than the neutralization production.

In summary, relatively short period covering kinetic test results suggest that waste pile rocks in the area do not have ARD production potential, but these rocks could create leachates with high concentrations under basic conditions. In addition, the pH values could be lower in the longer test periods because the trends have not reached to steady state condition yet. Indeed, NAG test results reflecting long-term extreme oxidation conditions suggest that the final pH values, although greater than the critical limit value of 4.5, could reach down to the range of 5.14-5.71.

EC Evaluation:

The electrical conductivity value distribution variation of test sample leachates is shown in Figure 9.4. Measured values reflect the water-mineral reactions related changes in the EC of deionized irrigation water whose value was determined to be between 1.5 and 3.4 µS/cm (average of 2.55 µS/cm). EC values of the leachates are in the ranges of 133.3-1473 µS/cm; 87.3-366.8 µS/cm and 129.3-573µS/cm for Sample I, Sample II and Sample III, respectively and are in the order of Bostantepe (I) > Upper Çavuşlar (III) > Lower Çavuşlar (II) sequence throughout the whole test period (Figure 9.4). The EC ordering among the sample leachates indicates that the ion releasing was higher at higher basic pH values. The values were initially very high due to oxidized parts related reactions, then continuously decreased to lower levels toward the last weeks and assumed flat positions indicating low level ion production in all sample leachates. This is related to the well-known lower level reaction relationship toward neutral pH conditions (Figure 9.5).

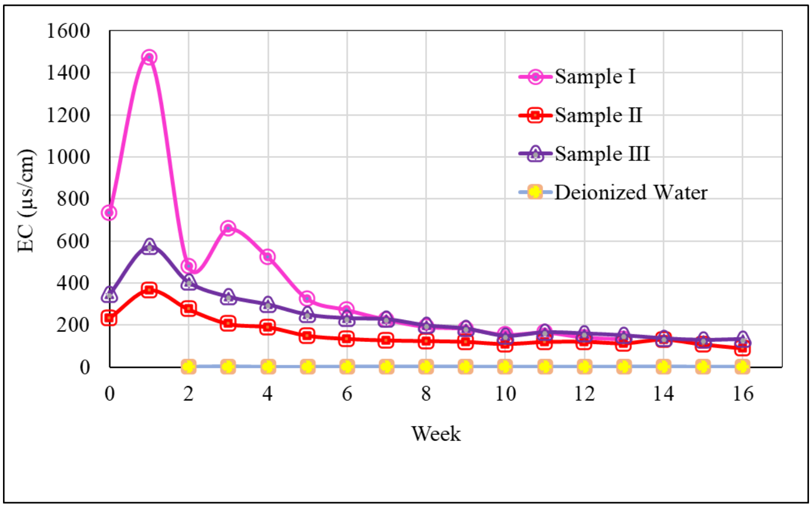


Figure 9.4. Variation of the EC values.

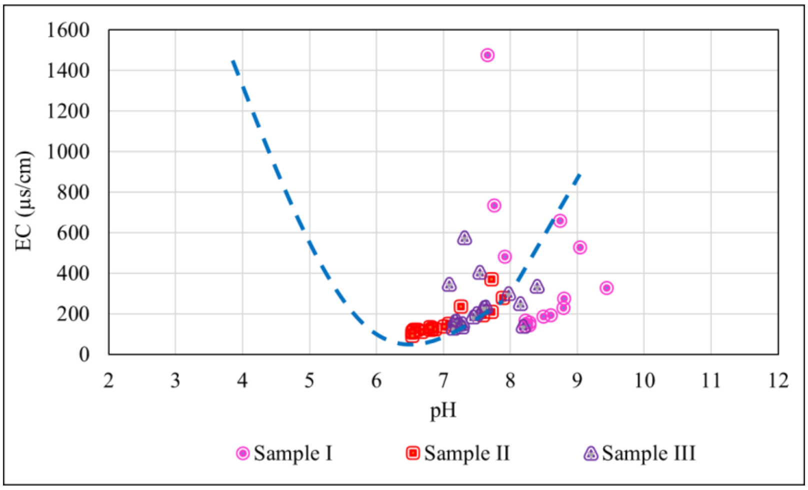


Figure 9.5. EC-pH relationship. The dashed line represents the expected trend.

According to the surface water quality regulation (MFW, 2016) limits for EC and pH values, Sample II and III leachates are in the near neutral and Class-I quality (except the 1st week leachate III, Class-II) (Figure 9.6). On the other hand, Sample I leachates are although in the near-neutral region, they are in Class I, II and III qualities in terms of EC values.

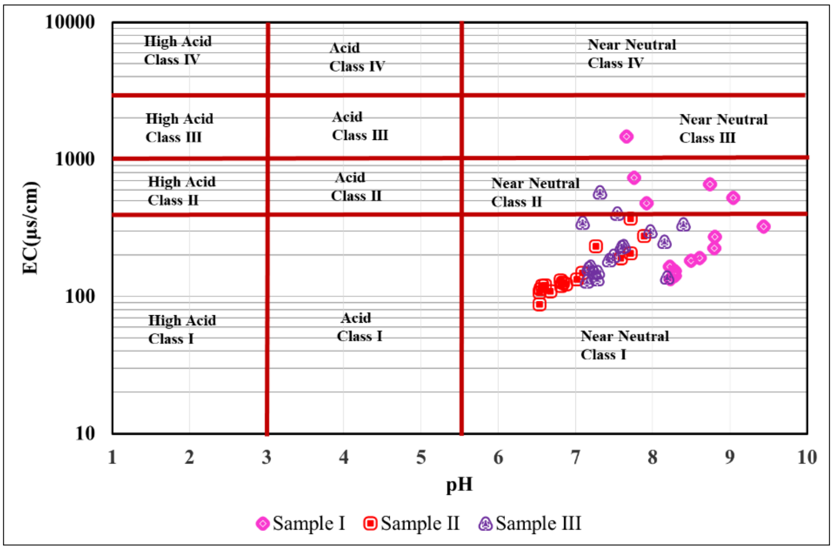


Figure 9.6. Kinetic test leachate classification according to EC-pH values.

Ions Concentrations:

Relatively high EC values measured in the leachates reflect basic environment water-rock reactions related ion concentrations and indicate possible ion release from the waste rocks.

The percent distribution of major ion concentrations is shown in Figure 9.7. In general, Sample I leachates changed from Ca-SO_4 to Na-HCO_3 facies through Ca-Na and SO_4-HCO_3 mixings and Sample II and III leachates changed from Mg-SO_4 to Mg-HCO_3 facies through SO_4-HCO_3 mixings during test period.

When the cations were considered, Ca cation facies exist in the first two weeks for sample I leachates. This could be explained by the dissolution of the Ca-bearing minerals (e.g. anorthite, margarite, polyhalite, volkonskoite and possibly calcite) as detected in the XRD analyses. minerals. The shifting of leachate cation facies to Na after first two weeks could be attributed to the clay minerals related exchange reactions in addition to the dissolution of the albite and nontronite minerals as detected in the sample. When the anions are considered, Sample I leachate was in the SO_4 facies in the early weeks probably due to the dissolution of polyhalite mineral and sulphide oxidation. The shifting of leachate anion facies to HCO_3 afterwards could be attributed to the dissolution of carbonate minerals (surite and possibly calcite) and decreasing polyhalite dissolution and sulphide oxidation.

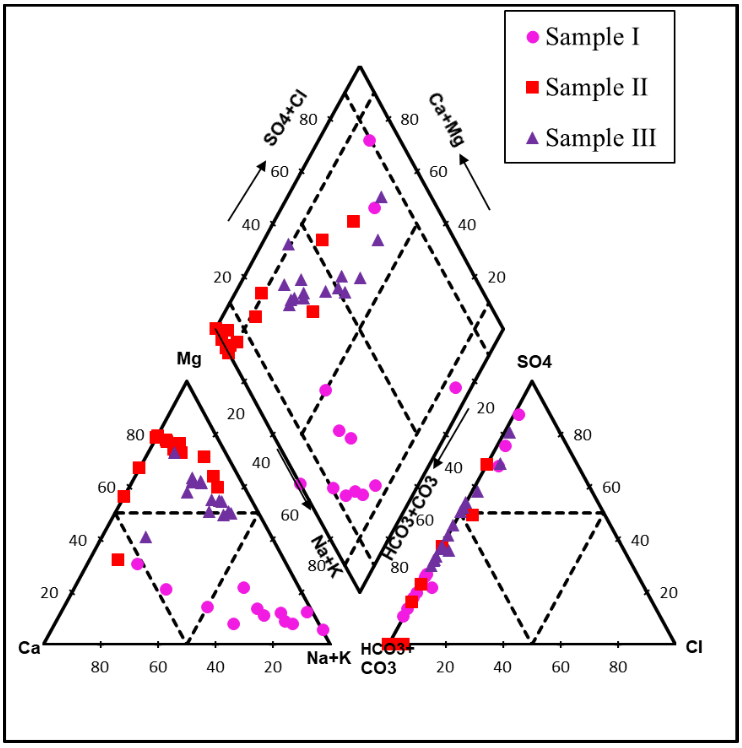


Figure 9.7. Kinetic test leachate facies of the samples on Piper plot.

The Mg characteristic of Sample II leachate is apparently related to the dominant Mg-bearing phases (dolomite, magnesite). Cation facies changed only once in the 13th week from Mg to Ca. This once shifting to Ca facies could be attributable to the Ca-enrichment due to Mg bearing phase precipitation. Anion facies of the Sample II leachate started with SO_4 and then shifted to the HCO_3 after the 2nd week. Lack of any SO_4 bearing mineral in this sample indicates that SO_4 content in leachates is related to sulphide mineral (teallite) oxidation. Apparently after the 2nd week, carbonate mineral dissolution was dominant resulting HCO_3 facies in the leachates.

The Mg characteristic of Sample III leachate is related to the dolomite dissolution. Cation facies changed a few times form Mg to mix types reflecting dissolution of non-Mg phases (e.g. sanidine, minrecordite). Anion facies of the leachates started with SO_4 and then was shifted to the HCO_3 after the 5nh week. In addition to SO_4 bearing mineral (lanarkite) in this sample, SO_4 content in leachates is related to sulphide mineral (argentopyrite, teallite) oxidation. Shifting after the 5th week indicates that carbonate mineral dissolution took over of sulphide mineral oxidation.

Average leachate concentrations of each test sample obtained in the kinetic tests other than continuously below detection limits values measured parameters are listed in Table 9.5 from higher to lower values. Concentrations of B, Be, Bi, Hg, Ni, P, Se (except 1st and 2nd weeks of Sample III), Sn, Ti, and Zr in all sample leachates are measured below the detection limits. In addition, concentrations Cd after the 2nd week and Co, U and Zn after the 3rd -5th weeks are below the detection limits in all leachates. Majority of total dissolved solid content of leachates from higher to lower concentrations is associated with alkalinity, SO_4, Na, Si, Ca, K, Cl, and Mg parameters additionally with Al, Sr, Fe, Mo, U, As, V, Li, Ba, Mn, Zn, Pb, Sb, and Cu trace ion parameters.

Table 9.5. Average concentrations above detection limit parameters in kinetic test leachates.

Unit mg/l	Sample I	Sample II	Sample III	Unit mg/l	Sample I	Sample II	Sample III
Alkalinity	103	64	61	**As**	0.13	0.02	0.07
SO4	95	18	60	**Ba**	0.034	0.009	0.023
Na	40	4	15	**Li**	0.02	0.05	0.15
Si	36	22	21	**Mn**	0.016	0.005	0.000
Ca	14	6	7	**V**	0.01	0.05	0.04
K	11	2	4	**Zn**	0.010	0.005	0.003
Cl	7	1	1	**Cu**	0.004	0.001	0.002
Mg	5	14	16	**Pb**	0.002	0.006	0.007
Al	1.67	0.01	0.01	**Cr. t**	0.0017	0.0001	0.0002
Fe	1.03	0.04	0.03	**Co**	0.0013	0.0002	0.0004
Sr	0.48	0.25	0.59	**Sb**	0.001	0.001	0.007
Mo	0.45	0.06	0.21	**Cd**	0.0004	0.0001	0.0003
U	0.32	0.04	0.09	**Se**	0.0000	0.0000	0.0026

The sample leachates are in the near-neutral and low metal region in the Ficklin graph in general (Figure 9.8). Sample I leachates plot are in both high metal and low metal region. However, if Fe concentration were neglected due to relatively higher values, sample I leachates also could be in low metal region.

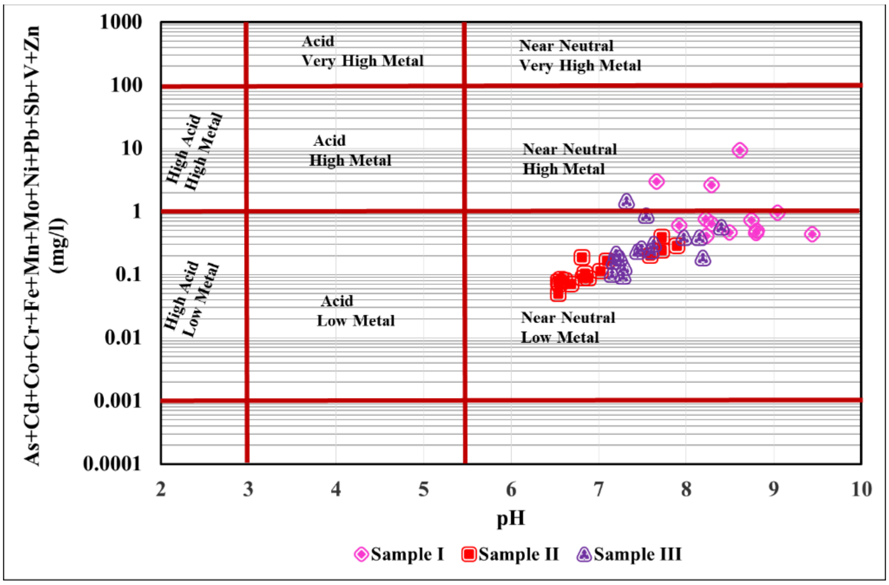


Figure 9.8. Kinetic test leachate classification based on pH and trace metal ion content.

Concentration Production Rates:

Concentration production rate of each parameter for each test sample is calculated and listed in Appendix-D. In order to eliminate deionized irrigation water alkalinity (basically carbonate alkalinity) contribution despite its lower contribution, the deionized water alkalinity was calculated and subtracted from the measured value for the alkalinity production rate calculations. In the determination of the deionized water alkalinity, the reaction relationships among the carbonate species are utilized.

$CO_2(g) + H_2O(l) = H_2CO_3^*$; $H_2CO_3^* = HCO_3^- + H^+$; $HCO_3^- = CO_3^{2-} + H^+$

Using equilibrium constant expressions for the above reactions, relationships among pH, P_{CO2} and activities of species could be expressed as:

$$\log a_{H2CO3} = \log p_{CO2} + \log K_{CO2}$$

$$\log a_{HCO3} = \log(K_1 K_{CO2} p_{CO2}) + pH$$

$$\log a_{CO3} = \log(\ K_2 K_1 K_{CO2} p_{CO2}) + 2pH$$

Where equilibrium constants K_{CO2}, K1 and K2 as calculated from Gibbs free energy data at 25 °C are equal to: $K_{CO2}= 10^{-1.6}$, $K1= 10^{-6.35}$ and $K2= 10^{-10.33}$.

Using these values, deionized pH value of 7 and the atmospheric partial pressure of CO_2 ($10^{-3.5}$) in the above equations, activities of the species in the deionized water were calculated. Taking activity coefficients of the species as one since it is deionized water, carbonate alkalinity of 2.17 mg/l was calculated using molalities of species in the following equation:

$$\text{Carbonate Alkalinity} = 2m_{CO3}^{2-} + m_{HCO3}^{-} + m_{OH}^{-} - m_{H}^{+}$$

Hydrogen concentration production rate calculations were performed using the activity of H^+ differences between the test leachate and the deionized irrigation water by incorporating activity coefficient of H^+ in each test solution using the extended Debye-Huckel equation.

Cumulative concentration production rate of 13 weeks (test period of Sample I) for each test sample are listed in Table 9.6. Highest production rates occurred for V and Zn in Sample II, for Mg, Sr, Li, Pb, Sb, Co and Se in Sample III and for the others in Sample I.

Weekly concentration production rate values for each test sample are shown in Figure 9.9 . Sulphate concentrations being sulphide mineral oxidation by product exhibit continuously decreasing trend beginning from the 1st week.

Table 9.6. Cumulative concentration production rates of samples in mg/kg/13 weeks.

Unit mg/kg/13 week	Sample I	Sample II	Sample III	Unit mg/kg/13 week	Sample I	Sample II	Sample III
Alkalinity	881	574	554	**As**	1.17	0.19	0.72
SO4	707	192	632	**Ba**	0.266	0.095	0.234
Si	194	56	64	**Li**	0.201	0.494	1.461
Na	310	35	125	**Mn**	0.116	0.065	0.000
Mg	39	116	134	**V**	0.052	0.455	0.334
Ca	93	50	61	**Zn**	0.044	0.050	0.032
K	68	16	33	**Cu**	0.026	0.009	0.016
Cl	54	9	15	**Pb**	0.020	0.071	0.079
Al	15	0	0	**Cr. t**	0.015	0.001	0.003
Fe	9.03	0.42	0.38	**Sb**	0.008	0.006	0.068
Sr	4	2	6	**Co**	0.003	0.002	0.004
Mo	3.60	0.58	2.27	**Cd**	0.003	0.001	0.003
U	2.058	0.297	0.746	**Se**	0.0000	0.0000	0.0245

However, it should be kept in mind that sulphate concentrations of leachates are also related to the dissolution of sulphate minerals. In any case production rate is in the order of I > III > II among the samples and sulphate minerals were determined in Sample I and III. Therefore, it is not possible to relate decreasing sulphate concentration directly to sulphide mineral oxidation. But in any case, sulphate production rates suggest that sulphide oxidation dependent acid production rate was decreased during the test period and metal hydroxide formation related acid production took place as decreasing pH values suggest.

Concentration production rates of parameters (except Al and V parameters of Sample I) in general change in the decreasing direction. There exist increasing/decreasing fluctuations in this general trend (Figure 9.9).

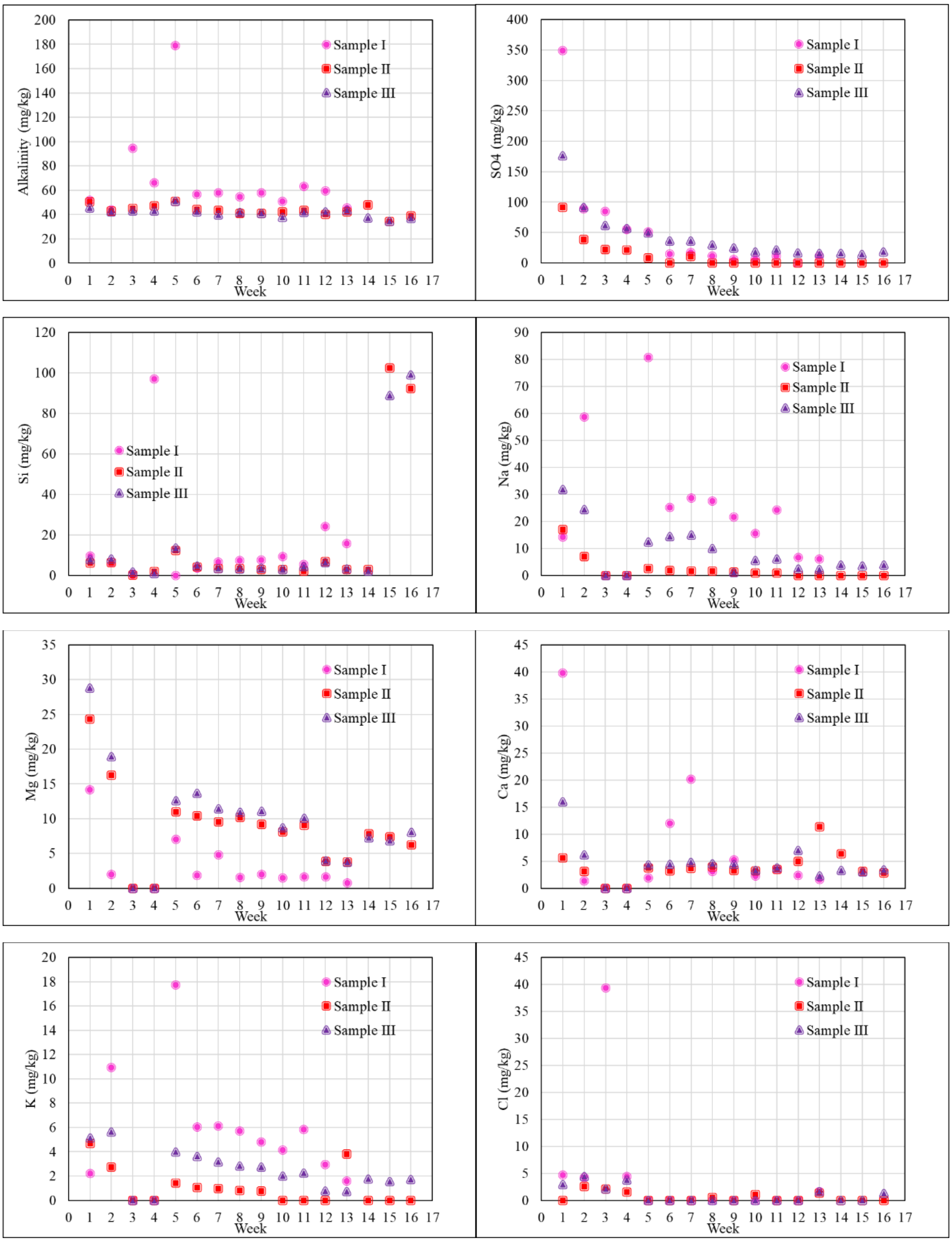


Figure 9.9. Concentration production rates of the samples through the weeks.

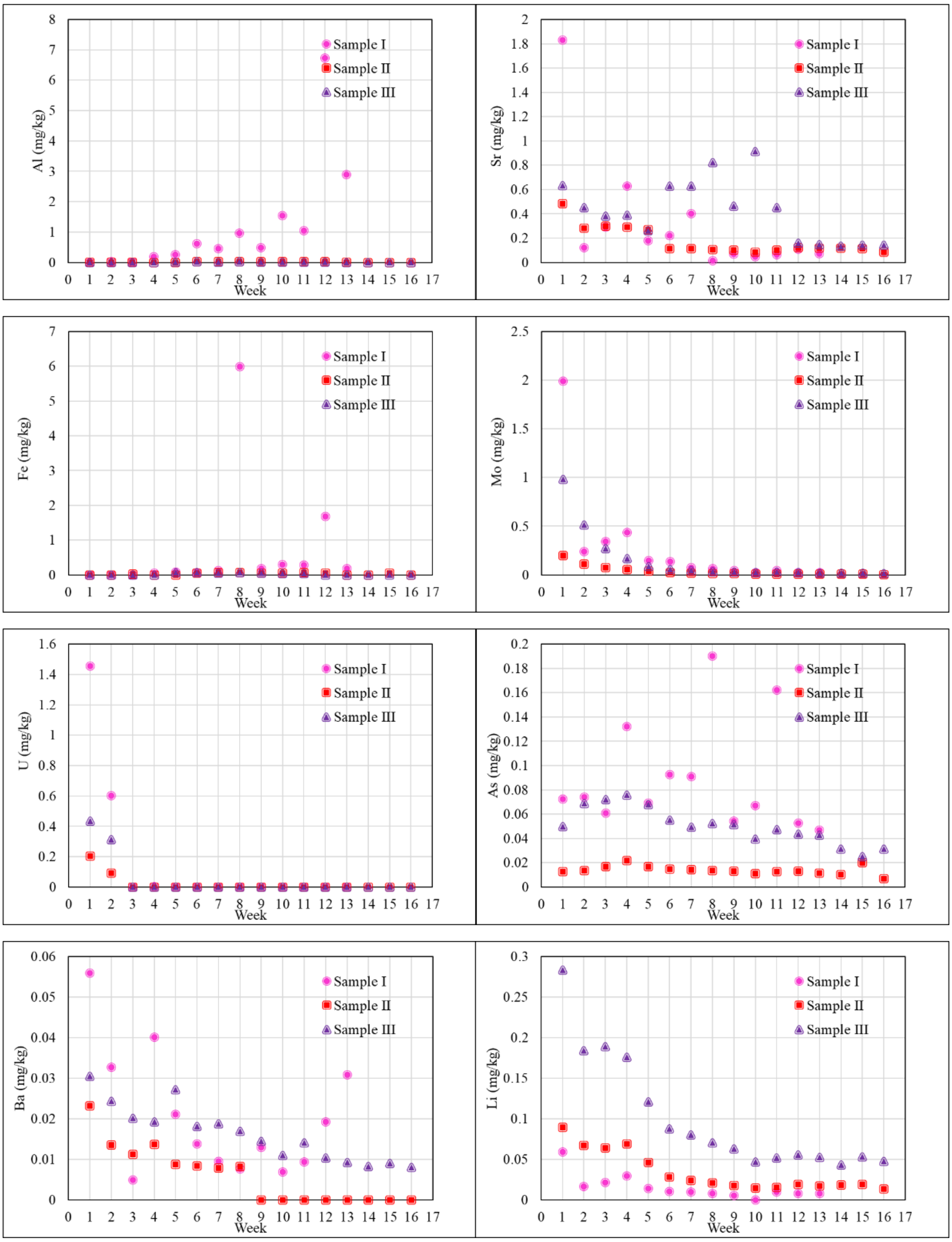


Figure 9.9. Cont'd

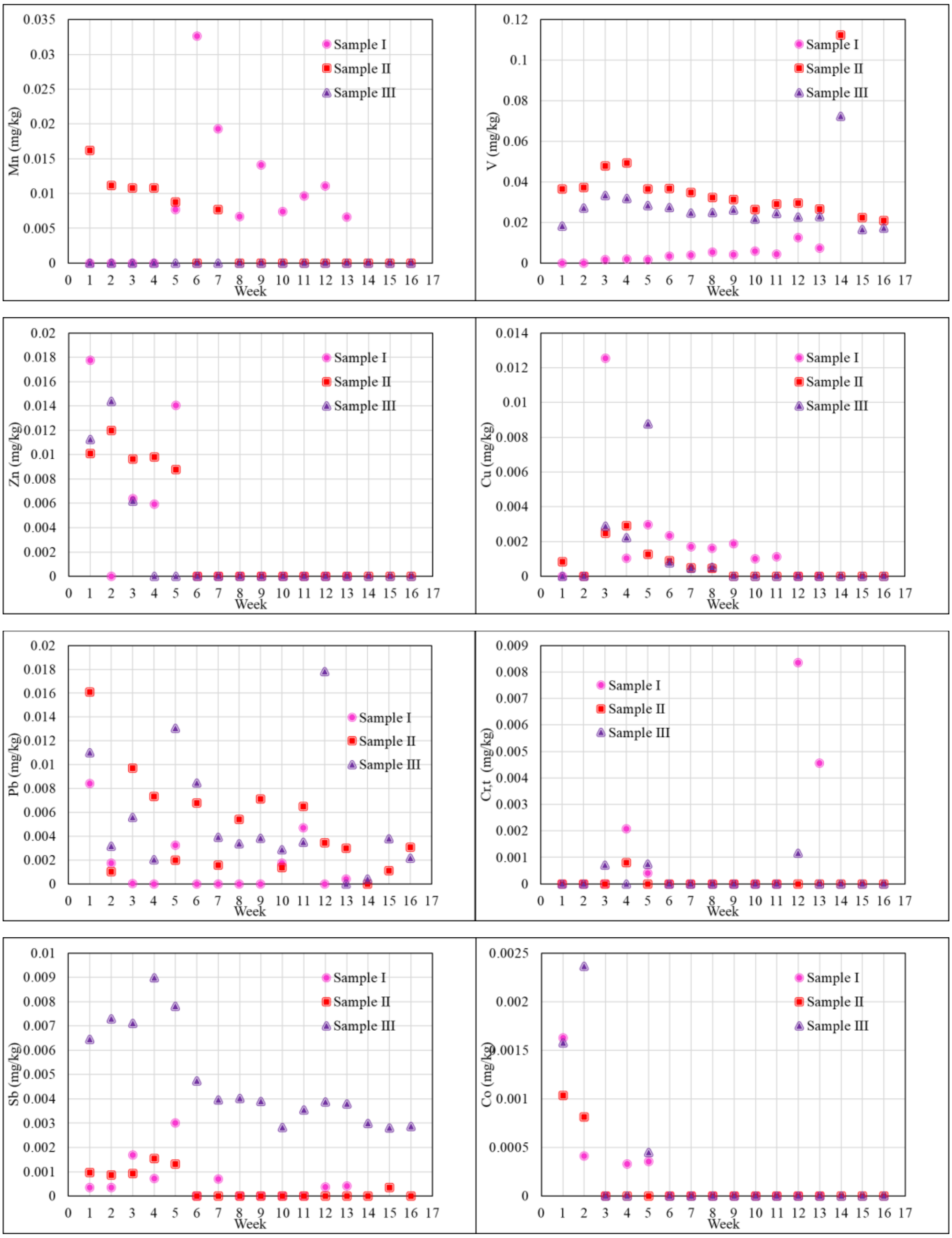


Figure 9.9 Cont’d

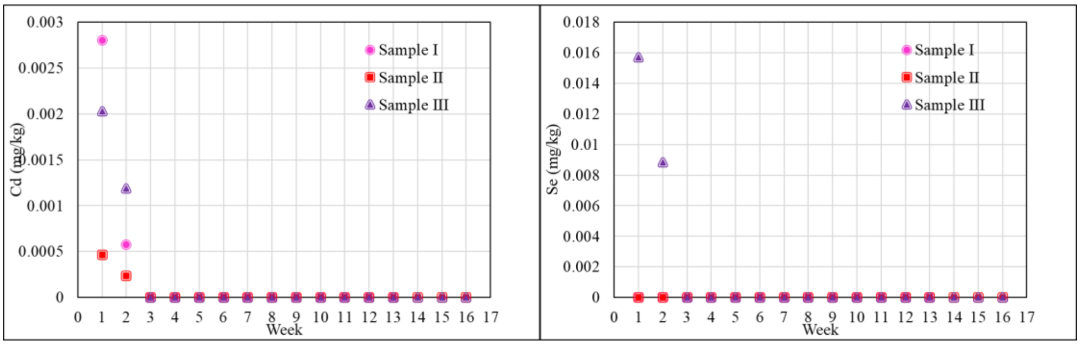


Figure 9.9 Cont'd

Kinetic test leachate quality:

In order to evaluate the leachate qualities, quality limits (a) for the surface water classification (SWC) and maximum environmental quality (MEQ) for rivers of MFW (2016) and (b) waste categorization (WC) limits of MEF (2010) were used and the results are given in (Table 9.7). According to the waste categorization limits, waste rocks generally are in "Non-Hazardous" class. The parameters with high concentrations causing this class are As, Mo and SO_4 in Sample I leachates, Mo in Sample II leachates and As, Mo, Sb and Se Sample III leachates. Sample II after the 5th week and Sample III after the 13th week are in "Inert" class. It should be kept in mind that these results represent individual week cycles meaning that cumulative effects are not reflected.

According to the surface water classification, Sample II is classified as Class I throughout the whole test period. Although Sample I was classified as Class II/III/IV due to high EC/low pH values in the first five weeks and Sample III was classified as Class II/IV due to high EC/Se values in the first and second weeks, the leachates are in Class I for Sample I and III in the other cycles. Concentrations of Al, As, Cd, Co, Cu, Fe and Si in Sample I, Al, Cd, Cu, Pb, Si and V in Sample II and Al, As, Cd, Co, Cu, Pb, Si and V in Sample III are higher than the maximum environmental quality limits. When compared with the short-term shake flask test (SFT) results, in

Table 9.7. Classification of kinetic test leachate results according to the surface water and waste categorization limits.

Sample Name	SWC (MFW,2016)	MEQ (MFW,2016)	WC (MEF, 2010)
I-0	Class II- EC	Al, As, Cd(III), Co, Cu, Fe, Si	Non-Hazardous - As, Mo, SO4
I-1	Class III- EC	As, Cd(IV), Si	Hazardous - Mo
I-2	Class II- EC	Al, As, Cd(IV), Si	Non-Hazardous - As, Mo, SO4
I-3	Class II- EC	As, Cu	Non-Hazardous - As, Mo, SO4
I-4	Class IV- pH	Al, As, Si	Hazardous - As
I-5	Class IV- pH	Al, As, Cu, Si	Non-Hazardous - As, Mo
I-6	Class I	Al, As, Cu, Fe, Si	Non-Hazardous - As, Mo
I-7	Class I	Al, As, Fe, Si	Non-Hazardous - As, Mo
I-8	Class I	Al, As, Fe, Si	Hazardous - As
I-9	Class I	Al, As, Fe, Si	Non-Hazardous- As, Mo
I-10	Class I	Al, As, Fe, Si	Non-Hazardous - As
I-11	Class I	Al, As, Fe, Si	Hazardous - As
I-12	Class I	Al, As, Fe, Si	Non-Hazardous - As
I-13	Class I	Al, As, Fe, Si	Non-Hazardous - As
II-0	Class I	Cu, Si	Non-Hazardous - Mo
II-1	Class I	Cd(III), Pb, Si	Non-hazardous - Mo, SO4
II-2	Class I	Si	Non-Hazardous - Mo
II-3	Class I	Cu	Non-Hazardous - Mo
II-4	Class I	Cu, Si	Non-Hazardous - Mo
II-5	Class I	Si	Non-Hazardous - Mo
II-6	Class I	Si	Inert
II-7	Class I	Si	Inert
II-8	Class I	Si	Inert
II-9	Class I	Si	Inert
II-10	Class I	Al, Si	Inert
II-11	Class I	Al, Si	Inert
II-12	Class I	Si	Inert
II-13	Class I	Si	Inert
II-14	Class I	Si, V	Inert
II-15	Class I	Si	Inert
II-16	Class I	Si	Inert
III-0	Class II- Se	Cu, Si	Non-Hazardous - Mo, Se
III-1	Class IV- Se	As, Cd(IV), Pb, Si	Hazardous - Mo
III-2	Class II- EC, Se	As, Cd(IV), Co, Si	Non-Hazardous - As, Mo, Sb, Se, SO4
III-3	Class I	As, Cu, Si	Non-Hazardous - As, Mo, Sb
III-4	Class I	As	Non-Hazardous - As, Mo, Sb
III-5	Class I	As, Cu, Pb, Si	Non-Hazardous - As, Mo, Sb
III-6	Class I	Al, As, Si	Non-Hazardous - As, Mo, Sb
III-7	Class I	As, Si	Non-Hazardous - As, Mo
III-8	Class I	Al, As, Si	Non-Hazardous - As
III-9	Class I	As, Si	Non-Hazardous - As
III-10	Class I	As, Si	Non-Hazardous - As
III-11	Class I	As, Si	Non-Hazardous - As
III-12	Class I	As, Pb, Si	Non-Hazardous - As
III-13	Class I	As, Si	Non-Hazardous - As
III-14	Class I	Si, V	Inert
III-15	Class I	Si	Inert
III-16	Class I	Si	Inert

SFT leachates concentrations of Al, Cu, Fe in Sample I; Al, Cd, Cu in Sample II; and Al in Sample III are relatively lower. Groundwaters also include above MEQ limit high concentrations of Al, Cu, Pb, Si in Lower Çavuşlar and Al, As, Si in Upper Çavuşlar units.

CHAPTER 10

HYDROGEOCHEMICAL MODELING OF PILE SEEPAGE QUALITY

In this chapter, evaluations related to waste rock pile pore water concentrations and seepage water quality are introduced. Predictions of the water quality have been carried out for the after operation (long-term) period because mining details of the operation period have not been established yet. Furthermore, due to lack of the mine closure plan, it is assumed that waste rocks will be left in the field without any remedial implementation.

Because there is not enough data to determine flow conditions in the pile using either numerical approach or analytical approach, waste rock pile pore water concentrations produced by interactions between infiltrating precipitation water and rock are estimated using the empirical approach of Morin and Hutt (1994) using weight of waste rocks in the pile, precipitation receiving surface area of the pile, annual amount of precipitation infiltration, number of precipitation days in a year and kinetic test concentration production rates. The empirical equation used for the predictions as follows;

$$Concentration\ (mg/kg) = \frac{Kinetic\ rate\ (mg/kg/day)\ x\ Number\ of\ precipitation\ days\ in\ a\ year\ x\ Waste\ rock\ weight\ (kg)}{Precipitation\ infiltration\ (L)}$$

Kinetic concentration rate of each parameter used in the predictions is listed in Appendix-D where below detection measurements were taken as zero. Waste rock amounts in the pre-feasibility studies (AMM, 2014) are given not in terms of lithological units but in terms of upper coal seam level (245.4 million bank cubic meter, Mbcm), lower coal seam level (5.1 Mbcm), third coal seam level (2.8 Mbcm) underlying the lower seam and behind fault (2.3 Mbcm). In the prediction modelling, it is assumed that the upper coal seam level waste rocks are represented by Upper Çavuşlar member rocks (Sample III), the lower coal seam level waste rocks are represented by Lower Çavuşlar member rocks (Sample II), third coal seam level waste rocks are represented by equal weight percentages of both Bostantepe and Lower Çavuşlar member rocks (Sample I and II, respectively) and behind fault waste rocks are represented by equal weight percentages of Bostantepe, Lower Çavuşlar and Upper Çavuşlar member rocks (Sample I, II and III, respectively). According to these assumptions, pile amounts of waste rocks represented by Sample I, II and III are estimated as 5330 kiloton, 18239 kiloton and 494795 kiloton, respectively, using previously measured densities. In the light of these weights, waste pile percentages of are 1%, 4% and 95% are represented by the samples I, II and III respectively.

10.1 Hydrology and Pile Precipitation Infiltration

The study area is located in the northeast part of Sakarya River basin in Central Anatolian Region and the area is characterized by the continental climate. Because it is close to the Black Sea region, relatively higher humidity exists in the area. Turkish State Meteorological Service classified the study area as semiarid-mesothermal climate according to Thornthwaite Climate Classification (McCabe and Wolock, 1999). In this type of climate, the weather is hot and dry in summers, cold and snowy in winters.

Meteorological data do not exist for the mine site and the nearest station (Çeltikçi) data were limited to rather short period of time (1987 and 1993). Therefore, the long term estimated average monthly temperature and precipitation data of (Yazıcıgil et. al, 2015) for the mine site (Çeltikçi) were used in order to determine precipitation infiltration into the waste rock pile. In the study of Yazıcıgil et. al (2015), meteorological data of Kızılcahamam station (covering period of 1957 and 2014) and Çeltikçi station were used for the long term site (Çeltikçi) estimations by comparing common year differences (Table 10.1).

Table 10.1. Long term monthly average precipitation and temperature (Yazıcıgil et. al, 2015).

Station/Months	**January**	**February**	**March**	**April**	**May**	**June**	**July**	**August**	**September**	**October**	**November**	**December**
Çeltikçi-Estimated (1957-2014) mm	59.4	40.9	33.7	38.7	37.3	27.8	14.5	10.1	9.3	31	30.5	58.9
Temperature (C°)	-1.0	0.1	4.1	9.3	13.9	17.8	20.7	20.3	16.1	10.5	5.2	1.1

Monthly average temperature distribution is shown in Figure 10.1. The values are in the range of -1^{o}C to 20.7 ^{o}C. Minimum and maximum values were recorded in January and July, respectively.

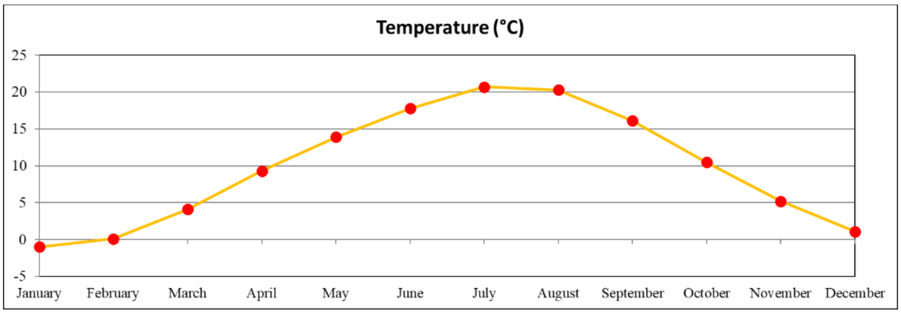


Figure 10.1. Monthly average temperature values.

The monthly average precipitation values are shown in Figure 10.2. The values are in the range of 9.3 mm to 59.4 mm. Minimum and maximum values were recorded in September and January, respectively. Winter and spring seasons have the highest precipitation. On the other hand, summer and autumn seasons have the lowest precipitation as expected from the climate classification of the area mentioned above.

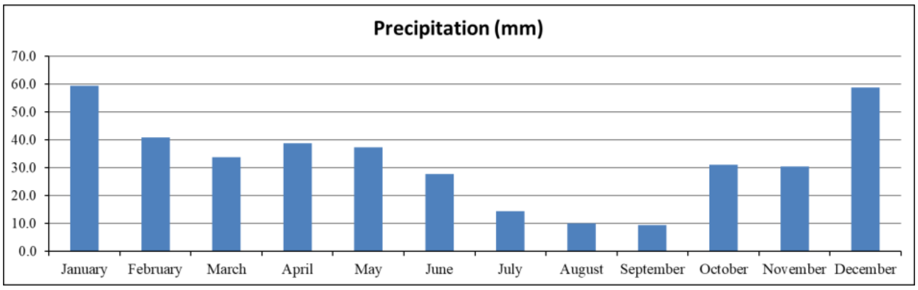


Figure 10.2. Monthly average precipitation values.

According to the average of 2013-2015 meteorological data, the number of rainy days in the area is equal to 122 in a year. The waste rock pile surface area which will receive precipitation is approximately estimated as 6000000 m^2 using a map of a pre-feasibility study.

Hydrologic Budget:

Water budget calculations are related to the relationships among precipitation, direct surface runoff, evapotranspiration, surplus runoff, soil-moisture storage capacity and infiltration components. In this study, Thornthwaite method (McCabe and Markstrom, 2007) is used to calculate potential evapotranspiration. The soil moisture capacity and direct surface runoff components are calculated using Curve Number (CN) method developed by the U.S. Soil Conservation Services (SCS, 1964).

The direct surface runoff amount (Q) could be estimated using the following Curve Number method equation.

$$Q = \frac{(P - 0.2S)^2}{P + 0.8S}$$

Where P is precipitation and S is potential maximum soil moisture retention which is determined using the Curve Number (CN) in the following equation:

$$S = \frac{1000}{CN} - 10$$

CN is the non-dimensional quantity depends on the land use, land cover and hydrologic soil groups. In this study, CN was assigned as 76 corresponding to disturbed quarries with high water transmission capacity hydrologic soil group (SCS,1964). The effect of adapting different CN numbers is evaluated in the sensitivity analyses by means of infiltration changes.

Monthly total precipitation is classified as rain or snow according to the mean monthly temperature. If the mean monthly temperature is less than the threshold temperature for snow [taken as T_{snow}= -10°C; as suggested by McCabe and Wolock, 1999) based on an analysis of water-balance results for a number of sites], all precipitation is regarded as snow. On the other hand, if the mean monthly temperature greater than threshold temperature for rain [taken as T_{rain}=3.3°C; as suggested by McCabe and Markstrom (2007) for elevations below 1000 m], all precipitation can be regarded as rain. When the monthly temperature is between these ranges, how much snow can be contributed to the total precipitation is calculated by the following formula.

$$P_{snow} = P \ * \ (\frac{T_{rain} - T}{T_{rain-}T_{snow}})$$

The fraction of snow melt (SMF) is calculated using the monthly average temperature, the maximum melt rate (Meltmax), T_{rain} and T_{snow} in the following formula. Meltmax is generally set to 0.5 (McCabe and Wolock, 1999) in this type of calculation.

$$SMF(Snow\,Melt\,Fraction) = (\frac{T - T_{snow}}{T_{rain-}T_{snow}}) * \ meltmax$$

If the SMF value is greater than the meltmax, SMF is equal to the meltmax.

Assuming 100 mm soil moisture capacity, the calculated monthly water budget is given in Table 10.2 where it is assumed that all calculated infiltration amount could infiltrate to subsurface. In other words, surplus runoff is taken as zero. The calculations suggest that about 23% (90.7 mm) of annual precipitation (392 mm) could infiltrate to the subsurface.

Table 10.2. Monthly water budget results.

Parameter	**J**	**F**	**M**	**A**	**M**	**J**	**J**	**A**	**S**	**O**	**N**	**D**	**Total**	**Percentage**
Monthly Average Temp.(°C)	-1	0.1	4.1	9.3	13.9	17.8	20.7	20.3	16.1	10.5	5.2	1.1		
Precipitation	59.40	40.90	33.70	38.70	37.30	27.80	14.50	10.10	9.30	31.00	30.50	58.90	392.10	
PET	0.00	0.18	16.08	44.66	78.76	105.67	127.85	117.06	78.92	44.44	17.26	2.80	633.68	
Direct Surface runoff	15.213	5.81	0.03	0	0	0	0	0	0	0	0	13.34	34.39	8.77%
Soil Moisture	100.00	100.00	100.00	100.00	58.54	12.95	0.00	0.00	0.00	0.00	13.20	56.00	540.70	
Change in soil moisture	0.00	0.00	0.00	0.00	-41.46	-45.59	-12.95	0.00	0.00	0.00	13.24	42.80	-43.96	11.21%
AET	0.00	0.18	16.08	44.66	78.76	73.39	27.45	10.10	9.30	31.00	17.26	2.80	310.97	79.31%
Subsurface Infiltration	31.48	33.63	24.59	1.03	0	0	0	0	0	0	0	0	90.73	23.14%
														100%

Monthly distributions of precipitation, AET, soil moisture content, direct surface runoff and infiltration are shown in Figure 10.3.

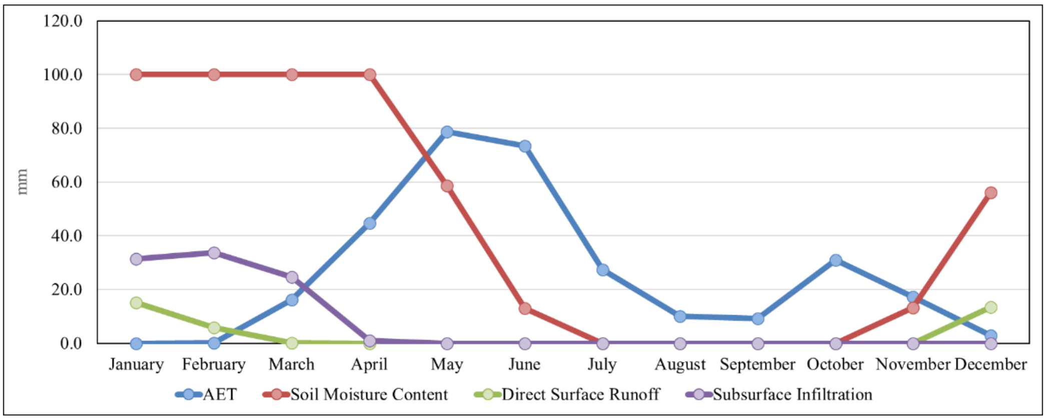


Figure 10.3. Graph of monthly water budget components.

10.2 Seepage Quality Prediction Results

Three different methods are used as kinetic concentration rates for each parameter in the prediction modeling. In the first method (Leachate 1), the average of the kinetic concentration rate for each parameter was used for each sample covering all weeks of the kinetic test. In the second method (Leachate 2), the average of the kinetic concentration rates for each parameter was used for each sample after the 5th week due to obtaining more reliable results for the long-term predictions. The 5th week approximately represents changing peak trends of pH, EC and concentration values (see the figures 9.3, 9.4 and 9.9). On the other hand, in the third method (Leachate 3), the percentile calculation with %75 confidence limit which is generally applied in these types of estimations, was used statistically using the concentrations of the 5th week and afterwards.

Furthermore, studies indicate that percentage of waste rocks in the pile flushed by the infiltrated water is in the range of 5-20% (Morin and Hutt, 1994). In this study, average of this range (12%) is taken as the reactive amount.

The initial concentrations for each leachate is estimated using the values stated earlier in this chapter in the empirical equation. Because these empirical concentrations do not include reaction effects, in the second step, the water-rock reaction effects are incorporated using PHREEQC software (Parkhust and Appelo, 1999) with MINTEQ.V4 thermodynamic database to estimate the leachate concentrations. In the thermodynamic modeling, saturation conditions of the mineral components with respect to the empirical concentrations in each leachate composition are evaluated and those solid components which are supersaturated are equilibrated by dissolution with the leachate without considering possible surface and exchange reactions. The saturation index of >0.1 is used instead of >0 for the supersaturation determinations just to be on the safe side and simulate worse conditions.

In these calculations, each leachate is subjected to two different cases: 1) It is assumed that the leachate in the pores is not open to atmospheric CO_2 conditions (Case I) and 2) the leachate in the pores is open to atmospheric CO2 conditions (Case II) and it is in equilibrium with CO_2 amount of the atmosphere (e.g. drainage conditions).

Moreover, all these estimations are carried out also using two different alkalinity rates due to the possible error (10%, see Table 9.2) associated with this parameter in the laboratory analyses. Apart from the analytical error, measured alkalinity values could also include measurement delay effects because of the pandemic work hour limitations. The estimations obtained with no error considered alkalinity rate and the 10% alkalinity error considered rate are later averaged.

The estimated leachate concentrations for the cases explained above are listed in Table 10.3 for each leachate. The thermodynamic model outputs of Leachate 2 for

Table 10.3. Calculated pile pore water concentrations.

mg/l	Case I			Case II		
	Leachate 1	Leachate 2	Leachate 3	Leachate 1	Leachate 2	Leachate 3
pH	4.45	4.40	4.31	7.48	7.54	7.42
pe	4.34	4.24	4.22	-1.35	-1.72	-1.74
Ag	0	0	0	0	0	0
Al	0.49	0.53	0.88	0.000	0.000	0.00
Alkalinity	41145.0	36212.5	41575.0	214.4	124.3	110.0
As	80.4	75.7	85.3	54.3	49.9	53.9
B	0	0	0	0	0	0
Ba	0.002	0.003	0.003	0.000	0.000	0.000
Be	0	0	0	0	0	0
Ca	686.5	919.3	924.8	103.2	61.0	90.6
Cd	0.319	0.000	0.000	0.008	0.000	0.000
Cl	1658.3	401.6	7.1	1267.8	297.4	5.1
Co	0.001	0.001	0.000	0.000	0.000	0.000
Cr	0.277	0.285	0.007	0.001	0.000	0.001
Cu	0.000	0.000	0.000	0.000	0.000	0.000
Fe	49.6	70.5	98.6	0.0	0.0	0.0
Hg	0	0	0	0	0	0
K	4370.9	3833.9	4819.5	3353.3	2855.7	3485.9
Li	158.3	106.8	118.5	121.0	79.1	85.2
Mg	15713.4	12555.5	16131.7	7734.9	4686.7	6986.3
Mn	0.38	0.31	0.24	0.29	0.23	0.18
Mo	229.72	52.39	57.30	15.08	23.77	12.56
Na	15731.3	11397.2	17638.5	12026.9	8440.3	12690.4
Ni	0	0	0	0	0	0
P	0	0	0	0	0	0
Pb	0.09	0.04	0.10	0.00	0.00	3.00
Sb	0.000	0.000	0.000	0.0000	0.0001	0.000
Se	0	0	0	0	0	0
Si	0.54	0.57	0.39	2.06	2.28	2.15
SO4	57597.4	35903.5	42223.0	51196.3	29406.2	35024.9
Sn	0	0	0	0	0	0
Sr	7.29	9.83	9.87	4.96	6.01	6.05
Ti	0	0	0	0	0	0
Tl	0	0	0	0	0	0
U	76.28	0.04	0.00	58.32	0.03	0.00
V	45.08	47.28	44.79	34.18	35.01	31.75
Zn	3.33	0.07	0.00	2.55	0.05	0.00

Alkalinity as $CaCO_3$; yellow color represents the parameter exceeding the quality limits of MFW (2016) and MEF (2010).

Case II are listed in Appendix E as an example. The results suggest that pile pore water under closed exchange CO2 conditions (Case I) could have acidic character (pH: 4.31-4.45). On the other hand, if the pore water becomes in equilibrium with the atmospheric CO2 value (Case II), it could be in basic/near neutral character (pH: 7.42-7.54). Gradual conditions would probably develop under field conditions.

In order to evaluate the leachate qualities, quality limits (a) for the surface water classification (SWC) and maximum environmental quality (MEQ) for rivers of MFW (2016) and (b) waste categorization (WC) limits of MEF (2010) are used and the results are given in Table 10.4. According to the MEF (2010) limits, all leachates including both Case I and II are in the ‘’Hazardous’’ class due to higher As, Mo, SO_4 concentrations.

Table 10.4. Classification of pile pore water concentration results according to the surface water and waste categorization limits.

	Sample Name	SWC (MFW,2016)	MEQ (MFW,2016)	WC (MEF, 2010)
Case I	Leachate 1	Class IV- pH	Al, As, Cd, Cr, Fe, Pb, V, Zn	Hazardous - As, Mo, SO4
	Leachate 2	Class IV- pH	Al, As,Cr, Fe, Pb, V	Hazardous - As, Mo, SO4
	Leachate 3	Class IV- pH	Al, As, Fe, Pb, V	Hazardous - As, Mo, SO4
Case II	Leachate 1	Class II- Mn	As, Cd, Si, V, Zn	Hazardous - As, Mo, SO4
	Leachate 2	Class II- Mn	As, Si, V	Hazardous - As, Mo, SO4
	Leachate 3	Class II- Mn	As, Pb, Si, V	Hazardous - As, Mo, SO4

According to the surface water classification, leachates are classified as Class IV (Highly Contaminated) due to their relatively low pH values in the absence of CO_2 equilibrium case. In addition, the concentrations of Al, As, Fe, Pb, V in all leachates, and Cd/Cr/Zn in some leachates are higher than the maximum environmental quality limits for the case. For the CO_2 equilibrium case, according to the surface water classification, leachates are classified as Class II (Slightly Contaminated) due to their relatively high Mn values. The maximum environmental quality limits of As, Si, V in all leachates and Cd/Pb/Zn parameters in some leachates are exceeded for the case. It should be kept in mind that there could a high error association with the lead laboratory measurements as discussed earlier.

10.3 Sensitivity Analyses

The estimated concentrations depend on different parameters some of which have potential error/range associated. In order to see the effects of these parameters separately on the estimated pore water concentrations, sensitivity analyses have been carried out for Leachate 3 with the CO_2 equilibrium case (Case II). Five different scenarios have been evaluated:

Scenario 1) The precipitation value was decreased by 50 mm which results about 80.2 mm infiltration. The infiltration was 90.7 mm in earlier run.

Scenario 2) The precipitation value was increased by 50 mm which results about 105.1 mm infiltration.

Scenario 3) The number of rainy days was decreased to 100 which was 122 earlier.

Scenario 4) The supersaturation determination criteria for the saturation index (SI) is set to >0.

Scenario 5) The supersaturation determination criteria for the saturation index (SI) is set to >0.3 which was >0.1 earlier.

The predicted pore water concentrations are listed in Table 10.5. The results show that leachates of all scenarios were in basic character (nearly neutral) and pH values (in the range of 7.41-7.48) are similar to that (7.42) of the original case. Concentrations slightly decrease when the infiltration amount increase, the number of rainy days decrease and the SI criteria (few parameters) decrease in general.

The quality limit comparisons are given in Table 10.6. The waste classifications of all sensitivity runs are the same as those of the original. The only difference is the addition of lead parameter in Scenario 5. Surface water classes of all sensitivity runs are also the same as those of the original. On the other hand, some parameters are added (Cd, Zn) or missing (Pb) in the comparison of the maximum environmental quality limits as shown in Table 10.6. This indicates that estimated values are relatively more sensitive to the possibly precipitating phases in the system.

Table 10.5. Calculated pile pore water concentrations of sensitivity runs for leachate 3 and Case II condition.

mg/l	Leachate 3	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5
pH	7.42	7.41	7.44	7.48	7.42	7.42
pe	-1.74	-1.72	-1.76	-1.35	-1.74	-1.74
Ag	0	0	0	0	0	0
Al	0.00	0.00	0.00	0.00	0.00	0.00
Alkalinity	110.0	111.7	108.6	108.0	109.9	110.0
As	53.9	58.5	49.4	54.3	53.9	53.9
B	0	0	0	0	0	0
Ba	0.000	0.000	0.000	0.000	0.000	0.000
Be	0	0	0	0	0	0
Ca	90.6	98.4	82.7	103.2	90.6	90.6
Cd	0.000	0.000	0.000	0.008	0.000	0.000
Cl	5.1	5.5	4.7	1267.8	5.1	5.1
Co	0.000	0.000	0.000	0.000	0.000	0.000
Cr	0.001	0.001	0.001	0.001	0.001	0.001
Cu	0.000	0.000	0.000	0.000	0.000	0.000
Fe	0.0	0.0	0.0	0.0	0.0	0.0
Hg	0	0	0	0	0	0
K	3485.9	3781.0	3190.3	3353.3	3485.9	3485.9
Li	85.2	92.5	78.0	121.0	85.2	85.2
Mg	6986.3	7564.1	6393.3	7734.9	6986.7	6986.0
Mn	0.18	0.19	0.16	0.29	0.18	0.18
Mo	12.56	11.17	14.13	15.08	12.56	12.56
Na	12690.4	13764.2	11614.6	12026.9	12690.5	12690.4
Ni	0	1	0	0	0	0
P	0	0	0	0	0	0
Pb	3.00	3.33	2.75	0.00	0.00	6.09
Sb	0.000	0.000	0.000	0.000	0.000	0.000
Se	0	0	0	0	0	0
Si	2.15	2.11	2.19	2.06	2.15	2.15
SO4	35024.9	37987.2	32056.1	51196.3	35025.0	35024.8
Sn	0	0	0	0	0	0
Sr	6.05	5.90	6.22	4.96	6.05	6.05
Ti	0	0	0	0	0	0
Tl	0	1	1	0	0	0
U	0.00	0.00	0.00	58.32	0.00	0.00
V	31.75	35.25	29.10	34.18	31.75	31.75
Zn	0.00	0.00	0.00	2.55	0.00	0.00

Alkalinity as $CaCO_3$; yellow color represents the parameter exceeding the quality limits of MFW (2016) or MEF (2010)

Table 10.6. Classification of sensitivity run results according to the surface water and waste categorization limits.

Sample Name	SWC (MFW,2016)	MEQ (MFW,2016)	WC (MEF, 2010)
Scenario 1	Class II- Mn	As, Pb, Si, V	Hazardous - As, Mo, SO4
Scenario 2	Class II- Mn	As, Pb, Si, V	Hazardous - As, Mo, SO4
Scenario 3	Class II- Mn	As, Cd, Si, V, Zn	Hazardous - As, Mo, SO4
Scenario 4	Class II- Mn	As, Si, V	Hazardous - As, Mo, SO4
Scenario 5	Class II- Mn	As, Pb, Si, V	Hazardous - As, Mo, Pb, SO4
Leachate 3 (Case II)	Class II- Mn	As, Pb, Si, V	Hazardous - As, Mo, SO4

CHAPTER 11

RESULTS AND CONCLUSIONS

The comparison of Çeltikçi formation whole rock concentrations with those of the Upper crustal average indicate that concentrations of As, Ca, Cd, Li, Mg, Mo, S and Sr in the rocks are higher.

Mineralogical studies showed that Bostantepe member Sample I contains high content of clay minerals in addition to the silicate and oxide minerals. There exist carbonate mineral (surite) and sulphate mineral (polyhalite) in the sample. In addition to commonly present major elements, Sample I contains As, Cr, Cu and Pb heavy metals that could create environmental problems. Lower Çavuşlar member Sample II contains carbonate minerals (dolomite, magnezite, ankerite) and sulphide mineral (teallite) in addition to the silicate mineral (quartz). In addition to commonly present major elements, Sample II contains Pb and Sn heavy metals. Upper Çavuşlar member Sample III contains carbonate minerals (dolomite, minrecordite), sulphate mineral (lanarkite) and sulphide minerals (teallite, argentopyrite) in addition to the silicate and hydroxide minerals. The sample also contains As, Pb, Sn, V and Zn heavy metals.

The static tests results show that ARD potential of the samples are in the order of I>II>III and the samples do not have significant acid production potential in the long term. The results indicate that any acidity produced will be neutralized by the minerals. NAG potential values suggest hydroxides related pH buffering and possible low-intermediate metal concentration release to the leachates upon excessive oxidation. According to MEU (2015) only static test criteria, the samples are classified as Inert.

The shake flask test results suggest that leachate pH and EC values are in the order of Bostantepe (I)>Lower Çavuşlar (II)>Upper Çavuşlar (III). According to the waste categorization limits, the test samples are in “Non-hazardous” class due to relatively high concentrations of As, Mo, SO_4 for Sample I; Mo for Sample II and Mo, Sb for Sample III. The surface water classification limits indicate that Sample I and Sample II are classified as Class IV (highly contaminated) due to the high pH values and Sample III is classified as Class II (slightly contaminated) due to relatively high EC value. Besides, the maximum environmental quality limits of As, Co, Si, Cd, and Pb in Sample I; Si concentration in Sample II; Si and Cd concentrations in Sample III are exceeded. Overall the results indicate low concentration metal release in short term (easily dissolvable) period under saturated test conditions.

Kinetic test result leachate pH values are in the order of Bostantepe (I)>Upper Çavuşlar (III)>Lower Çavuşlar (II). Through the test period, values of all leachates are in basic character in the ranges of 7.66-9.21, 7.09-8.40 and 6.54-7.89 and for samples I, III, and II, respectively. Increasing early week values later on decreased.

Kinetic test results showed that leachate EC values are in order of Bostantepe (I)>Upper Çavuşlar (III)>Lower Çavuşlar (II). Through the test period, EC values exist in the range 162.3-1473 µS/cm for Sample I; 129.3-573µS/cm for Sample III and 87.3-366.8 µS/cm for Sample II. The EC ordering among the sample leachates indicates that the ion release is higher at greater pH values. The values were initially very high due to oxidized parts related reactions, then continuously decreased to lower levels toward the last weeks and assumed flat positions indicating low level ion production in all sample leachates.

In kinetic test leachates, concentrations of B, Be, Bi, Hg, Ni, P, Se (except 1st and 2nd weeks of Sample III), Sn, Ti, and Zr in all sample leachates are measured below the detection limits. In addition, concentrations Cd after the 2nd week and Co, U and Zn after the 3rd -5th weeks are below the detection limits in all leachates.

According to the waste categorization limits, the leachate test samples are in “Non-hazardous” class due to higher concentrations of As, Mo and SO_4 in Sample I; Mo in Sample II and As, Mo, Sb and Se in sample III. The surface water classification limits indicate that Sample II is in Class I throughout the whole test period. Although Sample I is classified as Class II/III/IV due to high EC/low pH values in the first five weeks and Sample III is classified as Class II/IV due to high EC/Se values in the first and second weeks, the leachates in general are in Class I for samples I and III in the other cycles. The maximum environmental quality limits of Al, As, Cd, Co, Cu, Fe and Si in Sample I; Al, Cd, Cu, Pb, Si and V in Sample II; and Al, As, Cd, Co, Cu, Pb, Si and V in Sample III are exceeded.

Hydrogeochemical modeling results based on prefeasibility pile assumptions and no remediation implementations, suggest that pile leachates will be in acidic (4.31-4.5) character under closed CO_2 equilibrium conditions and in basic (7.42-7.54) character in equilibrium with atmospheric CO_2 conditions. Although waste classification and surface water classification limits are not used for waste rock piles according to the current regulations, the comparison of leachate concentrations indicate that they will be in ‘’Hazardous’’ class due to higher concentrations of As, Mo and SO_4. The leachates are classified as Class IV due to low pH values under the closed CO_2 equilibrium conditions but classified as Class II under equilibrium conditions with atmospheric CO_2. Besides, the maximum environmental quality limits of Al, As, Fe, Pb, V in all simulated leachates and Cd/Cr/Zn parameters in some simulated leachates for the closed CO_2 equilibrium conditions and As, Si, V in all simulated leachates and Cd/Pb/Zn parameters in some simulated leachates for the atmospheric CO_2 conditions are exceeded. Gradual conditions between the closed CO_2 and the open to atmospheric CO_2 cases would probably be developed under the field conditions.

Sensitivity analyses based on precipitation infiltration, number of rainy days and saturation index criteria indicate that concentrations would show in general slight tendency to decrease when the infiltration amount increase, the number of rainy days decrease and the SI criteria (few parameters) decrease.

CHAPTER 12

RECOMMENDATIONS

Based on the results of this study, following recommendations are made:

- Performing kinetic tests with longer period using more samples would increase the realibility and representativeness of the results.
- Revising pile seepage water calculations using updated kinetic data and pile data (types and amounts of waste rocks, pile dimensions,etc.) would improve the predictions.
- Sampling and analysis of the operational period seepage water under a monitoring program would provide means of evaluating predictions to the actual field occurences.
- Taking test and modeling data together with the recommended more data and revisions into consideration while making a closure plan would prevent possible environmental problems.
- Utilizing 3D groundwater numeric flow & mass transport modelings would provide means to determine the possible regional distribution of concenterations coming from the waste pile.
- Taking environmental precautions depending on the results from the groundwater numeric flow & mass transport models would decrease the possible problems.

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APPENDICES

APPENDIX-A Previous Study Whole Rock Chemistry Data

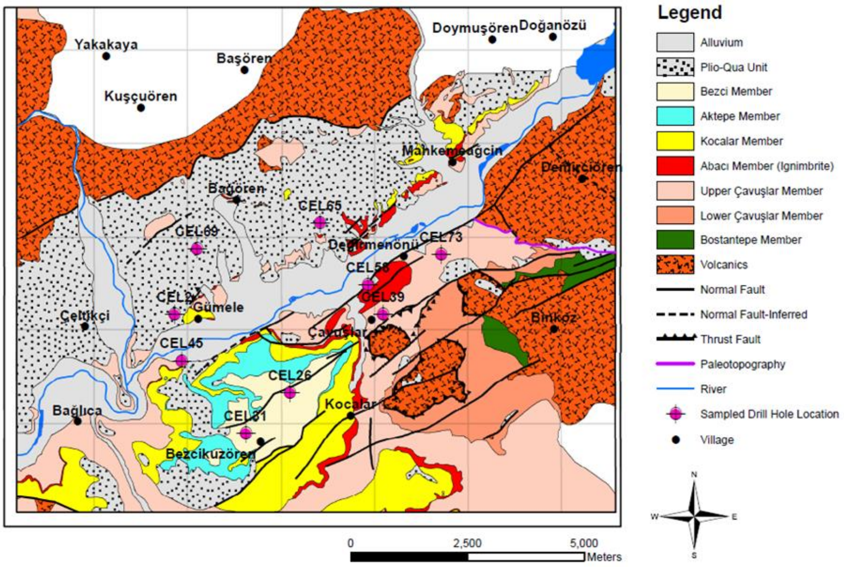

Figure A.1 Sampling locations of the wells

Table A-1. Well sampling interval information. U: Above the coal zone, B: Below the main coal zone

This Study ID	Well ID	From (m)	To (m)
U1	CEL0073	183.7	184.8
U7	CEL0065	286.94	288.7
U13	CEL0058	245.3	249.2
U19	CEL0039	158.8	161
U25	CEL0031	559	559.6
U31	CEL0026	519.6	520.5
U36	CEL0026	533.2	534.1
U38	CEL0045	338.6	339.5
U45	CEL0002	269.9	270.4
U51	CEL0069	303	304.1

This Study ID	Well ID	From (m)	To (m)
B3	CEL0073	188.64	190.2
B5	CEL0073	191.94	194.6
B6	CEL0073	194.6	195.4
B9	CEL0065	293.27	295
B11	CEL0065	297.64	299.7
B15	CEL0058	253.64	255.4
B17	CEL0058	258.25	259.8
B21	CEL0039	165.33	168.4
B23	CEL0039	170.68	173.1
B27	CEL0031	564.75	566
B29	CEL0031	569.1	570.4
B33	CEL0026	524.81	529.8
B35	CEL0026	531.73	533.2
B40	CEL0045	342.8	343
B42	CEL0045	346.14	347
B44	CEL0045	348.74	349
B47	CEL0002	275.1	276.8
B49	CEL0002	280.48	281.9
B53	CEL0069	308.77	309.9
B55	CEL0069	312.07	313.1

Table A-2. Whole rock chemistry (Gladwell et. al., 2014)

ppm	U1	U7	U13	U19	U25	U31	U36	U38	U45	U51	AVERAGE
Al	28200	20700	19400	16700	17800	28100	300	21000	22400	4100	17870
As	7	3	3	3	59	9	181	57	32	6	36
Au	0	0	0	0	0	0	0	0	0	0	0
Ba	247	214	161	165	118	135	19	70	95	215	143.9
Be	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
Bi	0.2	0.1	0.05	0.05	0.05	0.05	0.05	0.2	0.05	0.05	0.085
Ca	103100	138500	102100	129100	120200	98600	64500	48200	63100	226600	109400
Cd	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.3	0.1	0.05	0.08
Ce	20	18	14	13	14	12	0.5	16	11	12	13.05
Co	3.2	3	3.3	2.4	2.5	4.4	nd	3.9	2.3	1.1	2.9
Cr	26	28	14	13	57	58	198	164	39	10	60.7
Cu	8	5.6	5.1	4.6	4.5	5.7	1.8	6.4	4.1	3.4	4.92
Fe	6900	8300	6900	6000	6800	8200	10100	21600	7200	17700	9970
Hf	0.9	0.8	1	0.7	0.5	0.9	0.05	0.8	0.6	0.3	0.655
Hg	0.01	0.005	0.01	0.005	0.01	0.005	0.005	0.02	0.03	0.005	0.0105
In	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.025
K	15700	5600	8500	5500	14300	22200	100	19600	14800	1600	10790
La	10.3	9.1	7.5	6.6	7.1	6.3	0.2	7.8	6.2	5.7	6.68
Li	400	352.8	425.8	269.7	178.6	195	13.5	22.6	18.1	52.8	192.89
Mg	97800	107200	110100	98800	90100	88300	34900	30100	33400	98200	78890
Mn	334	367	270	239	450	414	200	592	719	613	419.8
Mo	2.9	2.4	2.1	2.3	2	2	23.7	12.6	3	1.5	5.45
Na	7590	4800	7160	5940	2690	2900	410	1830	3900	1400	3862
Nb	1.9	4.6	4.1	2.1	1.7	3.3	0.4	4	2.5	1.3	2.59
Ni	9.3	6.8	6.9	9.2	7.5	12.9	4.8	13	5.4	4.6	8.04
P	240	90	70	100	230	110	650	350	1220	340	340
Pb	6.6	5.3	5.6	5.2	5.4	6.9	0.4	22.3	2.9	2.1	6.27
Rb	57.7	43.3	42.8	30.7	46.8	68.8	0.4	52	52.2	8.4	40.31
S	500	500	500	500	3000	500	8000	24000	7000	2000	4650
Sb	0.1	0.1	0.2	0.05	0.1	0.1	0.05	0.4	0.2	0.05	0.135
Sc	2	3	2	2	1	2	0.5	0.5	1	3	1.7
Se	0	0	0	0	0	0	0	0	0	0	0
Si	128639	101808	131725	112513	134669	153180	308277	261953	225820	25102	158369
Sn	0.4	0.5	0.4	0.4	0.3	0.5	0.05	0.6	0.3	0.1	0.355
Sr	744	874	664	696	621	457	232	282	297	676	554.3
Ta	0.3	0.3	0.3	0.3	0.2	0.3	0.05	0.3	0.2	0.05	0.23
Th	3.6	3.7	2.4	2.5	7.8	3.4	0.1	4.6	2.5	23.5	5.41
Ti	390	960	820	560	430	790	60	860	720	390	598
Tl	0.25	0.25	0.25	0.25	0.25	0.25	0.25	1.9	0.25	0.25	0.415
U	1.1	1.2	0.7	0.6	3.1	1.2	0.7	4.1	3.3	8.8	2.48
V	13	31	29	18	12	22	5	39	12	11	19.2
W	0.05	0.2	0.2	0.4	0.2	0.2	0.1	0.4	0.6	0.2	0.255
Y	5.1	4.8	3.7	3.2	2.9	3.1	0.3	3.3	2.8	8	3.72
Zn	15	17	14	11	14	16	3	620	10	8	72.8
Zr	17.2	23.8	25.1	15.6	16.2	24.4	3.1	31.1	37.3	9.4	20.32

Table A-2. Cont'd

ppm	B3	B5	B6	B9	B11	B15	B17	B21	B23	B27
Al	12600	23600	11100	11300	3600	17100	3200	20700	4700	14700
As	3	4	44	7	3	2	3	2	3	41
Au	0	0	0	0	0	0	0	0	0	0
Ba	181	237	90	178	98	215	149	181	108	95
Be	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
Bi	0.3	0.2	0.1	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Ca	121300	126300	14500	168300	147100	174100	166500	111000	125700	166000
Cd	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.1
Ce	10	18	7	8	4	14	7	14	5	11
Co	1.9	2.9	2.7	2.8	0.7	2.2	0.8	3.9	1.6	2.7
Cr	87	25	45	15	50	14	30	21	31	193
Cu	4.6	5.8	5.4	3.3	1.7	5.4	1.9	7.2	2.4	5.8
Fe	6200	6700	7300	6400	3000	6900	5000	8600	3600	8900
Hf	0.5	0.7	0.3	0.8	0.3	0.7	0.5	0.7	0.3	0.6
Hg	0.02	0.04	0.04	0.02	0.005	0.02	0.01	0.01	0.005	0.005
In	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.025
K	3000	7100	10200	2000	900	8600	1700	4400	1300	5800
La	4.7	9.5	3.8	4.1	2.4	7.1	4.2	7.5	2.5	5.7
Li	183	185.2	30.2	77.8	45.1	105.3	66.5	365.5	321.3	96.8
Mg	89400	86200	8300	78800	78900	94000	88100	104400	105500	86100
Mn	323	264	146	535	298	357	252	271	217	582
Mo	1.8	1.2	8.8	1.8	1	2.2	1.6	1.6	2.1	3.2
Na	5350	10520	2170	1820	1200	5800	1650	6930	1730	1360
Nb	1.2	1.4	2	0.7	0.4	1.5	0.8	2.3	1	1.5
Ni	6.6	10.5	14.4	9.5	2.4	5.8	3.2	8.5	4.4	7
P	1050	360	820	3750	70	80	90	80	70	350
Pb	3.3	16.1	3.3	2.5	1.2	4.4	1.3	4.8	1.2	7.1
Rb	24.9	43.1	45.9	15.5	5	54.6	11.8	47.3	12.9	48.2
S	2000	3000	11000	2000	500	2000	2000	2000	500	3000
Sb	0.05	0.2	0.3	0.05	0.05	0.2	0.05	0.2	0.05	0.2
Sc	2	1	0.5	2	0.5	2	0.5	3	0.5	2
Se	0	0	0	0	0	0	0	0	0	0
Si	138082	138876	295235	120833	158976	88346	107137	126162	127705	103959
Sn	0.2	0.3	0.2	0.1	0.1	0.3	0.05	0.5	0.05	0.4
Sr	639	613	136	567	632	835	664	730	690	658
Ta	0.1	0.2	0.05	0.2	0.05	0.2	0.1	0.2	0.05	0.2
Th	2.3	1.6	2.1	8.8	0.4	2.1	1.3	1.9	0.8	1.9
Ti	510	520	380	330	110	560	180	890	290	580
Tl	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	1.1
U	1.1	0.4	1.9	4.5	0.4	0.7	1.2	0.4	0.3	0.8
V	20	16	12	23	8	20	12	34	17	54
W	0.1	0.1	0.6	0.2	0.6	0.1	0.05	0.2	0.2	0.2
Y	2.8	2.1	2	6.5	0.8	3.5	1.3	3.4	1.2	3.2
Zn	11	13	14	10	4	16	5	20	7	40
Zr	13	13	23.4	12.1	9.2	13.4	12.1	14.6	8.1	14.1

Table A-2. Cont'd

ppm	B29	B33	B35	B40	B42	B44	B47	B49	B53	B55	AVERAGE
Al	4200	14400	3500	10500	10700	2800	19000	11300	12100	8900	11000
As	23	11	11	0.5	11	182	11	10	4	4	19
Au	0	0	0	0	0	0	0	0	0	0	0
Ba	76	113	65	88	54	35	165	84	152	161	126
Be	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.50
Bi	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.1	0.05	0.05	0.08
Ca	184900	181800	234700	153000	76400	30400	144700	78700	99100	167400	133595
Cd	0.05	0.05	0.05	0.05	1.4	0.5	0.05	0.05	0.05	0.05	0.14
Ce	4	8	4	7	7	3	14	6	10	7	8
Co	0.9	2	0.7	1.6	1.3	1.3	3	1.5	1.9	1.6	1.90
Cr	59	8	21	16	56	73	22	117	49	8	47
Cu	2.3	3	1.2	2.6	2.4	2.1	6.4	4.1	4.3	2	4
Fe	5100	5300	4400	10500	18000	56100	10600	5000	5800	4200	9380
Hf	0.2	0.4	0.1	0.3	0.4	0.1	0.6	0.5	0.5	0.2	0.44
Hg	0.02	0.005	0.005	0.005	0.005	0.005	0.03	0.02	0.02	0.005	0.01
In	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.03
K	2400	3000	1000	3700	1500	900	4700	2800	3600	2600	3560
La	2.1	4.2	2	3.9	3.3	1.4	7.3	2.9	4.8	3.8	4.36
Li	45.7	46.6	24.4	66.7	33	13.9	36.1	38.9	58.2	60.1	95
Mg	89700	90800	111800	99200	56400	47500	90600	53100	66300	109200	81715
Mn	900	342	648	2725	1617	3118	479	210	437	448	708
Mo	4.3	2.3	22.8	1.8	6.4	22.1	1.9	3.8	3.6	1.5	4.79
Na	1030	1990	770	1220	1870	1320	1310	1000	1830	1780	2633
Nb	0.8	1.2	0.3	0.8	0.4	0.3	1.4	0.7	1.8	0.5	1.05
Ni	2.6	5.5	1.6	2.4	3.1	4.7	6.9	7	9.5	2.8	5.92
P	190	250	220	130	110	100	60	60	90	170	405
Pb	1.9	2.4	1.3	1.9	3.1	7.6	5	2.1	3.1	1.2	3.74
Rb	9.9	17.5	5	27.8	9.9	4.6	37.7	18.6	29	17.7	24.35
S	2000	2000	500	4000	7000	29000	5000	3000	2000	1000	4175
Sb	0.1	0.05	0.05	0.05	0.05	0.05	0.2	0.2	0.2	0.05	0.12
Sc	0.5	0.5	0.5	2	0.5	0.5	2	1	2	1	1.23
Se	0	0	0	0	0	0	0	0	0	0	0.00
Si	97975	76052	23606	35245	218248	258261	72173	243723	167858	24961	131171
Sn	0.2	0.1	0.05	0.2	0.1	0.1	0.4	0.2	0.3	0.1	0.20
Sr	613	781	623	568	412	180	651	397	635	957	599
Ta	0.05	0.2	0.05	0.1	0.1	0.05	0.2	0.2	0.2	0.1	0.13
Th	0.7	1.7	0.6	1.4	1.1	0.5	1.3	0.9	1.4	1.6	1.72
Ti	230	330	120	360	180	180	570	190	640	210	368
Tl	0.25	0.25	0.25	0.25	0.25	1.6	0.25	0.25	0.25	0.25	0.36
U	1.3	1.1	0.9	1	3.4	1.4	0.5	1.4	1.5	2.8	1.35
V	68	16	18	48	45	33	41	30	50	31	30
W	0.3	0.3	0.2	0.1	0.1	0.1	0.1	0.2	0.2	0.05	0.20
Y	1.2	1.9	1.2	2.3	1.9	0.8	2.8	1.5	2.2	2.5	2.26
Zn	16	14	24	67	420	399	17	6	11	7	56.05
Zr	6.7	12.6	8.9	8.8	11.1	8.4	12.7	9.2	14.7	5.4	11.58

APPENDIX-B Previous Study Shake Flask Test Data

Table B-1. Shake flask test data (Gladwell et. al., 2014) and the classification using the leaching limits of MEF (2010).

Parameter/ Sample	U1	B3	B5	B6	U7	B9	B11	U13	B15	B17	U19	B21	B23	U25	B27	B29
EC µS/cm at 25 °C	511	354	303	943	326	295	221	508	534	378	347	304	254	648	284	382
pH	8.8	8.7	8.3	7.8	8.8	8.8	8.8	9.2	8.7	8.3	9.2	9	8.4	8.1	8.9	8
Alkalinity	136	140	66	67	130	105	77	238	220	130	133	118	100	97	229	86
As	🟩 0.09	0.02	0.01	0.02	🟩 0.05	0.05	0.02	🟩 0.07	0.03	0.01	0.01	0.01	0.01	🟩 0.11	🟨 0.23	0.02
Ba	0.01	0.01	0.01	0.04	0.00	0.01	0.01	0.00	0.01	0.01	0.00	0.00	0.01	0.01	0.01	0.04
Cd	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cl	5.5	2.5	7.5	13.0	2.5	2.5	9.2	2.5	2.5	2.5	2.5	2.5	2.5	2.5	2.5	5.5
Cr, t	0.00	0.01	0.00	0.00	0.01	0.01	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cu	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
F	0.56	0.29	0.20	0.13	🟩 1.10	0.53	0.48	0.99	0.22	0.13	0.29	0.27	0.27	0.62	0.53	0.20
Hg	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mo	🟩 0.32	🟩 0.23	🟩 0.05	0.04	🟩 0.45	🟩 0.18	🟩 0.08	🟩 0.39	🟩 0.25	🟩 0.15	🟩 0.23	🟩 0.14	🟩 0.09	🟩 0.12	🟩 0.39	🟩 0.30
Ni	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pb	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Se	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Sb	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4	🟩 136	18	62	🟩 309	6	19	13	7	8	24	7	10	6	🟩 178	43	79
Zn	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Parameter/ Sample	U31	B33	B35	U36	U38	B40	B42	B44	U45	B47	B49	U51	B53	B55
EC µS/cm at 25 °C	482	444	273	96	2520	391	618	519	1440	778	598	392	612	410
pH	9.2	8.6	8.2	8	7.4	8.2	8	7.8	8.1	7.9	7.9	8.2	8.3	8.4
Alkalinity	176	124	110	40	83	134	91	54	117	58	59	119	196	190
As	🟨 0.70	🟩 0.20	🟨 0.40	🟩 0.12	0.01	0.04	0.02	0.01	0.03	0.02	0.02	🟩 0.14	🟩 0.08	0.05
Ba	0.00	0.02	0.01	0.01	0.06	0.00	0.01	0.02	0.03	0.03	0.03	0.01	0.01	0.00
Cd	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cl	6.5	2.5	5.7	5.1	15.0	7.5	12.0	10.0	9.3	12.0	6.2	7.7	7.6	5.6
Cr, t	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cu	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
F	0.63	0.31	0.27	0.16	0.49	🟩 1.10	0.73	0.17	0.28	0.42	0.28	0.63	0.40	0.86
Hg	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mo	🟩 0.26	🟩 0.28	🟥 3.90	🟩 0.63	0.02	🟩 0.32	🟨 1.17	🟨 1.08	🟩 0.05	🟩 0.20	🟩 0.20	🟩 0.21	🟩 0.37	🟩 0.25
Ni	0.00	0.00	0.00	0.00	🟩 0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
Pb	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Se	🟩 0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.00
Sb	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4	43	66	26	3	🟩 1340	53	🟩 161	🟩 158	🟩 500	🟩 215	🟩 139	46	83	6
Zn	0.00	0.00	0.00	0.00	🟩 0.98	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00

* No color: Inert, green: Non-Hazardous, yellow: Hazardous and red: Very Hazardous

APPENDIX-C Sample I Mixing Free Data Estimation

Related explanations were given in the page 62. The effect of remaining (previous week) solution on each parameter concentration [P0] to the following (current) cycle is estimated by considering remaining solution volume (V1) and concentration [P1] and the next cycle irrigation water volume (V2):

$$C_f = \frac{C_i V_i}{V_f}$$

[P0] contributed from the previous week solution into the current week solution

$$C_f = \frac{[P1]x(V1)}{(V2) + (V1)}$$

Then;
Previous week contribution free current week concentration [P] =
Current week concentration [P2] – [P0]

In the calculations, V1 (= 142 ml) is approximated by 1.5 cm height water column (out of 3 cm slurry) for each cycle. V2 is added volume of water in each cycle (Table 9.4). P1 for each parameter is listed in Table 15. In the case of pH calculations concentrations of H+ were subjected to the estimations and pH values were calculated afterwards.

The original laboratory measurements used for the estimations are listed in Table C-1. Both the mixing free and mixing effected values of some parameters are shown in Figure C.1. As can be seen from the figure the mixing effect is in fact negligible.

Table C-1. Sample I original laboratory measurements.

Sample No	Week	T °C	pH	EC (µS/cm)	Alkalinity	Cl	SO4	Al	As	Ba	Ca	Cd	Co	Cr. t	Cu	Fe
I-0	0		7.76	732	88	7	247.64	0.6855	0.082	0.078	30.95	0.0007	0.0141	0.001	0.015	1.140
I-1	1	25.8	7.66	1473	76.2	6.65	498.53	0	0.104	0.080	56.84	0.004	0.0023	0	0	0
I-2	2	27.7	7.81	715	96.6	9	246.14	0.0355	0.156	0.074	2.49	0.0017	0.0011	0	0	0
I-3	3	26.7	8.37	772	184	71	189.16	0.0197	0.133	0.021	nm	0	0	0	0.022	0
I-4	4	24.3	8.8	648	132	18	114.26	0.2890	0.223	0.065	nm	0	0.0005	0.003	0.005	0.085
I-5	5	20.7	9.21	427.7	264	0	86.57	0.3994	0.128	0.039	2.583	0	0.0006	0.00055	0.005	0.11962
I-6	6	22.4	8.78	340.2	128.1	0	35.15	0.9814	0.157	0.027	18.21	0	0	0	0.004	0.12069
I-7	7	20.7	8.73	279.8	107	0	31.08	0.8135	0.158	0.018	32.35	0	0	0	0.003	0.19364
I-8	8	20.5	8.56	236.3	99	0	21.31	1.57	0.307	0.014	9.705	0	0	0	0.003	8.899
I-9	9	21.6	8.44	220.1	107.6	0	12.35	1.01	0.134	0.022	9.746	0	0	0	0.003	1.70659
I-10	10	21.9	8.24	190	99	0	12.35	2.60	0.128	0.015	5.23	0	0	0	0.002	0.75543
I-11	11	22	8.16	196.6	111.4	0	18.62	1.98	0.259	0.016	5.991	0	0	0	0.002	0.54717
I-12	12	21.6	8.2	174.4	109.6	0	0	10.38	0.122	0.031	4.524	0	0	0.012	0	2.593
I-13	13	22.4	8.16	162.3	87.2	2.4	16.42	5.96	0.089	0.051	3.193	0	0	0.00877	0	0.70665

Sample No	Week	K	Li	Mg	Mn	Mo	Na	Ni	Pb	Sb	Si	Sr	U	V	Zn
I-0	0	23.18	0.044	8.35	0.048695	0.884	10.78	0.0169	0.0047	0	207.7	0.708	1.261	0.0036	0.0705
I-1	1	3.161	0.085	20.24	0	2.847	20.24	0	0.0120	0.0005	13.66	2.617	2.079	0	0.0254
I-2	2	21.06	0.044	6.97	0	0.909	113.3	0	0.0052	0.0008	14.52	0.649	1.461	0	0
I-3	3	nm	0.045	nm	0	0.753	nm	0	0.0009	0.0031	3.57	0.621	0.002	0.0029	0.0113
I-4	4	nm	0.053	nm	0	0.781	nm	0	0	0.001602	148.8	1.059	0.003	0.0034	0.0109
I-5	5	23.88	0.027	9.42	0.010375	0.322	108.6	0	0.0044	0.0043	15.06	0.410	0.001	0.002954	0.0206
I-6	6	12.73	0.020	4.29	0.050045	0.253	54.56	0	0	0	7.618	0.391	0	0.005351	0
I-7	7	10.95	0.017	7.736	0.036232	0.151	50.64	0	0	0.001	11	0.648	0	0.0066	0
I-8	8	10.19	0.014	3.504	0.015689	0.119	48.87	0	0	0	12.48	0.124	0	0.0089	0
I-9	9	9.085	0.011	3.69	0.024425	0.086	41.34	0	0	0	13.85	0.126	0	0.008033	0
I-10	10	8.038	0.000	2.92	0.015687	0.055	31.39	0	0.0028	0	17.01	0.095	0	0.010563	0
I-11	11	9.926	0.014	2.9	0.016823	0.075	40.83	0	0.0073	0	10.71	0.111	0	0.0081	0
I-12	12	6.059	0.014	2.894	0.019424	0.045	16.69	0	0.0008	0.000571	37.84	0.181	0	0.0200	0
I-13	13	3.355	0.014	1.57	0.012914	0.042	11.57	0	0.0007	0.0007	29.57	0.139	0	0.014297	0

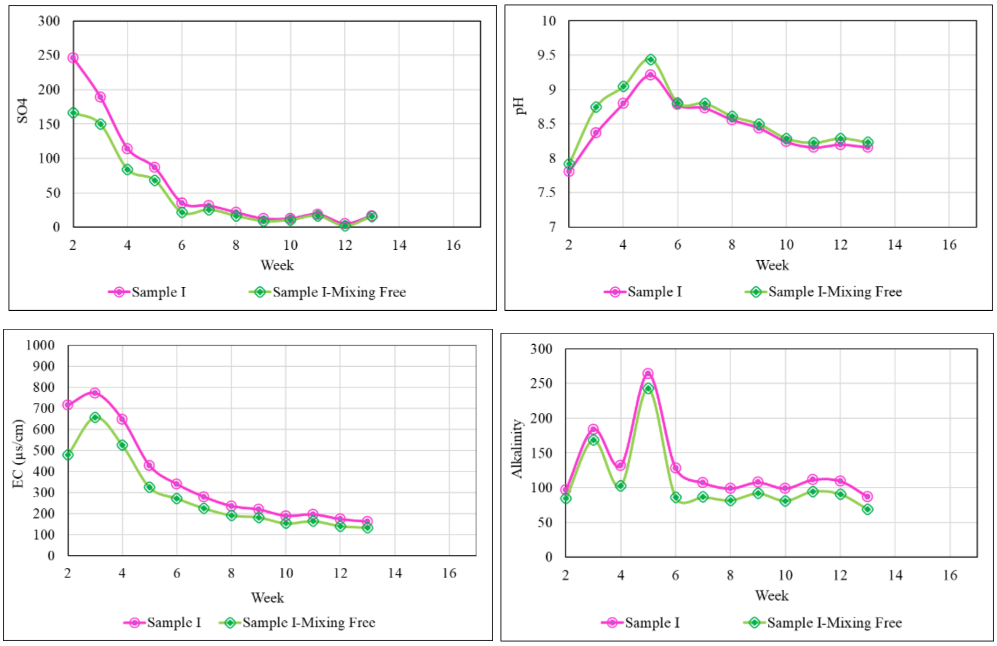

Figure C-1. Mixing free and mixing effected values of SO_4, pH, EC and Alkalinity.

APPENDIX-D Kinetic Test Rate Values

Table D-1. Kinetic test concentration rates (nm represents not measured)

Unit mg/kg/week	Sample No	Week	*Alkalinity	Cl	SO4	Al	As	B	Ba	Ca	Cd	Co	Cr. t	Cu	Fe	K
SAMPLE-I	**I-1**	1	51.8	4.7	349.0	0.00	0.07	0	0.056	39.8	0.003	0.0016	0.000	0.000	0.00	2.2
	I-2	2	43.8	4.2	88.7	0.02	0.07	0	0.033	1.3	0.001	0.0004	0.000	0.000	0.00	10.9
	I-3	3	94.0	39.5	85.0	0.01	0.06	0.0	0.005	nm	0.000	0.0000	0.000	0.013	0.00	nm
	I-4	4	66.1	4.4	55.3	0.19	0.13	0.0	0.040	nm	0.000	0.0003	0.002	0.001	0.06	nm
	I-5	5	179.2	0	50.8	0.26	0.07	0	0.021	1.9	0.000	0.0004	0.000	0.003	0.08	17.8
	I-6	6	56.7	0	14.4	0.62	0.09	0	0.014	12.0	0.000	0.0000	0.000	0.002	0.07	6.0
	I-7	7	57.9	0	17.5	0.45	0.09	0	0.009	20.2	0.000	0.0000	0.000	0.002	0.12	6.1
	I-8	8	54.5	0	11.2	0.98	0.19	0	0.008	3.1	0.000	0.0000	0.000	0.002	6.06	5.8
	I-9	9	57.7	0	5.8	0.49	0.05	0	0.013	5.3	0.000	0.0000	0.000	0.002	0.18	4.8
	I-10	10	50.7	0	6.6	1.56	0.07	0	0.007	2.3	0.000	0.0000	0.000	0.001	0.30	4.2
	I-11	11	63.2	0	11.3	1.05	0.16	0	0.009	3.5	0.000	0.0000	0.000	0.001	0.29	5.9
	I-12	12	59.5	0	0	6.75	0.05	0	0.019	2.4	0.000	0.0000	0.008	0.000	1.68	2.9
	I-13	13	45.6	1.6	11.2	2.89	0.05	0.0	0.031	1.7	0.000	0.0000	0.005	0.000	0.19	1.6
SAMPLE-II	**II-1**	1	50.6	0	91.1	0.01	0.01	0	0.023	5.6	0.000	0.0010	0.000	0.001	0.00	4.7
	II-2	2	43.0	2.6	38.4	0.01	0.01	0	0.014	3.2	0.000	0.0008	0.000	0.000	0.00	2.7
	II-3	3	45.1	2.1	22.1	0.01	0.02	0	0.011	nm	0.000	0.0000	0.000	0.002	0.02	nm
	II-4	4	47.3	1.6	21.1	0.00	0.02	0	0.014	nm	0.000	0.0000	0.001	0.003	0.00	nm
	II-5	5	50.7	0	8.2	0.00	0.02	0	0.009	3.8	0.000	0.0000	0.000	0.001	0.00	1.4
	II-6	6	44.1	0	0	0.02	0.01	0	0.008	3.2	0.000	0.0000	0.000	0.001	0.05	1.1
	II-7	7	43.3	0	10.8	0.02	0.01	0	0.008	3.6	0.000	0.0000	0.000	0.000	0.06	1.0
	II-8	8	40.9	0.5	0	0.02	0.01	0	0.008	3.9	0.000	0.0000	0.000	0.000	0.07	0.8
	II-9	9	40.8	0	0	0.02	0.01	0	0.000	3.3	0.000	0.0000	0.000	0.000	0.06	0.8
	II-10	10	42.3	1.1	0	0.02	0.01	0	0.000	3.2	0.000	0.0000	0.000	0.000	0.05	0.0
	II-11	11	43.6	0	0	0.02	0.01	0	0.000	3.5	0.000	0.0000	0.000	0.000	0.06	0.0
	II-12	12	40.0	0	0	0.02	0.01	0	0.000	5.0	0.000	0.0000	0.000	0.000	0.06	0.0
	II-13	13	42.0	1.4	0	0.01	0.01	0	0.000	11.3	0.000	0.0000	0.000	0.000	0.00	3.8
	II-14	14	48.1	0	0	0.00	0.01	0	0.000	6.3	0.000	0.0000	0.000	0.000	0.00	0.0
	II-15	15	34.4	0	0	0.00	0.02	0	0.000	3.1	0.000	0.0000	0.000	0.000	0.05	0.0
	II-16	16	39.0	0	0	0.00	0.01	0	0.000	2.8	0.000	0.0000	0.000	0.000	0.00	0.0
SAMPLE-III	**III-1**	1	45.4	3.0	176.5	0.00	0.05	0	0.030	16.0	0.002	0.0016	0.000	0.000	0.00	5.1
	III-2	2	42.3	4.4	91.3	0.00	0.07	0	0.024	6.2	0.001	0.0024	0.000	0.000	0.00	5.6
	III-3	3	43.2	2.1	61.5	0.00	0.07	0	0.020	nm	0.000	0.0000	0.001	0.003	0.00	nm
	III-4	4	43.0	3.7	56.5	0.00	0.08	0	0.019	nm	0.000	0.0000	0.000	0.002	0.00	nm
	III-5	5	50.8	0	49.4	0.02	0.07	0	0.027	4.3	0.000	0.0004	0.001	0.009	0.06	4.0
	III-6	6	42.1	0	36.0	0.03	0.06	0	0.018	4.4	0.000	0.0000	0.000	0.001	0.07	3.6
	III-7	7	39.7	0	36.3	0.01	0.05	0	0.019	4.8	0.000	0.0000	0.000	0.000	0.05	3.2
	III-8	8	41.8	0	29.1	0.03	0.05	0	0.017	4.5	0.000	0.0000	0.000	0.001	0.07	2.8
	III-9	9	40.9	0	24.4	0.02	0.05	0	0.014	4.4	0.000	0.0000	0.000	0.000	0.05	2.8
	III-10	10	37.5	0	18.0	0.01	0.04	0	0.011	3.3	0.000	0.0000	0.000	0.000	0.03	2.0
	III-11	11	41.7	0	20.9	0.01	0.05	0	0.014	3.7	0.000	0.0000	0.000	0.000	0.04	2.3
	III-12	12	42.0	0	16.7	0.00	0.04	0	0.010	7.0	0.000	0.0000	0.001	0.000	0.00	0.8
	III-13	13	43.4	1.6	15.6	0.00	0.04	0	0.009	2.2	0.000	0.0000	0.000	0.000	0.00	0.7
	III-14	14	37.1	0	15.6	0.00	0.03	0	0.008	3.3	0.000	0.0000	0.000	0.000	0.00	1.7
	III-15	15	34.4	0	13.5	0.00	0.03	0	0.009	3.1	0.000	0.0000	0.000	0.000	0.00	1.5
	III-16	16	36.7	1.2	18.1	0.00	0.03	0	0.008	3.4	0.000	0.0000	0.000	0.000	0.00	1.7

* Irrigation water contribution free values

Table D-1. Cont'd

Unit mg/kg/week	Sample No	Week	Li	Mg	Mn	Mo	Na	Ni	Pb	Sb	Se	Si	Sr	U	V	Zn
SAMPLE-I	**I-1**	1	0.06	14.2	0.00	1.99	14.2	0	0.008	0.000	0.000	9.6	1.83	1.45	0.000	0.018
	I-2	2	0.02	2.0	0.00	0.24	58.6	0	0.002	0.000	0.000	6.6	0.12	0.60	0.000	0.000
	I-3	3	0.02	nm	0.00	0.34	nm	0	0.000	0.002	0.000	0.7	0.29	0.00	0.002	0.006
	I-4	4	0.03	nm	0.00	0.43	nm	0	0.000	0.001	0.000	97.5	0.63	0.00	0.002	0.006
	I-5	5	0.01	7.0	0.01	0.15	80.8	0	0.003	0.003	0.000	0.0	0.18	0.00	0.002	0.014
	I-6	6	0.01	1.9	0.03	0.14	25.2	0	0.000	0.000	0.000	3.5	0.22	0.00	0.003	0.000
	I-7	7	0.01	4.8	0.02	0.08	28.8	0	0.000	0.001	0.000	6.7	0.40	0.00	0.004	0.000
	I-8	8	0.01	1.6	0.01	0.07	27.9	0	0.000	0.000	0.000	7.3	0.01	0.00	0.005	0.000
	I-9	9	0.01	2.0	0.01	0.04	21.6	0	0.000	0.000	0.000	7.6	0.07	0.00	0.004	0.000
	I-10	10	0.00	1.5	0.01	0.03	15.8	0	0.002	0.000	0.000	9.4	0.05	0.00	0.006	0.000
	I-11	11	0.01	1.6	0.01	0.05	24.3	0	0.005	0.000	0.000	5.4	0.06	0.00	0.004	0.000
	I-12	12	0.01	1.6	0.01	0.02	6.6	0	0.000	0.000	0.000	24.2	0.11	0.00	0.013	0.000
	I-13	13	0.01	0.7	0.01	0.02	6.0	0.0	0.000	0.000	0.000	15.9	0.07	0.00	0.007	0.000
SAMPLE-II	**II-1**	1	0.09	24.4	0.02	0.20	16.9	0	0.016	0.001	0.000	6.0	0.48	0.20	0.037	0.010
	II-2	2	0.07	16.3	0.01	0.11	7.1	0	0.001	0.001	0.000	6.4	0.28	0.09	0.037	0.012
	II-3	3	0.06	nm	0.01	0.07	nm	0	0.010	0.001	0.000	0.1	0.30	0.00	0.048	0.010
	II-4	4	0.07	nm	0.01	0.05	nm	0	0.007	0.002	0.000	2.0	0.29	0.00	0.049	0.010
	II-5	5	0.05	11.0	0.01	0.04	2.5	0	0.002	0.001	0.000	12.2	0.27	0.00	0.037	0.009
	II-6	6	0.03	10.4	0.00	0.02	1.8	0	0.007	0.000	0.000	4.2	0.11	0.00	0.037	0.000
	II-7	7	0.02	9.5	0.01	0.02	1.7	0	0.002	0.000	0.000	3.5	0.11	0.00	0.035	0.000
	II-8	8	0.02	10.2	0.00	0.01	1.6	0	0.005	0.000	0.000	3.3	0.11	0.00	0.032	0.000
	II-9	9	0.02	9.2	0.00	0.01	1.2	0	0.007	0.000	0.000	2.9	0.10	0.00	0.031	0.000
	II-10	10	0.01	8.1	0.00	0.01	0.9	0	0.001	0.000	0.000	2.8	0.09	0.00	0.026	0.000
	II-11	11	0.02	9.0	0.00	0.01	0.9	0	0.007	0.000	0.000	2.3	0.10	0.00	0.029	0.000
	II-12	12	0.02	3.9	0.00	0.01	0.0	0	0.003	0.000	0.000	6.9	0.12	0.00	0.030	0.000
	II-13	13	0.02	3.8	0.00	0.01	0.0	0	0.003	0.000	0.000	3.0	0.12	0.00	0.027	0.000
	II-14	14	0.02	7.8	0.00	0.01	0.0	0	0.000	0.000	0.000	2.9	0.12	0.00	0.112	0.000
	II-15	15	0.02	7.4	0.00	0.01	0.0	0	0.001	0.000	0.000	102.4	0.11	0.00	0.022	0.000
	II-16	16	0.01	6.3	0.00	0.00	0.0	0	0.003	0.000	0.000	92.4	0.09	0.00	0.021	0.000
SAMPLE-III	**III-1**	1	0.28	28.8	0.00	0.98	31.8	0	0.011	0.006	0.016	7.9	0.63	0.43	0.018	0.011
	III-2	2	0.18	18.9	0.00	0.51	24.4	0	0.003	0.007	0.009	8.1	0.45	0.31	0.027	0.014
	III-3	3	0.19	nm	0.00	0.27	nm	0	0.006	0.007	0.000	1.8	0.38	0.00	0.033	0.006
	III-4	4	0.18	nm	0.00	0.17	nm	0	0.002	0.009	0.000	0.8	0.39	0.00	0.032	0.000
	III-5	5	0.12	12.6	0.00	0.09	12.4	0	0.013	0.008	0.000	13.6	0.26	0.00	0.028	0.000
	III-6	6	0.09	13.7	0.00	0.05	14.5	0	0.008	0.005	0.000	4.7	0.63	0.00	0.027	0.000
	III-7	7	0.08	11.5	0.00	0.04	14.9	0	0.004	0.004	0.000	3.3	0.63	0.00	0.025	0.000
	III-8	8	0.07	10.9	0.00	0.03	10.0	0	0.003	0.004	0.000	3.2	0.82	0.00	0.025	0.000
	III-9	9	0.06	11.0	0.00	0.03	1.0	0	0.004	0.004	0.000	3.6	0.47	0.00	0.026	0.000
	III-10	10	0.05	8.7	0.00	0.02	5.4	0	0.003	0.003	0.000	2.9	0.91	0.00	0.022	0.000
	III-11	11	0.05	10.0	0.00	0.03	6.0	0	0.003	0.004	0.000	4.5	0.45	0.00	0.025	0.000
	III-12	12	0.06	3.9	0.00	0.02	2.3	0	0.018	0.004	0.000	6.3	0.16	0.00	0.023	0.000
	III-13	13	0.05	3.7	0.00	0.02	2.1	0	0.000	0.004	0.000	3.3	0.15	0.00	0.023	0.000
	III-14	14	0.04	7.3	0.00	0.02	3.8	0	0.000	0.003	0.000	2.2	0.13	0.00	0.072	0.000
	III-15	15	0.05	6.8	0.00	0.02	3.4	0	0.004	0.003	0.000	88.9	0.14	0.00	0.017	0.000
	III-16	16	0.05	8.0	0.00	0.02	3.8	0	0.002	0.003	0.000	98.9	0.14	0.00	0.017	0.000

APPENDIX-E Example Thermodynamic Model Run Output

Table E-1. Thermodynamic model run of Leachate 3 and Case II Output

```
Initial solution 1.   WSEEPAGE-1 KIN ORT

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

       Elements           Molality       Moles

       Al                 2.348e-03   2.348e-03
       Alkalinity         1.380e+00   1.380e+00
       As                 1.348e-03   1.348e-03
       Ba                 2.452e-04   2.452e-04
       Ca                 2.212e-01   2.212e-01
       Cl                 2.361e-04   2.361e-04
       Cr                 1.600e-07   1.600e-07
       Cu                 1.561e-05   1.561e-05
       Fe                 2.105e-03   2.105e-03
       K                  1.467e-01   1.467e-01
       Li                 2.021e-02   2.021e-02
       Mg                 9.018e-01   9.018e-01
       Mn                 5.262e-06   5.262e-06
       Mo                 7.548e-04   7.548e-04
       Na                 9.082e-01   9.082e-01
       Pb                 4.839e-05   4.839e-05
       S(6)               6.135e-01   6.135e-01
       Sb                 6.204e-05   6.204e-05
       Si                 2.700e-01   2.700e-01
       Sr                 1.375e-02   1.375e-02
       V                  1.041e-03   1.041e-03

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

                                       pH  =   4.481
                                       pe  =   4.000
                        Activity of water  =   0.430
                 Ionic strength (mol/kgw)  =   1.457e+00
                       Mass of water (kg)  =   1.000e+00
                 Total carbon (mol/kg)  =   3.171e+01
                    Total CO2 (mol/kg)  =   3.171e+01
                      Temperature (°C)  =  25.00
                  Electrical balance (eq)  =   7.518e-01
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  29.43
                               Iterations  =  68
                                  Total H  = 1.741380e+02
                                  Total O  = 1.541820e+02
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```
----------------------------Distribution of species----------------------------

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

   H+              3.756e-05   3.301e-05    -4.425    -4.481    -0.056      0.00
   OH-             2.377e-10   1.313e-10    -9.624    -9.882    -0.258     (0)
   H2O             5.551e+01   4.304e-01     1.744    -0.366     0.000     18.07
Al            2.348e-03
   AlSO4+          1.799e-03   1.081e-03    -2.745    -2.966    -0.221     (0)
   Al(SO4)2-       5.285e-04   3.176e-04    -3.277    -3.498    -0.221     (0)
   Al+3            1.623e-05   5.082e-06    -4.790    -5.294    -0.504     (0)
   AlOH+2          4.056e-06   6.671e-07    -5.392    -6.176    -0.784     (0)
   Al(OH)2+        1.092e-07   6.956e-08    -6.962    -7.158    -0.196     (0)
   AlMo6O21-3      1.276e-09   3.676e-15    -8.894   -14.435    -5.540     (0)
   Al(OH)3         1.822e-10   1.822e-10    -9.739    -9.739     0.000     (0)
   Al(OH)4-        5.009e-12   3.011e-12   -11.300   -11.521    -0.221     (0)
As(3)         2.480e-04
   H3AsO3          2.480e-04   2.480e-04    -3.606    -3.606     0.000     (0)
   H4AsO3+         1.674e-08   4.056e-09    -7.776    -8.392    -0.616     (0)
   H2AsO3-         1.590e-08   3.852e-09    -7.799    -8.414    -0.616     (0)
   HAsO3-2         3.086e-14   1.064e-16   -13.511   -15.973    -2.462     (0)
   AsO3-3          4.313e-20   1.243e-25   -19.365   -24.906    -5.540     (0)
As(5)         1.100e-03
   H2AsO4-         8.908e-04   2.159e-04    -3.050    -3.666    -0.616     (0)
   HAsO4-2         2.079e-04   7.169e-07    -3.682    -6.145    -2.462     (0)
   H3AsO4          8.855e-07   1.238e-06    -6.053    -5.907     0.146     (0)
   AsO4-3          2.384e-08   6.867e-14    -7.623   -13.163    -5.540     (0)
Ba            2.452e-04
   BaHCO3+         1.912e-04   1.257e-04    -3.718    -3.901    -0.182     (0)
   Ba+2            5.398e-05   3.222e-05    -4.268    -4.492    -0.224     (0)
   BaCO3           9.586e-09   9.586e-09    -8.018    -8.018     0.000     (0)
   BaOH+           2.970e-14   1.846e-14   -13.527   -13.734    -0.206     (0)
C(4)          3.171e+01
   H2CO3           3.033e+01   3.033e+01     1.482     1.482     0.000     (0)
   HCO3-           6.414e-01   4.085e-01    -0.193    -0.389    -0.196     (0)
   MgHCO3+         4.693e-01   2.713e-01    -0.329    -0.567    -0.238     (0)
   CaHCO3+         1.311e-01   8.618e-02    -0.882    -1.065    -0.182     (0)
   NaHCO3          1.305e-01   1.305e-01    -0.884    -0.884     0.000     (0)
   SrHCO3+         8.044e-03   5.288e-03    -2.095    -2.277    -0.182     (0)
   BaHCO3+         1.912e-04   1.257e-04    -3.718    -3.901    -0.182     (0)
   FeHCO3+         5.407e-05   3.555e-05    -4.267    -4.449    -0.182     (0)
   PbHCO3+         3.167e-05   7.675e-06    -4.499    -5.115    -0.616     (0)
   MgCO3           3.131e-05   3.131e-05    -4.504    -4.504     0.000     (0)
   CuHCO3+         1.389e-05   3.367e-06    -4.857    -5.473    -0.616     (0)
   CaCO3           1.042e-05   1.042e-05    -4.982    -4.982     0.000     (0)
   NaCO3-          9.636e-06   6.136e-06    -5.016    -5.212    -0.196     (0)
   CO3-2           9.717e-07   5.801e-07    -6.012    -6.237    -0.224     (0)
   CuCO3           4.462e-07   4.462e-07    -6.350    -6.350     0.000     (0)
   SrCO3           2.989e-07   2.989e-07    -6.524    -6.524     0.000     (0)
   MnHCO3+         2.240e-07   1.392e-07    -6.650    -6.856    -0.206     (0)
   Cu(CO3)2-2      2.020e-07   6.966e-10    -6.695    -9.157    -2.462     (0)
   PbCO3           4.410e-08   4.410e-08    -7.356    -7.356     0.000     (0)
   Pb(CO3)2-2      2.139e-08   7.377e-11    -7.670   -10.132    -2.462     (0)
   BaCO3           9.586e-09   9.586e-09    -8.018    -8.018     0.000     (0)
Ca            2.212e-01
   CaHCO3+         1.311e-01   8.618e-02    -0.882    -1.065    -0.182     (0)
   CaSO4           7.115e-02   7.115e-02    -1.148    -1.148     0.000     (0)
   Ca+2            1.898e-02   1.133e-02    -1.722    -1.946    -0.224     (0)
   CaCO3           1.042e-05   1.042e-05    -4.982    -4.982     0.000     (0)
   CaOH+           4.514e-11   2.967e-11   -10.345   -10.528    -0.182     (0)
Cl            2.361e-04
   Cl-             2.361e-04   2.075e-04    -3.627    -3.683    -0.056     (0)
   VOCl+           4.743e-09   1.149e-09    -8.324    -8.940    -0.616     (0)
   CuCl            1.671e-09   1.671e-09    -8.777    -8.777     0.000     (0)
   PbCl+           7.683e-10   1.862e-10    -9.114    -9.730    -0.616     (0)
   CuCl2-          1.254e-10   7.246e-11    -9.902   -10.140    -0.238     (0)
   CuCl+           7.432e-11   4.296e-11   -10.129   -10.367    -0.238     (0)
   MnCl+           7.178e-12   4.463e-12   -11.144   -11.350    -0.206     (0)
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   PbCl2           1.726e-13   1.726e-13   -12.763   -12.763     0.000     (0)
   CrCl+2          3.579e-14   1.234e-16   -13.446   -15.909    -2.462     (0)
   CuCl3-2         2.151e-14   3.214e-15   -13.667   -14.493    -0.826     (0)
   CuCl2           3.091e-15   3.091e-15   -14.510   -14.510     0.000     (0)
   MnCl2           1.308e-15   1.308e-15   -14.883   -14.883     0.000     (0)
   FeCl+2          2.693e-16   4.024e-17   -15.570   -16.395    -0.826     (0)
   PbCl3-          5.882e-17   1.425e-17   -16.230   -16.846    -0.616     (0)
   PbCl4-2         3.921e-19   1.352e-21   -18.407   -20.869    -2.462     (0)
   MnCl3-          1.202e-19   7.475e-20   -18.920   -19.126    -0.206     (0)
   FeCl2+          5.998e-20   3.729e-20   -19.222   -19.428    -0.206     (0)
   CuCl3-          1.035e-20   5.985e-21   -19.985   -20.223    -0.238     (0)
   CrCl2+          1.003e-20   2.430e-21   -19.999   -20.614    -0.616     (0)
   CrOHCl2         6.389e-23   6.389e-23   -22.195   -22.195     0.000     (0)
   FeCl3           7.738e-25   7.738e-25   -24.111   -24.111     0.000     (0)
   CuCl4-2         4.166e-26   6.224e-27   -25.380   -26.206    -0.826     (0)
   CrO3Cl-         0.000e+00   0.000e+00   -47.252   -47.867    -0.616     (0)
Cr(2)         3.184e-21
   Cr+2            3.184e-21   1.098e-23   -20.497   -22.959    -2.462     (0)
Cr(3)         1.600e-07
   Cr+3            1.595e-07   4.596e-13    -6.797   -12.338    -5.540     (0)
   Cr(OH)+2        3.828e-10   1.320e-12    -9.417   -11.879    -2.462     (0)
   CrSO4+          1.214e-10   2.942e-11    -9.916   -10.531    -0.616     (0)
   CrOHSO4         8.586e-12   8.586e-12   -11.066   -11.066     0.000     (0)
   Cr(OH)2+        8.699e-14   2.108e-14   -13.061   -13.676    -0.616     (0)
   CrCl+2          3.579e-14   1.234e-16   -13.446   -15.909    -2.462     (0)
   Cr(OH)3         1.040e-18   1.040e-18   -17.983   -17.983     0.000     (0)
   Cr2(OH)2SO4+2   2.971e-19   1.024e-21   -18.527   -20.990    -2.462     (0)
   CrCl2+          1.003e-20   2.430e-21   -19.999   -20.614    -0.616     (0)
   Cr2(OH)2(SO4)2   1.668e-21   1.668e-21   -20.778   -20.778     0.000     (0)
   CrO2-           1.434e-22   3.474e-23   -21.844   -22.459    -0.616     (0)
   CrOHCl2         6.389e-23   6.389e-23   -22.195   -22.195     0.000     (0)
   Cr(OH)4-        2.242e-23   5.433e-24   -22.649   -23.265    -0.616     (0)
Cr(6)         0.000e+00
   HCrO4-          0.000e+00   0.000e+00   -40.252   -40.868    -0.616     (0)
   CrO3SO4-2       0.000e+00   0.000e+00   -41.599   -44.061    -2.462     (0)
   NaCrO4-         0.000e+00   0.000e+00   -41.830   -42.446    -0.616     (0)
   CrO4-2          0.000e+00   0.000e+00   -42.673   -42.897    -0.224     (0)
   KCrO4-          0.000e+00   0.000e+00   -42.704   -43.319    -0.616     (0)
   H2CrO4          0.000e+00   0.000e+00   -45.440   -45.440     0.000     (0)
   CrO3Cl-         0.000e+00   0.000e+00   -47.252   -47.867    -0.616     (0)
   Cr2O7-2         0.000e+00   0.000e+00   -77.367   -79.830    -2.462     (0)
Cu(1)         2.820e-08
   Cu+             2.640e-08   6.398e-09    -7.578    -8.194    -0.616     (0)
   CuCl            1.671e-09   1.671e-09    -8.777    -8.777     0.000     (0)
   CuCl2-          1.254e-10   7.246e-11    -9.902   -10.140    -0.238     (0)
   CuCl3-2         2.151e-14   3.214e-15   -13.667   -14.493    -0.826     (0)
Cu(2)         1.558e-05
   CuHCO3+         1.389e-05   3.367e-06    -4.857    -5.473    -0.616     (0)
   CuSO4           8.204e-07   8.204e-07    -6.086    -6.086     0.000     (0)
   CuCO3           4.462e-07   4.462e-07    -6.350    -6.350     0.000     (0)
   Cu+2            2.188e-07   1.306e-07    -6.660    -6.884    -0.224     (0)
   Cu(CO3)2-2      2.020e-07   6.966e-10    -6.695    -9.157    -2.462     (0)
   CuOH+           9.382e-11   5.423e-11   -10.028   -10.266    -0.238     (0)
   CuCl+           7.432e-11   4.296e-11   -10.129   -10.367    -0.238     (0)
   Cu2(OH)2+2      2.142e-14   7.387e-17   -13.669   -16.132    -2.462     (0)
   CuCl2           3.091e-15   3.091e-15   -14.510   -14.510     0.000     (0)
   Cu(OH)2         1.420e-15   1.420e-15   -14.848   -14.848     0.000     (0)
   CuCl3-          1.035e-20   5.985e-21   -19.985   -20.223    -0.238     (0)
   Cu(OH)3-        1.578e-21   3.824e-22   -20.802   -21.417    -0.616     (0)
   CuCl4-2         4.166e-26   6.224e-27   -25.380   -26.206    -0.826     (0)
   Cu(OH)4-2       1.146e-28   3.951e-31   -27.941   -30.403    -2.462     (0)
Fe(2)         2.105e-03
   Fe+2            2.005e-03   6.912e-06    -2.698    -5.160    -2.462     (0)
   FeHCO3+         5.407e-05   3.555e-05    -4.267    -4.449    -0.182     (0)
   FeSO4           4.651e-05   4.651e-05    -4.332    -4.332     0.000     (0)
   FeOH+           5.810e-11   3.612e-11   -10.236   -10.442    -0.206     (0)
   Fe(OH)2         3.766e-18   3.766e-18   -17.424   -17.424     0.000     (0)
   Fe(OH)3-        2.515e-22   1.563e-22   -21.599   -21.806    -0.206     (0)
Fe(3)         5.540e-11
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   Fe(OH)2+         4.364e-11   2.779e-11   -10.360   -10.556    -0.196     (0)
   Fe(SO4)2-        4.777e-12   1.158e-12   -11.321   -11.936    -0.616     (0)
   FeOH+2           3.643e-12   5.442e-13   -11.439   -12.264    -0.826     (0)
   FeSO4+           3.177e-12   1.975e-12   -11.498   -11.704    -0.206     (0)
   Fe2(OH)2+4       6.938e-14   9.807e-24   -13.159   -23.008    -9.850     (0)
   Fe+3             2.050e-14   6.421e-15   -13.688   -14.192    -0.504     (0)
   Fe(OH)3          3.918e-15   3.918e-15   -14.407   -14.407     0.000     (0)
   FeCl+2           2.693e-16   4.024e-17   -15.570   -16.395    -0.826     (0)
   Fe3(OH)4+5       9.675e-18   3.940e-33   -17.014   -32.405   -15.390     (0)
   Fe(OH)4-         7.520e-20   4.789e-20   -19.124   -19.320    -0.196     (0)
   FeCl2+           5.998e-20   3.729e-20   -19.222   -19.428    -0.206     (0)
   FeCl3            7.738e-25   7.738e-25   -24.111   -24.111     0.000     (0)
H(0)             1.103e-20
   H2               5.517e-21   7.716e-21   -20.258   -20.113     0.146     (0)
K                1.467e-01
   K+               1.157e-01   1.017e-01    -0.937    -0.993    -0.056     (0)
   KSO4-            3.099e-02   1.974e-02    -1.509    -1.705    -0.196     (0)
   KCrO4-           0.000e+00   0.000e+00   -42.704   -43.319    -0.616     (0)
Li               2.021e-02
   Li+              1.728e-02   1.519e-02    -1.762    -1.818    -0.056     (0)
   LiSO4-           2.924e-03   1.818e-03    -2.534    -2.740    -0.206     (0)
Mg               9.018e-01
   MgHCO3+          4.693e-01   2.713e-01    -0.329    -0.567    -0.238     (0)
   MgSO4            3.237e-01   3.237e-01    -0.490    -0.490     0.000     (0)
   Mg+2             1.087e-01   6.490e-02    -0.964    -1.188    -0.224     (0)
   MgCO3            3.131e-05   3.131e-05    -4.504    -4.504     0.000     (0)
   MgOH+            5.041e-09   3.391e-09    -8.298    -8.470    -0.172     (0)
Mn(2)            5.262e-06
   Mn+2             4.955e-06   1.708e-08    -5.305    -7.767    -2.462     (0)
   MnHCO3+          2.240e-07   1.392e-07    -6.650    -6.856    -0.206     (0)
   MnSO4            8.329e-08   8.329e-08    -7.079    -7.079     0.000     (0)
   MnCl+            7.178e-12   4.463e-12   -11.144   -11.350    -0.206     (0)
   MnOH+            9.061e-15   5.633e-15   -14.043   -14.249    -0.206     (0)
   MnCl2            1.308e-15   1.308e-15   -14.883   -14.883     0.000     (0)
   MnCl3-           1.202e-19   7.475e-20   -18.920   -19.126    -0.206     (0)
   Mn(OH)3-         9.649e-31   5.999e-31   -30.015   -30.222    -0.206     (0)
   Mn(OH)4-2        1.702e-39   2.542e-40   -38.769   -39.595    -0.826     (0)
Mn(3)            2.437e-29
   Mn+3             2.437e-29   7.632e-30   -28.613   -29.117    -0.504     (0)
Mn(6)            0.000e+00
   MnO4-2           0.000e+00   0.000e+00   -74.978   -75.804    -0.826     (0)
Mn(7)            0.000e+00
   MnO4-            0.000e+00   0.000e+00   -80.894   -81.176    -0.281     (0)
Mo               7.548e-04
   Mo7O24-6         1.076e-04   7.410e-27    -3.968   -26.130   -22.162     (0)
   HMoO4-           1.103e-06   2.672e-07    -5.958    -6.573    -0.616     (0)
   MoO4-2           6.815e-07   4.068e-07    -6.167    -6.391    -0.224     (0)
   H2MoO4           6.462e-08   6.462e-08    -7.190    -7.190     0.000     (0)
   HMo7O24-5        1.464e-09   5.961e-25    -8.835   -24.225   -15.390     (0)
   AlMo6O21-3       1.276e-09   3.676e-15    -8.894   -14.435    -5.540     (0)
   H2Mo7O24-4       8.432e-15   1.192e-24   -14.074   -23.924    -9.850     (0)
   H3Mo7O24-3       2.406e-20   6.933e-26   -19.619   -25.159    -5.540     (0)
Na               9.082e-01
   Na+              6.463e-01   5.681e-01    -0.190    -0.246    -0.056     (0)
   NaSO4-           1.313e-01   8.364e-02    -0.882    -1.078    -0.196     (0)
   NaHCO3           1.305e-01   1.305e-01    -0.884    -0.884     0.000     (0)
   NaCO3-           9.636e-06   6.136e-06    -5.016    -5.212    -0.196     (0)
   NaCrO4-          0.000e+00   0.000e+00   -41.830   -42.446    -0.616     (0)
O(0)             0.000e+00
   O2               0.000e+00   0.000e+00   -52.948   -52.802     0.146     (0)
Pb               4.839e-05
   PbHCO3+          3.167e-05   7.675e-06    -4.499    -5.115    -0.616     (0)
   Pb(SO4)2-2       1.627e-05   5.608e-08    -4.789    -7.251    -2.462     (0)
   PbSO4            3.395e-07   3.395e-07    -6.469    -6.469     0.000     (0)
   PbCO3            4.410e-08   4.410e-08    -7.356    -7.356     0.000     (0)
   Pb+2             4.237e-08   2.529e-08    -7.373    -7.597    -0.224     (0)
   Pb(CO3)2-2       2.139e-08   7.377e-11    -7.670   -10.132    -2.462     (0)
   PbCl+            7.683e-10   1.862e-10    -9.114    -9.730    -0.616     (0)
   PbOH+            3.441e-11   8.339e-12   -10.463   -11.079    -0.616     (0)
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   Pb2OH+3          1.160e-12   3.342e-18   -11.936   -17.476    -5.540      (0)
   PbCl2            1.726e-13   1.726e-13   -12.763   -12.763     0.000      (0)
   PbCl3-           5.882e-17   1.425e-17   -16.230   -16.846    -0.616      (0)
   Pb(OH)2          3.461e-17   3.461e-17   -16.461   -16.461     0.000      (0)
   PbCl4-2          3.921e-19   1.352e-21   -18.407   -20.869    -2.462      (0)
   Pb(OH)3-         1.875e-23   4.544e-24   -22.727   -23.343    -0.616      (0)
   Pb4(OH)4+4       8.592e-25   1.214e-34   -24.066   -33.916    -9.850      (0)
   Pb3(OH)4+2       1.753e-28   6.046e-31   -27.756   -30.219    -2.462      (0)
   Pb(OH)4-2        4.236e-29   1.461e-31   -28.373   -30.835    -2.462      (0)
S(6)             6.135e-01
   MgSO4            3.237e-01   3.237e-01    -0.490    -0.490     0.000      (0)
   NaSO4-           1.313e-01   8.364e-02    -0.882    -1.078    -0.196      (0)
   CaSO4            7.115e-02   7.115e-02    -1.148    -1.148     0.000      (0)
   SO4-2            4.592e-02   2.741e-02    -1.338    -1.562    -0.224      (0)
   KSO4-            3.099e-02   1.974e-02    -1.509    -1.705    -0.196      (0)
   SrSO4            4.366e-03   4.366e-03    -2.360    -2.360     0.000      (0)
   LiSO4-           2.924e-03   1.818e-03    -2.534    -2.740    -0.206      (0)
   AlSO4+           1.799e-03   1.081e-03    -2.745    -2.966    -0.221      (0)
   Al(SO4)2-        5.285e-04   3.176e-04    -3.277    -3.498    -0.221      (0)
   HSO4-            1.471e-04   8.844e-05    -3.832    -4.053    -0.221      (0)
   FeSO4            4.651e-05   4.651e-05    -4.332    -4.332     0.000      (0)
   Pb(SO4)2-2       1.627e-05   5.608e-08    -4.789    -7.251    -2.462      (0)
   VOSO4            1.491e-05   1.491e-05    -4.827    -4.827     0.000      (0)
   CuSO4            8.204e-07   8.204e-07    -6.086    -6.086     0.000      (0)
   PbSO4            3.395e-07   3.395e-07    -6.469    -6.469     0.000      (0)
   MnSO4            8.329e-08   8.329e-08    -7.079    -7.079     0.000      (0)
   VO2SO4-          2.633e-10   6.380e-11    -9.580   -10.195    -0.616      (0)
   CrSO4+           1.214e-10   2.942e-11    -9.916   -10.531    -0.616      (0)
   VSO4+            1.326e-11   3.213e-12   -10.877   -11.493    -0.616      (0)
   CrOHSO4          8.586e-12   8.586e-12   -11.066   -11.066     0.000      (0)
   Fe(SO4)2-        4.777e-12   1.158e-12   -11.321   -11.936    -0.616      (0)
   FeSO4+           3.177e-12   1.975e-12   -11.498   -11.704    -0.206      (0)
   Cr2(OH)2SO4+2    2.971e-19   1.024e-21   -18.527   -20.990    -2.462      (0)
   Cr2(OH)2(SO4)2    1.668e-21   1.668e-21   -20.778   -20.778     0.000      (0)
   CrO3SO4-2        0.000e+00   0.000e+00   -41.599   -44.061    -2.462      (0)
Sb(3)            2.519e-05
   HSbO2            1.741e-05   1.741e-05    -4.759    -4.759     0.000      (0)
   Sb(OH)3          7.675e-06   7.675e-06    -5.115    -5.115     0.000      (0)
   Sb(OH)2+         5.899e-08   1.430e-08    -7.229    -7.845    -0.616      (0)
   SbO+             4.726e-08   1.145e-08    -7.326    -7.941    -0.616      (0)
   SbO2-            3.524e-12   8.539e-13   -11.453   -12.069    -0.616      (0)
   Sb(OH)4-         3.741e-13   9.064e-14   -12.427   -13.043    -0.616      (0)
Sb(5)            3.685e-05
   SbO3-            3.685e-05   8.930e-06    -4.434    -5.049    -0.616      (0)
   Sb(OH)6-         9.475e-10   8.328e-10    -9.023    -9.079    -0.056      (0)
   SbO2+            2.677e-14   6.486e-15   -13.572   -14.188    -0.616      (0)
Si               2.700e-01
   H4SiO4           2.700e-01   3.776e-01    -0.569    -0.423     0.146      (0)
   H3SiO4-          2.860e-06   1.653e-06    -5.544    -5.782    -0.238      (0)
   H2SiO4-2         1.921e-14   3.159e-15   -13.716   -14.500    -0.784      (0)
Sr               1.375e-02
   SrHCO3+          8.044e-03   5.288e-03    -2.095    -2.277    -0.182      (0)
   SrSO4            4.366e-03   4.366e-03    -2.360    -2.360     0.000      (0)
   Sr+2             1.337e-03   7.982e-04    -2.874    -3.098    -0.224      (0)
   SrCO3            2.989e-07   2.989e-07    -6.524    -6.524     0.000      (0)
   SrOH+            1.113e-12   6.923e-13   -11.953   -12.160    -0.206      (0)
V(2)             3.527e-19
   V+2              3.527e-19   1.216e-21   -18.453   -20.915    -2.462      (0)
   VOH+             2.132e-23   5.166e-24   -22.671   -23.287    -0.616      (0)
V(3)             4.531e-04
   V(OH)3           4.530e-04   4.530e-04    -3.344    -3.344     0.000      (0)
   V+3              8.618e-08   2.483e-13    -7.065   -12.605    -5.540      (0)
   VOH+2            4.737e-09   1.634e-11    -8.324   -10.787    -2.462      (0)
   V(OH)2+          9.266e-11   2.245e-11   -10.033   -10.649    -0.616      (0)
   VSO4+            1.326e-11   3.213e-12   -10.877   -11.493    -0.616      (0)
   V2(OH)2+4        1.191e-11   1.684e-21   -10.924   -20.774    -9.850      (0)
   V2(OH)3+3        3.604e-18   1.038e-23   -17.443   -22.984    -5.540      (0)
V(4)             5.877e-04
   VO+2             5.726e-04   1.974e-06    -3.242    -5.705    -2.462      (0)
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   VOSO4           1.491e-05   1.491e-05    -4.827    -4.827     0.000      (0)
   V(OH)3+         9.184e-08   2.226e-08    -7.037    -7.653    -0.616      (0)
   H2V2O4+2        3.887e-08   1.340e-10    -7.410    -9.873    -2.462      (0)
   VOCl+           4.743e-09   1.149e-09    -8.324    -8.940    -0.616      (0)
V(5)          4.121e-09
   H2VO4-          3.426e-09   8.302e-10    -8.465    -9.081    -0.616      (0)
   H3VO4           2.741e-10   2.741e-10    -9.562    -9.562     0.000      (0)
   VO2SO4-         2.633e-10   6.380e-11    -9.580   -10.195    -0.616      (0)
   VO2+            1.109e-10   9.747e-11    -9.955   -10.011    -0.056      (0)
   HVO4-2          1.832e-11   6.317e-14   -10.737   -13.200    -2.462      (0)
   H3V2O7-         1.409e-11   3.414e-12   -10.851   -11.467    -0.616      (0)
   HV2O7-3         1.433e-14   4.129e-20   -13.844   -19.384    -5.540      (0)
   V3O9-3          2.609e-15   7.517e-21   -14.584   -20.124    -5.540      (0)
   V2O7-4          2.381e-16   3.366e-26   -15.623   -25.473    -9.850      (0)
   V4O12-4         4.276e-17   6.045e-27   -16.369   -26.219    -9.850      (0)
   VO4-3           3.329e-18   9.590e-24   -17.478   -23.018    -5.540      (0)
   V10O28-6        5.346e-34   0.000e+00   -33.272   -55.434   -22.162      (0)
   HV10O28-5       4.589e-37   0.000e+00   -36.338   -51.728   -15.390      (0)
   H2V10O28-4      0.000e+00   0.000e+00   -41.152   -51.002    -9.850      (0)

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

  Phase               SI** log IAP   log K(298 K,   1 atm)

  Al(OH)3(am)      -3.75      7.05   10.80  Al(OH)3
  Al2(MoO4)3      -32.13    -29.76    2.37  Al2(MoO4)3
  Al2O3            -4.45     15.20   19.65  Al2O3
  Al4(OH)10SO4     -4.29     18.41   22.70  Al4(OH)10SO4
  AlAsO4:2H2O      -3.29      1.51    4.80  AlAsO4:2H2O
  AlOHSO4           0.49     -2.74   -3.23  AlOHSO4
  AlSb           -112.38    -46.75   65.62  AlSb
  Alunite           6.09      4.69   -1.40  KAl3(SO4)2(OH)6
  Anglesite        -1.37     -9.16   -7.79  PbSO4
  Anhydrite         0.85     -3.51   -4.36  CaSO4
  Antlerite       -14.54     -5.75    8.79  Cu3(OH)4SO4
  Aragonite         0.12     -8.18   -8.30  CaCO3
  Arsenolite       -9.47    -12.23   -2.76  As4O6
  Artinite        -11.08     -1.48    9.60  MgCO3:Mg(OH)2:3H2O
  As2O5           -17.42    -10.72    6.71  As2O5
  Atacamite       -12.50     -5.11    7.39  Cu2(OH)3Cl
  Azurite          -7.99    -24.89  -16.91  Cu3(OH)2(CO3)2
  Ba(OH)2:8H2O    -23.58      0.81   24.39  Ba(OH)2:8H2O
  Ba2V2O7:2H2O    -19.82     -3.95   15.87  Ba2V2O7:2H2O
  Ba3(AsO4)2       10.51      1.60   -8.91  Ba3(AsO4)2
  Ba3(VO4)2:4H2O  -33.52     -0.58   32.94  Ba3(VO4)2:4H2O
  BaCrO4          -37.72    -47.39   -9.67  BaCrO4
  BaMoO4           -3.92    -10.88   -6.96  BaMoO4
  Barite            3.93     -6.05   -9.98  BaSO4
  Birnessite      -26.02     -7.92   18.09  MnO2
  Bixbyite        -31.80    -32.45   -0.64  Mn2O3
  Boehmite         -1.16      7.42    8.58  AlOOH
  Brochantite     -19.63     -4.41   15.22  Cu4(OH)6SO4
  Brucite          -9.80      7.04   16.84  Mg(OH)2
  Ca(VO3)2        -10.44     -4.78    5.66  Ca(VO3)2
  Ca2V2O7         -15.62      1.88   17.50  Ca2V2O7
  Ca2V2O7:2H2O    -20.41      1.14   21.55  Ca2V2O7:2H2O
  Ca3(AsO4)2:4H2O -14.53      7.77   22.30  Ca3(AsO4)2:4H2O
  Ca3(VO4)2       -30.43      8.53   38.96  Ca3(VO4)2
  Ca3(VO4)2:4H2O  -32.80      7.06   39.86  Ca3(VO4)2:4H2O
  Ca3Sb2         -231.73    -88.76  142.97  Ca3Sb2
  CaCrO4          -42.58    -44.84   -2.27  CaCrO4
  Calcite           0.30     -8.18   -8.48  CaCO3
  CaMoO4           -0.39     -8.34   -7.95  CaMoO4
  Celestite         1.96     -4.66   -6.62  SrSO4
  Cerussite        -0.70    -13.83  -13.13  PbCO3
  CH4(g)          -40.91    -81.95  -41.05  CH4
  Chalcanthite     -7.64    -10.28   -2.64  CuSO4:5H2O
  Chalcedony        3.86      0.31   -3.55  SiO2
  Chrysotile      -10.09     22.11   32.20  Mg3Si2O5(OH)4
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Claudetite       -9.16    -12.23   -3.06  As4O6
CO2(g)            3.31    -14.83  -18.15  CO2
Cotunnite       -10.18    -14.96   -4.78  PbCl2
Cr(OH)2         -25.55    -14.73   10.82  Cr(OH)2
Cr(OH)3         -10.90     -9.56    1.34  Cr(OH)3
Cr(OH)3(am)      -8.81     -9.56   -0.75  Cr(OH)3
Cr2O3           -15.67    -18.02   -2.36  Cr2O3
CrCl2           -44.42    -30.33   14.09  CrCl2
CrCl3           -48.07    -32.96   15.11  CrCl3
Cristobalite      3.66      0.31   -3.35  SiO2
Crmetal         -61.44    -30.96   30.48  Cr
CrO3            -48.28    -51.49   -3.21  CrO3
Cu(OH)2          -7.33      1.35    8.67  Cu(OH)2
Cu(SbO3)2       -19.44     25.77   45.21  Cu(SbO3)2
Cu2Sb:3H2O      -22.75    -57.64  -34.88  Cu2Sb:3H2O
Cu2SO4          -16.00    -17.95   -1.95  Cu2SO4
Cu3(AsO4)2:2H2O -12.41     -6.31    6.10  Cu3(AsO4)2:2H2O
Cu3Sb           -23.45    -66.04  -42.59  Cu3Sb
CuCO3            -1.62    -13.12  -11.50  CuCO3
CuCrO4          -44.34    -49.78   -5.44  CuCrO4
Cumetal          -3.44    -12.19   -8.76  Cu
CuMoO4           -0.20    -13.27  -13.08  CuMoO4
CuOCuSO4        -17.04     -6.73   10.30  CuOCuSO4
Cupricferrite    -6.87     -0.88    5.99  CuFe2O4
Cuprite          -6.39     -7.79   -1.41  Cu2O
Cuprousferrite    3.72     -5.19   -8.92  CuFeO2
CuSO4           -11.39     -8.45    2.94  CuSO4
Diaspore          0.54      7.42    6.87  AlOOH
Dolomite(disordered)   0.93    -15.61  -16.54  CaMg(CO3)2
Dolomite(ordered)   1.48    -15.61  -17.09  CaMg(CO3)2
Epsomite         -3.19     -5.31   -2.13  MgSO4:7H2O
Fe(OH)2         -10.49      3.07   13.56  Fe(OH)2
Fe(OH)2.7Cl.3    -1.15     -4.19   -3.04  Fe(OH)2.7Cl.3
Fe(VO3)2         -4.27     -7.99   -3.72  Fe(VO3)2
Fe2(SO4)3       -29.34    -33.07   -3.73  Fe2(SO4)3
Fe3(OH)8        -20.85     -0.62   20.22  Fe3(OH)8
FeAsO4:2H2O      -7.79     -7.39    0.40  FeAsO4:2H2O
FeCr2O4         -21.79    -14.59    7.20  FeCr2O4
FeMoO4           -1.46    -11.55  -10.09  FeMoO4
Ferrihydrite     -5.04     -1.85    3.19  Fe(OH)3
Gibbsite         -1.24      7.05    8.29  Al(OH)3
Goethite         -1.97     -1.48    0.49  FeOOH
Greenalite      -10.62     10.19   20.81  Fe3Si2O5(OH)4
Gypsum            0.37     -4.24   -4.61  CaSO4:2H2O
H-Jarosite      -13.76    -25.86  -12.10  (H3O)Fe3(SO4)2(OH)6
H2MoO4           -2.48    -15.35  -12.88  H2MoO4
Halite           -5.53     -3.93    1.60  NaCl
Halloysite        5.51     15.09    9.57  Al2Si2O5(OH)4
Hausmannite     -41.95     19.08   61.03  Mn3O4
Hematite         -1.18     -2.60   -1.42  Fe2O3
Hercynite        -4.26     18.64   22.89  FeAl2O4
Huntite          -0.49    -30.46  -29.97  CaMg3(CO3)4
Hydrocerussite   -8.26    -27.03  -18.77  Pb3(OH)2(CO3)2
Hydromagnesite  -15.35    -24.12   -8.77  Mg5(CO3)4(OH)2:4H2O
K-Alum           -8.63    -13.80   -5.17  KAl(SO4)2:12H2O
K-Jarosite       -7.20    -22.00  -14.80  KFe3(SO4)2(OH)6
K2Cr2O7         -79.13    -96.38  -17.24  K2Cr2O7
K2CrO4          -44.37    -44.88   -0.51  K2CrO4
K2MoO4          -11.64     -8.38    3.26  K2MoO4
Kaolinite         7.65     15.09    7.43  Al2Si2O5(OH)4
Langite         -22.26     -4.77   17.49  Cu4(OH)6SO4:H2O
Larnakite        -7.73     -8.16   -0.43  PbO:PbSO4
Laurionite       -7.79     -7.16    0.62  PbOHCl
Lepidocrocite    -2.85     -1.48    1.37  FeOOH
Li2CrO4         -51.39    -46.53    4.86  Li2CrO4
Li2MoO4         -12.47    -10.03    2.44  Li2MoO4
Lime            -26.05      6.65   32.70  CaO
Litharge        -11.69      1.00   12.69  PbO
Maghemite        -8.98     -2.60    6.39  Fe2O3
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Magnesioferrite -12.05      4.81   16.86  Fe2MgO4
Magnesite         0.04     -7.42   -7.46  MgCO3
Magnetite        -2.56      0.84    3.40  Fe3O4
Malachite        -6.47    -11.77   -5.31  Cu2(OH)2CO3
Manganite       -16.40      8.94   25.34  MnOOH
Massicot        -11.89      1.00   12.89  PbO
Melanothallite  -20.51    -14.25    6.26  CuCl2
Melanterite      -7.08     -9.29   -2.21  FeSO4:7H2O
Mg(OH)2(active) -11.75      7.04   18.79  Mg(OH)2
Mg(VO3)2        -15.30     -4.02   11.28  Mg(VO3)2
Mg2Sb3         -181.44   -106.76   74.68  Mg2Sb3
Mg2V2O7         -22.97      3.39   26.36  Mg2V2O7
MgCr2O4         -26.82    -10.61   16.20  MgCr2O4
MgCrO4          -49.46    -44.08    5.38  MgCrO4
MgMoO4           -5.73     -7.58   -1.85  MgMoO4
Minium          -53.93     19.59   73.52  Pb3O4
Mirabilite       -4.60     -5.71   -1.11  Na2SO4:10H2O
Mn(VO3)2        -15.50    -10.60    4.90  Mn(VO3)2
Mn2(SO4)3       -57.21    -62.92   -5.71  Mn2(SO4)3
Mn2Sb          -122.07    -61.00   61.08  Mn2Sb
Mn3(AsO4)2:8H2O -23.66    -11.16   12.50  Mn3(AsO4)2:8H2O
MnCl2:4H2O      -19.31    -16.60    2.72  MnCl2:4H2O
MnSb            -67.67    -70.58   -2.91  MnSb
MnSO4           -11.91     -9.33    2.58  MnSO4
MoO3             -6.99    -14.99   -8.00  MoO3
Na-Jarosite     -10.06    -21.26  -11.20  NaFe3(SO4)2(OH)6
Na2Cr2O7        -84.99    -94.88   -9.90  Na2Cr2O7
Na2CrO4         -46.32    -43.39    2.93  Na2CrO4
Na2Mo2O7         -5.27    -21.87  -16.60  Na2Mo2O7
Na2MoO4          -8.37     -6.88    1.49  Na2MoO4
Na2MoO4:2H2O     -8.84     -7.61    1.22  Na2MoO4:2H2O
Na3Sb          -136.65    -42.20   94.45  Na3Sb
Na3VO4          -30.24      6.45   36.68  Na3VO4
Na4V2O7         -32.62      4.78   37.40  Na4V2O7
Nantokite        -5.15    -11.88   -6.73  CuCl
NaSb            -56.87    -33.71   23.17  NaSb
Natron           -9.08    -10.39   -1.31  Na2CO3:10H2O
NaVO3            -5.52     -1.66    3.86  NaVO3
Nesquehonite     -3.85     -8.52   -4.67  MgCO3:3H2O
Nsutite         -25.43     -7.92   17.50  MnO2
O2(g)           -49.90     33.19   83.09  O2
Pb(OH)2          -7.52      0.63    8.15  Pb(OH)2
Pb10(OH)6O(CO3)6 -71.34     -80.10    -8.76  Pb10(OH)6O(CO3)6
Pb2(OH)3Cl      -15.32     -6.53    8.79  Pb2(OH)3Cl
Pb2O(OH)2       -24.56      1.63   26.19  Pb2O(OH)2
Pb2O3           -42.44     18.60   61.04  Pb2O3
Pb2OCO3         -12.28    -12.83   -0.56  Pb2OCO3
Pb2V2O7          -7.53     -9.43   -1.90  Pb2V2O7
Pb3(AsO4)2      -13.52     -7.72    5.80  Pb3(AsO4)2
Pb3(VO4)2       -14.57     -8.43    6.14  Pb3(VO4)2
Pb3O2CO3        -22.85    -11.83   11.02  Pb3O2CO3
Pb3O2SO4        -17.85     -7.16   10.69  Pb3O2SO4
Pb4(OH)6SO4     -28.36     -7.26   21.10  Pb4(OH)6SO4
Pb4O3SO4        -28.04     -6.16   21.88  Pb4O3SO4
PbCrO4          -37.89    -50.49  -12.60  PbCrO4
Pbmetal         -19.84    -15.60    4.25  Pb
PbMoO4            1.63    -13.99  -15.62  PbMoO4
PbO:0.3H2O      -12.10      0.88   12.98  PbO:0.33H2O
Periclase       -14.18      7.41   21.58  MgO
Phosgenite       -8.99    -28.80  -19.81  PbCl2:PbCO3
Plattnerite     -32.00     17.60   49.60  PbO2
Portlandite     -16.52      6.28   22.80  Ca(OH)2
Pyrochroite     -14.73      0.46   15.19  Mn(OH)2
Pyrolusite      -23.95     17.43   41.38  MnO2
Quartz            4.31      0.31   -4.00  SiO2
Rhodochrosite    -3.42    -14.00  -10.58  MnCO3
Sb(OH)3           1.99     -5.11   -7.11  Sb(OH)3
Sb2O4             4.06      7.47    3.40  Sb2O4
Sb2O5           -14.89    -24.56   -9.67  Sb2O5
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  Sb4O6(cubic)     -0.00    -18.26  -18.26  Sb4O6
  Sb4O6(orth)      -0.36    -18.26  -17.90  Sb4O6
  SbCl3           -29.08    -28.51    0.57  SbCl3
  Sbmetal         -17.77    -29.46  -11.69  Sb
  SbO2              7.25    -20.58  -27.82  SbO2
  Senarmontite      3.23     -9.13  -12.37  Sb2O3
  Sepiolite        -1.30     14.46   15.76  Mg2Si3O7.5OH:3H2O
  Sepiolite(A)     -4.32     14.46   18.78  Mg2Si3O7.5OH:3H2O
  Siderite         -1.16    -11.40  -10.24  FeCO3
  SiO2(am-gel)      3.02      0.31   -2.71  SiO2
  SiO2(am-ppt)      3.05      0.31   -2.74  SiO2
  Spinel          -14.24     22.61   36.85  MgAl2O4
  SrCrO4          -41.34    -45.99   -4.65  SrCrO4
  Strontianite     -0.06     -9.33   -9.27  SrCO3
  Tenorite         -5.93      1.71    7.64  CuO
  Thenardite       -2.37     -2.05    0.32  Na2SO4
  Thermonatrite    -7.73     -7.09    0.64  Na2CO3:H2O
  V(OH)3           -7.85     -0.26    7.59  V(OH)3
  V2O5            -10.07    -11.43   -1.36  V2O5
  V3O5             -9.76     -7.92    1.84  V3O5
  V4O7            -12.22     -5.03    7.19  V4O7
  V6O13            -6.61    -67.47  -60.86  V6O13
  Valentinite      -0.65     -9.13   -8.48  Sb2O3
  VCl2            -42.85    -23.97   18.87  VCl2
  VCl3            -47.09    -23.65   23.43  VCl3
  Vmetal          -68.63    -24.61   44.03  V
  VO              -22.76     -8.01   14.76  VO
  VO(OH)2          -2.62      2.53    5.15  VO(OH)2
  VO2Cl           -16.54    -13.69    2.84  VO2Cl
  VOCl            -18.84     -7.69   11.15  VOCl
  VOCl2           -25.83    -13.07   12.76  VOCl2
  VOSO4           -10.88     -7.27    3.61  VOSO4
  Witherite        -2.16    -10.73   -8.57  BaCO3

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

Initial solution 2.	WSEEPAGE2-alk% KIN ORT

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

	Elements           Molality       Moles

	Al                2.348e-03   2.348e-03
	Alkalinity        1.237e+00   1.237e+00
	As                1.348e-03   1.348e-03
	Ba                2.452e-04   2.452e-04
	Ca                2.212e-01   2.212e-01
	Cl                2.361e-04   2.361e-04
	Cr                1.600e-07   1.600e-07
	Cu                1.561e-05   1.561e-05
	Fe                2.105e-03   2.105e-03
	K                 1.467e-01   1.467e-01
	Li                2.021e-02   2.021e-02
	Mg                9.018e-01   9.018e-01
	Mn                5.262e-06   5.262e-06
	Mo                7.548e-04   7.548e-04
	Na                9.082e-01   9.082e-01
	Pb                4.839e-05   4.839e-05
	S(6)              6.135e-01   6.135e-01
	Sb                6.204e-05   6.204e-05
	Si                2.700e-01   2.700e-01
	Sr                1.375e-02   1.375e-02
	V                 1.041e-03   1.041e-03

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

                                       pH  =   4.452
                                       pe  =   4.000
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                      Activity of water  =   0.479
              Ionic strength (mol/kgw)  =   1.433e+00
                     Mass of water (kg)  =   1.000e+00
               Total carbon (mol/kg)  =   2.883e+01
                  Total CO2 (mol/kg)  =   2.883e+01
                      Temperature (°C)  =  25.00
              Electrical balance (eq)  =   8.947e-01
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  36.14
                            Iterations  =  56 (124 overall)
                               Total H  = 1.685122e+02
                               Total O  = 1.455285e+02

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

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

   H+              4.039e-05   3.529e-05    -4.394    -4.452    -0.059      0.00
   OH-             2.468e-10   1.366e-10    -9.608    -9.865    -0.257     (0)
   H2O             5.551e+01   4.787e-01     1.744    -0.320     0.000     18.07
Al           2.348e-03
   AlSO4+          1.829e-03   1.101e-03    -2.738    -2.958    -0.220     (0)
   Al(SO4)2-       4.951e-04   2.980e-04    -3.305    -3.526    -0.220     (0)
   Al+3            1.891e-05   5.617e-06    -4.723    -5.251    -0.527     (0)
   AlOH+2          4.643e-06   7.671e-07    -5.333    -6.115    -0.782     (0)
   Al(OH)2+        1.305e-07   8.321e-08    -6.884    -7.080    -0.195     (0)
   AlMo6O21-3      1.790e-09   5.717e-15    -8.747   -14.243    -5.496     (0)
   Al(OH)3         2.267e-10   2.267e-10    -9.644    -9.644     0.000     (0)
   Al(OH)4-        6.476e-12   3.898e-12   -11.189   -11.409    -0.220     (0)
As(3)        2.740e-04
   H3AsO3          2.740e-04   2.740e-04    -3.562    -3.562     0.000     (0)
   H4AsO3+         1.955e-08   4.791e-09    -7.709    -8.320    -0.611     (0)
   H2AsO3-         1.624e-08   3.981e-09    -7.789    -8.400    -0.611     (0)
   HAsO3-2         2.850e-14   1.029e-16   -13.545   -15.988    -2.443     (0)
   AsO3-3          3.518e-20   1.124e-25   -19.454   -24.949    -5.496     (0)
As(5)        1.074e-03
   H2AsO4-         8.858e-04   2.171e-04    -3.053    -3.663    -0.611     (0)
   HAsO4-2         1.869e-04   6.745e-07    -3.728    -6.171    -2.443     (0)
   H3AsO4          9.573e-07   1.332e-06    -6.019    -5.876     0.143     (0)
   AsO4-3          1.892e-08   6.043e-14    -7.723   -13.219    -5.496     (0)
Ba           2.452e-04
   BaHCO3+         1.830e-04   1.204e-04    -3.738    -3.919    -0.182     (0)
   Ba+2            6.222e-05   3.628e-05    -4.206    -4.440    -0.234     (0)
   BaCO3           8.589e-09   8.589e-09    -8.066    -8.066     0.000     (0)
   BaOH+           3.474e-14   2.163e-14   -13.459   -13.665    -0.206     (0)
C(4)         2.883e+01
   H2CO3           2.759e+01   2.759e+01     1.441     1.441     0.000     (0)
   HCO3-           5.451e-01   3.476e-01    -0.263    -0.459    -0.195     (0)
   MgHCO3+         4.448e-01   2.575e-01    -0.352    -0.589    -0.237     (0)
   CaHCO3+         1.255e-01   8.259e-02    -0.901    -1.083    -0.182     (0)
   NaHCO3          1.143e-01   1.143e-01    -0.942    -0.942     0.000     (0)
   SrHCO3+         7.686e-03   5.058e-03    -2.114    -2.296    -0.182     (0)
   BaHCO3+         1.830e-04   1.204e-04    -3.738    -3.919    -0.182     (0)
   FeHCO3+         4.829e-05   3.178e-05    -4.316    -4.498    -0.182     (0)
   PbHCO3+         3.204e-05   7.854e-06    -4.494    -5.105    -0.611     (0)
   MgCO3           2.781e-05   2.781e-05    -4.556    -4.556     0.000     (0)
   CuHCO3+         1.385e-05   3.395e-06    -4.859    -5.469    -0.611     (0)
   CaCO3           9.337e-06   9.337e-06    -5.030    -5.030     0.000     (0)
   NaCO3-          7.887e-06   5.029e-06    -5.103    -5.299    -0.195     (0)
   CO3-2           7.918e-07   4.617e-07    -6.101    -6.336    -0.234     (0)
   CuCO3           4.208e-07   4.208e-07    -6.376    -6.376     0.000     (0)
   SrCO3           2.675e-07   2.675e-07    -6.573    -6.573     0.000     (0)
   MnHCO3+         2.003e-07   1.247e-07    -6.698    -6.904    -0.206     (0)
   Cu(CO3)2-2      1.449e-07   5.229e-10    -6.839    -9.282    -2.443     (0)
   PbCO3           4.221e-08   4.221e-08    -7.375    -7.375     0.000     (0)
   Pb(CO3)2-2      1.557e-08   5.620e-11    -7.808   -10.250    -2.443     (0)
   BaCO3           8.589e-09   8.589e-09    -8.066    -8.066     0.000     (0)
Ca           2.212e-01
   CaHCO3+         1.255e-01   8.259e-02    -0.901    -1.083    -0.182     (0)
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   CaSO4           7.383e-02   7.383e-02    -1.132    -1.132     0.000     (0)
   Ca+2            2.189e-02   1.276e-02    -1.660    -1.894    -0.234     (0)
   CaCO3           9.337e-06   9.337e-06    -5.030    -5.030     0.000     (0)
   CaOH+           5.284e-11   3.477e-11   -10.277   -10.459    -0.182     (0)
Cl            2.361e-04
   Cl-             2.361e-04   2.063e-04    -3.627    -3.686    -0.059     (0)
   VOCl+           4.471e-09   1.096e-09    -8.350    -8.960    -0.611     (0)
   CuCl            1.969e-09   1.969e-09    -8.706    -8.706     0.000     (0)
   PbCl+           9.081e-10   2.226e-10    -9.042    -9.653    -0.611     (0)
   CuCl2-          1.466e-10   8.486e-11    -9.834   -10.071    -0.237     (0)
   CuCl+           8.741e-11   5.061e-11   -10.058   -10.296    -0.237     (0)
   MnCl+           7.500e-12   4.669e-12   -11.125   -11.331    -0.206     (0)
   PbCl2           2.051e-13   2.051e-13   -12.688   -12.688     0.000     (0)
   CrCl+2          3.767e-14   1.360e-16   -13.424   -15.867    -2.443     (0)
   CuCl3-2         2.492e-14   3.742e-15   -13.603   -14.427    -0.823     (0)
   CuCl2           3.620e-15   3.620e-15   -14.441   -14.441     0.000     (0)
   MnCl2           1.360e-15   1.360e-15   -14.866   -14.866     0.000     (0)
   FeCl+2          2.798e-16   4.203e-17   -15.553   -16.376    -0.823     (0)
   PbCl3-          6.871e-17   1.684e-17   -16.163   -16.774    -0.611     (0)
   PbCl4-2         4.399e-19   1.588e-21   -18.357   -20.799    -2.443     (0)
   MnCl3-          1.242e-19   7.729e-20   -18.906   -19.112    -0.206     (0)
   FeCl2+          6.220e-20   3.872e-20   -19.206   -19.412    -0.206     (0)
   CuCl3-          1.203e-20   6.968e-21   -19.920   -20.157    -0.237     (0)
   CrCl2+          1.086e-20   2.661e-21   -19.964   -20.575    -0.611     (0)
   CrOHCl2         7.280e-23   7.280e-23   -22.138   -22.138     0.000     (0)
   FeCl3           7.987e-25   7.987e-25   -24.098   -24.098     0.000     (0)
   CuCl4-2         4.797e-26   7.204e-27   -25.319   -26.142    -0.823     (0)
   CrO3Cl-         0.000e+00   0.000e+00   -47.250   -47.861    -0.611     (0)
Cr(2)         3.371e-21
   Cr+2            3.371e-21   1.217e-23   -20.472   -22.915    -2.443     (0)
Cr(3)         1.600e-07
   Cr+3            1.595e-07   5.093e-13    -6.797   -12.293    -5.496     (0)
   Cr(OH)+2        4.216e-10   1.522e-12    -9.375   -11.818    -2.443     (0)
   CrSO4+          1.225e-10   3.004e-11    -9.912   -10.522    -0.611     (0)
   CrOHSO4         9.120e-12   9.120e-12   -11.040   -11.040     0.000     (0)
   Cr(OH)2+        1.032e-13   2.529e-14   -12.986   -13.597    -0.611     (0)
   CrCl+2          3.767e-14   1.360e-16   -13.424   -15.867    -2.443     (0)
   Cr(OH)3         1.297e-18   1.297e-18   -17.887   -17.887     0.000     (0)
   Cr2(OH)2SO4+2   3.475e-19   1.254e-21   -18.459   -20.902    -2.443     (0)
   CrCl2+          1.086e-20   2.661e-21   -19.964   -20.575    -0.611     (0)
   Cr2(OH)2(SO4)2   1.882e-21   1.882e-21   -20.725   -20.725     0.000     (0)
   CrO2-           1.488e-22   3.647e-23   -21.827   -22.438    -0.611     (0)
   CrOHCl2         7.280e-23   7.280e-23   -22.138   -22.138     0.000     (0)
   Cr(OH)4-        2.877e-23   7.053e-24   -22.541   -23.152    -0.611     (0)
Cr(6)         0.000e+00
   HCrO4-          0.000e+00   0.000e+00   -40.231   -40.842    -0.611     (0)
   CrO3SO4-2       0.000e+00   0.000e+00   -41.645   -44.088    -2.443     (0)
   NaCrO4-         0.000e+00   0.000e+00   -41.825   -42.436    -0.611     (0)
   CrO4-2          0.000e+00   0.000e+00   -42.665   -42.899    -0.234     (0)
   KCrO4-          0.000e+00   0.000e+00   -42.706   -43.317    -0.611     (0)
   H2CrO4          0.000e+00   0.000e+00   -45.385   -45.385     0.000     (0)
   CrO3Cl-         0.000e+00   0.000e+00   -47.250   -47.861    -0.611     (0)
   Cr2O7-2         0.000e+00   0.000e+00   -77.381   -79.823    -2.443     (0)
Cu(1)         3.305e-08
   Cu+             3.093e-08   7.582e-09    -7.510    -8.120    -0.611     (0)
   CuCl            1.969e-09   1.969e-09    -8.706    -8.706     0.000     (0)
   CuCl2-          1.466e-10   8.486e-11    -9.834   -10.071    -0.237     (0)
   CuCl3-2         2.492e-14   3.742e-15   -13.603   -14.427    -0.823     (0)
Cu(2)         1.558e-05
   CuHCO3+         1.385e-05   3.395e-06    -4.859    -5.469    -0.611     (0)
   CuSO4           8.957e-07   8.957e-07    -6.048    -6.048     0.000     (0)
   CuCO3           4.208e-07   4.208e-07    -6.376    -6.376     0.000     (0)
   Cu+2            2.655e-07   1.548e-07    -6.576    -6.810    -0.234     (0)
   Cu(CO3)2-2      1.449e-07   5.229e-10    -6.839    -9.282    -2.443     (0)
   CuOH+           1.155e-10   6.685e-11    -9.938   -10.175    -0.237     (0)
   CuCl+           8.741e-11   5.061e-11   -10.058   -10.296    -0.237     (0)
   Cu2(OH)2+2      3.110e-14   1.123e-16   -13.507   -15.950    -2.443     (0)
   CuCl2           3.620e-15   3.620e-15   -14.441   -14.441     0.000     (0)
   Cu(OH)2         1.822e-15   1.822e-15   -14.740   -14.740     0.000     (0)
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   CuCl3-          1.203e-20   6.968e-21  -19.920   -20.157    -0.237      (0)
   Cu(OH)3-        2.082e-21   5.103e-22  -20.682   -21.292    -0.611      (0)
   CuCl4-2         4.797e-26   7.204e-27  -25.319   -26.142    -0.823      (0)
   Cu(OH)4-2       1.519e-28   5.485e-31  -27.818   -30.261    -2.443      (0)
Fe(2)           2.105e-03
   Fe+2            2.012e-03   7.262e-06   -2.696    -5.139    -2.443      (0)
   FeHCO3+         4.829e-05   3.178e-05   -4.316    -4.498    -0.182      (0)
   FeSO4           4.502e-05   4.502e-05   -4.347    -4.347     0.000      (0)
   FeOH+           6.342e-11   3.948e-11  -10.198   -10.404    -0.206      (0)
   Fe(OH)2         4.283e-18   4.283e-18  -17.368   -17.368     0.000      (0)
   Fe(OH)3-        2.971e-22   1.850e-22  -21.527   -21.733    -0.206      (0)
Fe(3)           6.098e-11
   Fe(OH)2+        4.957e-11   3.160e-11  -10.305   -10.500    -0.195      (0)
   Fe(SO4)2-       4.211e-12   1.032e-12  -11.376   -11.986    -0.611      (0)
   FeOH+2          3.961e-12   5.949e-13  -11.402   -12.226    -0.823      (0)
   FeSO4+          3.071e-12   1.912e-12  -11.513   -11.719    -0.206      (0)
   Fe2(OH)2+4      6.902e-14   1.172e-23  -13.161   -22.931    -9.770      (0)
   Fe+3            2.271e-14   6.746e-15  -13.644   -14.171    -0.527      (0)
   Fe(OH)3         4.635e-15   4.635e-15  -14.334   -14.334     0.000      (0)
   FeCl+2          2.798e-16   4.203e-17  -15.553   -16.376    -0.823      (0)
   Fe3(OH)4+5      9.873e-18   5.353e-33  -17.006   -32.271   -15.266      (0)
   Fe(OH)4-        9.245e-20   5.894e-20  -19.034   -19.230    -0.195      (0)
   FeCl2+          6.220e-20   3.872e-20  -19.206   -19.412    -0.206      (0)
   FeCl3           7.987e-25   7.987e-25  -24.098   -24.098     0.000      (0)
H(0)            1.268e-20
   H2              6.340e-21   8.819e-21  -20.198   -20.055     0.143      (0)
K               1.467e-01
   K+              1.178e-01   1.029e-01   -0.929    -0.987    -0.059      (0)
   KSO4-           2.887e-02   1.841e-02   -1.540    -1.735    -0.195      (0)
   KCrO4-          0.000e+00   0.000e+00  -42.706   -43.317    -0.611      (0)
Li              2.021e-02
   Li+             1.750e-02   1.529e-02   -1.757    -1.816    -0.059      (0)
   LiSO4-          2.708e-03   1.686e-03   -2.567    -2.773    -0.206      (0)
Mg              9.018e-01
   MgHCO3+         4.448e-01   2.575e-01   -0.352    -0.589    -0.237      (0)
   MgSO4           3.328e-01   3.328e-01   -0.478    -0.478     0.000      (0)
   Mg+2            1.242e-01   7.241e-02   -0.906    -1.140    -0.234      (0)
   MgCO3           2.781e-05   2.781e-05   -4.556    -4.556     0.000      (0)
   MgOH+           5.846e-09   3.937e-09   -8.233    -8.405    -0.172      (0)
Mn(2)           5.262e-06
   Mn+2            4.981e-06   1.798e-08   -5.303    -7.745    -2.443      (0)
   MnHCO3+         2.003e-07   1.247e-07   -6.698    -6.904    -0.206      (0)
   MnSO4           8.075e-08   8.075e-08   -7.093    -7.093     0.000      (0)
   MnCl+           7.500e-12   4.669e-12  -11.125   -11.331    -0.206      (0)
   MnOH+           9.908e-15   6.168e-15  -14.004   -14.210    -0.206      (0)
   MnCl2           1.360e-15   1.360e-15  -14.866   -14.866     0.000      (0)
   MnCl3-          1.242e-19   7.729e-20  -18.906   -19.112    -0.206      (0)
   Mn(OH)3-        1.142e-30   7.109e-31  -29.942   -30.148    -0.206      (0)
   Mn(OH)4-2       2.087e-39   3.134e-40  -38.680   -39.504    -0.823      (0)
Mn(3)           2.704e-29
   Mn+3            2.704e-29   8.031e-30  -28.568   -29.095    -0.527      (0)
Mn(6)           0.000e+00
   MnO4-2          0.000e+00   0.000e+00  -75.005   -75.829    -0.823      (0)
Mn(7)           0.000e+00
   MnO4-           0.000e+00   0.000e+00  -80.921   -81.201    -0.280      (0)
Mo              7.548e-04
   Mo7O24-6        1.075e-04   1.119e-26   -3.968   -25.951   -21.983      (0)
   HMoO4-          1.217e-06   2.983e-07   -5.915    -6.525    -0.611      (0)
   MoO4-2          7.286e-07   4.248e-07   -6.138    -6.372    -0.234      (0)
   H2MoO4          7.712e-08   7.712e-08   -7.113    -7.113     0.000      (0)
   AlMo6O21-3      1.790e-09   5.717e-15   -8.747   -14.243    -5.496      (0)
   HMo7O24-5       1.774e-09   9.620e-25   -8.751   -24.017   -15.266      (0)
   H2Mo7O24-4      1.211e-14   2.056e-24  -13.917   -23.687    -9.770      (0)
   H3Mo7O24-3      4.004e-20   1.279e-25  -19.398   -24.893    -5.496      (0)
Na              9.082e-01
   Na+             6.694e-01   5.850e-01   -0.174    -0.233    -0.059      (0)
   NaSO4-          1.244e-01   7.934e-02   -0.905    -1.101    -0.195      (0)
   NaHCO3          1.143e-01   1.143e-01   -0.942    -0.942     0.000      (0)
   NaCO3-          7.887e-06   5.029e-06   -5.103    -5.299    -0.195      (0)
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   NaCrO4-          0.000e+00   0.000e+00   -41.825   -42.436    -0.611     (0)
O(0)          0.000e+00
   O2               0.000e+00   0.000e+00   -52.969   -52.826     0.143     (0)
Pb            4.839e-05
   PbHCO3+          3.204e-05   7.854e-06    -4.494    -5.105    -0.611     (0)
   Pb(SO4)2-2       1.586e-05   5.725e-08    -4.800    -7.242    -2.443     (0)
   PbSO4            3.762e-07   3.762e-07    -6.425    -6.425     0.000     (0)
   Pb+2             5.216e-08   3.041e-08    -7.283    -7.517    -0.234     (0)
   PbCO3            4.221e-08   4.221e-08    -7.375    -7.375     0.000     (0)
   Pb(CO3)2-2       1.557e-08   5.620e-11    -7.808   -10.250    -2.443     (0)
   PbCl+            9.081e-10   2.226e-10    -9.042    -9.653    -0.611     (0)
   PbOH+            4.256e-11   1.043e-11   -10.371   -10.982    -0.611     (0)
   Pb2OH+3          1.575e-12   5.029e-18   -11.803   -17.299    -5.496     (0)
   PbCl2            2.051e-13   2.051e-13   -12.688   -12.688     0.000     (0)
   PbCl3-           6.871e-17   1.684e-17   -16.163   -16.774    -0.611     (0)
   Pb(OH)2          4.505e-17   4.505e-17   -16.346   -16.346     0.000     (0)
   PbCl4-2          4.399e-19   1.588e-21   -18.357   -20.799    -2.443     (0)
   Pb(OH)3-         2.510e-23   6.153e-24   -22.600   -23.211    -0.611     (0)
   Pb4(OH)4+4       1.753e-24   2.976e-34   -23.756   -33.526    -9.770     (0)
   Pb3(OH)4+2       3.412e-28   1.232e-30   -27.467   -29.909    -2.443     (0)
   Pb(OH)4-2        5.701e-29   2.058e-31   -28.244   -30.687    -2.443     (0)
S(6)          6.135e-01
   MgSO4            3.328e-01   3.328e-01    -0.478    -0.478     0.000     (0)
   NaSO4-           1.244e-01   7.934e-02    -0.905    -1.101    -0.195     (0)
   CaSO4            7.383e-02   7.383e-02    -1.132    -1.132     0.000     (0)
   SO4-2            4.332e-02   2.526e-02    -1.363    -1.598    -0.234     (0)
   KSO4-            2.887e-02   1.841e-02    -1.540    -1.735    -0.195     (0)
   SrSO4            4.522e-03   4.522e-03    -2.345    -2.345     0.000     (0)
   LiSO4-           2.708e-03   1.686e-03    -2.567    -2.773    -0.206     (0)
   AlSO4+           1.829e-03   1.101e-03    -2.738    -2.958    -0.220     (0)
   Al(SO4)2-        4.951e-04   2.980e-04    -3.305    -3.526    -0.220     (0)
   HSO4-            1.447e-04   8.711e-05    -3.839    -4.060    -0.220     (0)
   FeSO4            4.502e-05   4.502e-05    -4.347    -4.347     0.000     (0)
   Pb(SO4)2-2       1.586e-05   5.725e-08    -4.800    -7.242    -2.443     (0)
   VOSO4            1.317e-05   1.317e-05    -4.880    -4.880     0.000     (0)
   CuSO4            8.957e-07   8.957e-07    -6.048    -6.048     0.000     (0)
   PbSO4            3.762e-07   3.762e-07    -6.425    -6.425     0.000     (0)
   MnSO4            8.075e-08   8.075e-08    -7.093    -7.093     0.000     (0)
   VO2SO4-          2.238e-10   5.486e-11    -9.650   -10.261    -0.611     (0)
   CrSO4+           1.225e-10   3.004e-11    -9.912   -10.522    -0.611     (0)
   VSO4+            1.190e-11   2.917e-12   -10.924   -11.535    -0.611     (0)
   CrOHSO4          9.120e-12   9.120e-12   -11.040   -11.040     0.000     (0)
   Fe(SO4)2-        4.211e-12   1.032e-12   -11.376   -11.986    -0.611     (0)
   FeSO4+           3.071e-12   1.912e-12   -11.513   -11.719    -0.206     (0)
   Cr2(OH)2SO4+2    3.475e-19   1.254e-21   -18.459   -20.902    -2.443     (0)
   Cr2(OH)2(SO4)2    1.882e-21   1.882e-21   -20.725   -20.725     0.000     (0)
   CrO3SO4-2        0.000e+00   0.000e+00   -41.645   -44.088    -2.443     (0)
Sb(3)         2.729e-05
   HSbO2            1.824e-05   1.824e-05    -4.739    -4.739     0.000     (0)
   Sb(OH)3          8.943e-06   8.943e-06    -5.049    -5.049     0.000     (0)
   Sb(OH)2+         6.533e-08   1.601e-08    -7.185    -7.796    -0.611     (0)
   SbO+             4.705e-08   1.153e-08    -7.327    -7.938    -0.611     (0)
   SbO2-            3.414e-12   8.369e-13   -11.467   -12.077    -0.611     (0)
   Sb(OH)4-         4.483e-13   1.099e-13   -12.348   -12.959    -0.611     (0)
Sb(5)         3.475e-05
   SbO3-            3.475e-05   8.517e-06    -4.459    -5.070    -0.611     (0)
   Sb(OH)6-         1.251e-09   1.093e-09    -8.903    -8.961    -0.059     (0)
   SbO2+            2.593e-14   6.357e-15   -13.586   -14.197    -0.611     (0)
Si            2.700e-01
   H4SiO4           2.700e-01   3.756e-01    -0.569    -0.425     0.143     (0)
   H3SiO4-          2.656e-06   1.538e-06    -5.576    -5.813    -0.237     (0)
   H2SiO4-2         1.664e-14   2.750e-15   -13.779   -14.561    -0.782     (0)
Sr            1.375e-02
   SrHCO3+          7.686e-03   5.058e-03    -2.114    -2.296    -0.182     (0)
   SrSO4            4.522e-03   4.522e-03    -2.345    -2.345     0.000     (0)
   Sr+2             1.539e-03   8.973e-04    -2.813    -3.047    -0.234     (0)
   SrCO3            2.675e-07   2.675e-07    -6.573    -6.573     0.000     (0)
   SrOH+            1.301e-12   8.096e-13   -11.886   -12.092    -0.206     (0)
V(2)          3.321e-19
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   V+2            3.320e-19   1.199e-21   -18.479   -20.921    -2.443     (0)
   VOH+           2.161e-23   5.297e-24   -22.665   -23.276    -0.611     (0)
V(3)         5.029e-04
   V(OH)3         5.028e-04   5.028e-04    -3.299    -3.299     0.000     (0)
   V+3            7.662e-08   2.447e-13    -7.116   -12.611    -5.496     (0)
   VOH+2          4.640e-09   1.675e-11    -8.333   -10.776    -2.443     (0)
   V(OH)2+        9.772e-11   2.395e-11   -10.010   -10.621    -0.611     (0)
   VSO4+          1.190e-11   2.917e-12   -10.924   -11.535    -0.611     (0)
   V2(OH)2+4      1.043e-11   1.770e-21   -10.982   -20.752    -9.770     (0)
   V2(OH)3+3      3.556e-18   1.136e-23   -17.449   -22.945    -5.496     (0)
V(4)         5.380e-04
   VO+2           5.246e-04   1.894e-06    -3.280    -5.723    -2.443     (0)
   VOSO4          1.317e-05   1.317e-05    -4.880    -4.880     0.000     (0)
   V(OH)3+        1.008e-07   2.470e-08    -6.997    -7.607    -0.611     (0)
   H2V2O4+2       3.697e-08   1.334e-10    -7.432    -9.875    -2.443     (0)
   VOCl+          4.471e-09   1.096e-09    -8.350    -8.960    -0.611     (0)
V(5)         4.090e-09
   H2VO4-         3.422e-09   8.387e-10    -8.466    -9.076    -0.611     (0)
   H3VO4          2.960e-10   2.960e-10    -9.529    -9.529     0.000     (0)
   VO2SO4-        2.238e-10   5.486e-11    -9.650   -10.261    -0.611     (0)
   VO2+           1.041e-10   9.098e-11    -9.982   -10.041    -0.059     (0)
   HVO4-2         1.654e-11   5.969e-14   -10.782   -13.224    -2.443     (0)
   H3V2O7-        1.366e-11   3.349e-12   -10.864   -11.475    -0.611     (0)
   HV2O7-3        1.110e-14   3.544e-20   -13.955   -19.451    -5.496     (0)
   V3O9-3         1.764e-15   5.633e-21   -14.754   -20.249    -5.496     (0)
   V2O7-4         1.592e-16   2.703e-26   -15.798   -25.568    -9.770     (0)
   V4O12-4        2.424e-17   4.114e-27   -16.616   -26.386    -9.770     (0)
   VO4-3          2.654e-18   8.476e-24   -17.576   -23.072    -5.496     (0)
   V10O28-6       1.429e-34   0.000e+00   -33.845   -55.828   -21.983     (0)
   HV10O28-5      1.487e-37   0.000e+00   -36.828   -52.093   -15.266     (0)
   H2V10O28-4     0.000e+00   0.000e+00   -41.568   -51.338    -9.770     (0)

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

  Phase               SI** log IAP   log K(298 K,   1 atm)

  Al(OH)3(am)       -3.65      7.15   10.80  Al(OH)3
  Al2(MoO4)3       -31.98    -29.62    2.37  Al2(MoO4)3
  Al2O3             -4.40     15.25   19.65  Al2O3
  Al4(OH)10SO4      -3.98     18.72   22.70  Al4(OH)10SO4
  AlAsO4:2H2O       -3.21      1.59    4.80  AlAsO4:2H2O
  AlOHSO4            0.51     -2.72   -3.23  AlOHSO4
  AlSb            -112.32    -46.70   65.62  AlSb
  Alunite            6.26      4.86   -1.40  KAl3(SO4)2(OH)6
  Anglesite         -1.32     -9.11   -7.79  PbSO4
  Anhydrite          0.87     -3.49   -4.36  CaSO4
  Antlerite        -14.29     -5.50    8.79  Cu3(OH)4SO4
  Aragonite          0.07     -8.23   -8.30  CaCO3
  Arsenolite        -9.57    -12.33   -2.76  As4O6
  Artinite         -10.91     -1.31    9.60  MgCO3:Mg(OH)2:3H2O
  As2O5            -17.50    -10.79    6.71  As2O5
  Atacamite        -12.30     -4.91    7.39  Cu2(OH)3Cl
  Azurite           -7.93    -24.84  -16.91  Cu3(OH)2(CO3)2
  Ba(OH)2:8H2O     -23.13      1.26   24.39  Ba(OH)2:8H2O
  Ba2V2O7:2H2O     -19.72     -3.85   15.87  Ba2V2O7:2H2O
  Ba3(AsO4)2        10.55      1.64   -8.91  Ba3(AsO4)2
  Ba3(VO4)2:4H2O   -33.28     -0.34   32.94  Ba3(VO4)2:4H2O
  BaCrO4           -37.67    -47.34   -9.67  BaCrO4
  BaMoO4            -3.85    -10.81   -6.96  BaMoO4
  Barite             3.94     -6.04   -9.98  BaSO4
  Birnessite       -26.02     -7.93   18.09  MnO2
  Bixbyite         -31.79    -32.44   -0.64  Mn2O3
  Boehmite          -1.11      7.47    8.58  AlOOH
  Brochantite      -19.27     -4.04   15.22  Cu4(OH)6SO4
  Brucite           -9.72      7.12   16.84  Mg(OH)2
  Ca(VO3)2         -10.47     -4.81    5.66  Ca(VO3)2
  Ca2V2O7          -15.62      1.88   17.50  Ca2V2O7
  Ca2V2O7:2H2O     -20.31      1.24   21.55  Ca2V2O7:2H2O
  Ca3(AsO4)2:4H2O -14.30      8.00   22.30  Ca3(AsO4)2:4H2O
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Ca3(VO4)2       -30.39      8.57   38.96  Ca3(VO4)2
Ca3(VO4)2:4H2O  -32.57      7.29   39.86  Ca3(VO4)2:4H2O
Ca3Sb2         -231.55    -88.57  142.97  Ca3Sb2
CaCrO4          -42.53    -44.79   -2.27  CaCrO4
Calcite           0.25     -8.23   -8.48  CaCO3
CaMoO4           -0.32     -8.27   -7.95  CaMoO4
Celestite         1.98     -4.64   -6.62  SrSO4
Cerussite        -0.72    -13.85  -13.13  PbCO3
CH4(g)          -40.85    -81.90  -41.05  CH4
Chalcanthite     -7.37    -10.01   -2.64  CuSO4:5H2O
Chalcedony        3.76      0.21   -3.55  SiO2
Chrysotile      -10.08     22.12   32.20  Mg3Si2O5(OH)4
Claudetite       -9.26    -12.33   -3.06  As4O6
CO2(g)            3.23    -14.92  -18.15  CO2
Cotunnite       -10.11    -14.89   -4.78  PbCl2
Cr(OH)2         -25.47    -14.65   10.82  Cr(OH)2
Cr(OH)3         -10.80     -9.46    1.34  Cr(OH)3
Cr(OH)3(am)      -8.71     -9.46   -0.75  Cr(OH)3
Cr2O3           -15.61    -17.97   -2.36  Cr2O3
CrCl2           -44.38    -30.29   14.09  CrCl2
CrCl3           -48.03    -32.92   15.11  CrCl3
Cristobalite      3.56      0.21   -3.35  SiO2
Crmetal         -61.40    -30.91   30.48  Cr
CrO3            -48.27    -51.48   -3.21  CrO3
Cu(OH)2          -7.22      1.45    8.67  Cu(OH)2
Cu(SbO3)2       -19.40     25.81   45.21  Cu(SbO3)2
Cu2Sb:3H2O      -22.45    -57.34  -34.88  Cu2Sb:3H2O
Cu2SO4          -15.89    -17.84   -1.95  Cu2SO4
Cu3(AsO4)2:2H2O -12.21     -6.11    6.10  Cu3(AsO4)2:2H2O
Cu3Sb           -23.21    -65.81  -42.59  Cu3Sb
CuCO3            -1.65    -13.15  -11.50  CuCO3
CuCrO4          -44.27    -49.71   -5.44  CuCrO4
Cumetal          -3.36    -12.12   -8.76  Cu
CuMoO4           -0.11    -13.18  -13.08  CuMoO4
CuOCuSO4        -16.94     -6.63   10.30  CuOCuSO4
Cupricferrite    -6.80     -0.81    5.99  CuFe2O4
Cuprite          -6.25     -7.66   -1.41  Cu2O
Cuprousferrite    3.80     -5.12   -8.92  CuFeO2
CuSO4           -11.35     -8.41    2.94  CuSO4
Diaspore          0.59      7.47    6.87  AlOOH
Dolomite(disordered)   0.83    -15.71  -16.54  CaMg(CO3)2
Dolomite(ordered)   1.38    -15.71  -17.09  CaMg(CO3)2
Epsomite         -2.85     -4.98   -2.13  MgSO4:7H2O
Fe(OH)2         -10.44      3.13   13.56  Fe(OH)2
Fe(OH)2.7Cl.3    -1.08     -4.12   -3.04  Fe(OH)2.7Cl.3
Fe(VO3)2         -4.33     -8.05   -3.72  Fe(VO3)2
Fe2(SO4)3       -29.40    -33.13   -3.73  Fe2(SO4)3
Fe3(OH)8        -20.64     -0.42   20.22  Fe3(OH)8
FeAsO4:2H2O      -7.73     -7.33    0.40  FeAsO4:2H2O
FeCr2O4         -21.72    -14.52    7.20  FeCr2O4
FeMoO4           -1.42    -11.51  -10.09  FeMoO4
Ferrihydrite     -4.96     -1.77    3.19  Fe(OH)3
Gibbsite         -1.14      7.15    8.29  Al(OH)3
Goethite         -1.94     -1.45    0.49  FeOOH
Greenalite      -10.68     10.13   20.81  Fe3Si2O5(OH)4
Gypsum            0.48     -4.13   -4.61  CaSO4:2H2O
H-Jarosite      -13.59    -25.69  -12.10   (H3O)Fe3(SO4)2(OH)6
H2MoO4           -2.40    -15.28  -12.88  H2MoO4
Halite           -5.52     -3.92    1.60  NaCl
Halloysite        5.47     15.04    9.57  Al2Si2O5(OH)4
Hausmannite     -41.93     19.10   61.03  Mn3O4
Hematite         -1.17     -2.59   -1.42  Fe2O3
Hercynite        -4.19     18.70   22.89  FeAl2O4
Huntite          -0.69    -30.66  -29.97  CaMg3(CO3)4
Hydrocerussite   -8.19    -26.96  -18.77  Pb3(OH)2(CO3)2
Hydromagnesite  -15.29    -24.06   -8.77  Mg5(CO3)4(OH)2:4H2O
K-Alum           -8.10    -13.27   -5.17  KAl(SO4)2:12H2O
K-Jarosite       -7.10    -21.90  -14.80  KFe3(SO4)2(OH)6
K2Cr2O7         -79.12    -96.36  -17.24  K2Cr2O7
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K2CrO4          -44.36    -44.87   -0.51  K2CrO4
K2MoO4          -11.61     -8.35    3.26  K2MoO4
Kaolinite         7.61     15.04    7.43  Al2Si2O5(OH)4
Langite         -21.85     -4.36   17.49  Cu4(OH)6SO4:H2O
Larnakite        -7.61     -8.05   -0.43  PbO:PbSO4
Laurionite       -7.69     -7.07    0.62  PbOHCl
Lepidocrocite    -2.82     -1.45    1.37  FeOOH
Li2CrO4         -51.39    -46.53    4.86  Li2CrO4
Li2MoO4         -12.44    -10.00    2.44  Li2MoO4
Lime            -26.01      6.69   32.70  CaO
Litharge        -11.63      1.07   12.69  PbO
Maghemite        -8.97     -2.59    6.39  Fe2O3
Magnesioferrite -12.00      4.86   16.86  Fe2MgO4
Magnesite        -0.02     -7.48   -7.46  MgCO3
Magnetite        -2.55      0.86    3.40  Fe3O4
Malachite        -6.39    -11.69   -5.31  Cu2(OH)2CO3
Manganite       -16.37      8.97   25.34  MnOOH
Massicot        -11.83      1.07   12.89  PbO
Melanothallite  -20.44    -14.18    6.26  CuCl2
Melanterite      -6.77     -8.98   -2.21  FeSO4:7H2O
Mg(OH)2(active) -11.67      7.12   18.79  Mg(OH)2
Mg(VO3)2        -15.33     -4.05   11.28  Mg(VO3)2
Mg2Sb3         -181.30   -106.62   74.68  Mg2Sb3
Mg2V2O7         -22.97      3.39   26.36  Mg2V2O7
MgCr2O4         -26.73    -10.53   16.20  MgCr2O4
MgCrO4          -49.42    -44.04    5.38  MgCrO4
MgMoO4           -5.66     -7.51   -1.85  MgMoO4
Minium          -53.73     19.79   73.52  Pb3O4
Mirabilite       -4.15     -5.26   -1.11  Na2SO4:10H2O
Mn(VO3)2        -15.56    -10.66    4.90  Mn(VO3)2
Mn2(SO4)3       -57.27    -62.98   -5.71  Mn2(SO4)3
Mn2Sb          -122.02    -60.94   61.08  Mn2Sb
Mn3(AsO4)2:8H2O -23.33    -10.83   12.50  Mn3(AsO4)2:8H2O
MnCl2:4H2O      -19.11    -16.40    2.72  MnCl2:4H2O
MnSb            -67.63    -70.54   -2.91  MnSb
MnSO4           -11.93     -9.34    2.58  MnSO4
MoO3             -6.96    -14.96   -8.00  MoO3
Na-Jarosite      -9.95    -21.15  -11.20  NaFe3(SO4)2(OH)6
Na2Cr2O7        -84.95    -94.85   -9.90  Na2Cr2O7
Na2CrO4         -46.30    -43.36    2.93  Na2CrO4
Na2Mo2O7         -5.20    -21.79  -16.60  Na2Mo2O7
Na2MoO4          -8.33     -6.84    1.49  Na2MoO4
Na2MoO4:2H2O     -8.70     -7.48    1.22  Na2MoO4:2H2O
Na3Sb          -136.60    -42.14   94.45  Na3Sb
Na3VO4          -30.25      6.43   36.68  Na3VO4
Na4V2O7         -32.66      4.74   37.40  Na4V2O7
Nantokite        -5.08    -11.81   -6.73  CuCl
NaSb            -56.84    -33.68   23.17  NaSb
Natron           -8.69    -10.00   -1.31  Na2CO3:10H2O
NaVO3            -5.55     -1.69    3.86  NaVO3
Nesquehonite     -3.77     -8.44   -4.67  MgCO3:3H2O
Nsutite         -25.43     -7.93   17.50  MnO2
O2(g)           -49.92     33.17   83.09  O2
Pb(OH)2          -7.40      0.75    8.15  Pb(OH)2
Pb10(OH)6O(CO3)6 -71.04    -79.80   -8.76   Pb10(OH)6O(CO3)6
Pb2(OH)3Cl      -15.12     -6.32    8.79  Pb2(OH)3Cl
Pb2O(OH)2       -24.37      1.82   26.19  Pb2O(OH)2
Pb2O3           -42.32     18.72   61.04  Pb2O3
Pb2OCO3         -12.23    -12.78   -0.56  Pb2OCO3
Pb2V2O7          -7.46     -9.36   -1.90  Pb2V2O7
Pb3(AsO4)2      -13.39     -7.59    5.80  Pb3(AsO4)2
Pb3(VO4)2       -14.43     -8.29    6.14  Pb3(VO4)2
Pb3O2CO3        -22.74    -11.72   11.02  Pb3O2CO3
Pb3O2SO4        -17.67     -6.98   10.69  Pb3O2SO4
Pb4(OH)6SO4     -27.97     -6.87   21.10  Pb4(OH)6SO4
Pb4O3SO4        -27.79     -5.91   21.88  Pb4O3SO4
PbCrO4          -37.82    -50.42  -12.60  PbCrO4
Pbmetal         -19.76    -15.52    4.25  Pb
PbMoO4            1.73    -13.89  -15.62  PbMoO4
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  PbO:0.3H2O      -12.02      0.96   12.98  PbO:0.33H2O
  Periclase       -14.14      7.44   21.58  MgO
  Phosgenite       -8.93    -28.74  -19.81  PbCl2:PbCO3
  Plattnerite     -31.95     17.65   49.60  PbO2
  Portlandite     -16.43      6.37   22.80  Ca(OH)2
  Pyrochroite     -14.67      0.52   15.19  Mn(OH)2
  Pyrolusite      -23.96     17.42   41.38  MnO2
  Quartz            4.21      0.21   -4.00  SiO2
  Rhodochrosite    -3.50    -14.08  -10.58  MnCO3
  Sb(OH)3           2.06     -5.05   -7.11  Sb(OH)3
  Sb2O4             4.05      7.45    3.40  Sb2O4
  Sb2O5           -14.92    -24.59   -9.67  Sb2O5
  Sb4O6(cubic)     -0.01    -18.27  -18.26  Sb4O6
  Sb4O6(orth)      -0.37    -18.27  -17.90  Sb4O6
  SbCl3           -29.07    -28.50    0.57  SbCl3
  Sbmetal         -17.76    -29.45  -11.69  Sb
  SbO2              7.24    -20.59  -27.82  SbO2
  Senarmontite      3.23     -9.14  -12.37  Sb2O3
  Sepiolite        -1.35     14.41   15.76  Mg2Si3O7.5OH:3H2O
  Sepiolite(A)     -4.37     14.41   18.78  Mg2Si3O7.5OH:3H2O
  Siderite         -1.23    -11.47  -10.24  FeCO3
  SiO2(am-gel)      2.92      0.21   -2.71  SiO2
  SiO2(am-ppt)      2.95      0.21   -2.74  SiO2
  Spinel          -14.15     22.70   36.85  MgAl2O4
  SrCrO4          -41.30    -45.95   -4.65  SrCrO4
  Strontianite     -0.11     -9.38   -9.27  SrCO3
  Tenorite         -5.87      1.77    7.64  CuO
  Thenardite       -2.39     -2.06    0.32  Na2SO4
  Thermonatrite    -7.76     -7.12    0.64  Na2CO3:H2O
  V(OH)3           -7.81     -0.21    7.59  V(OH)3
  V2O5            -10.14    -11.50   -1.36  V2O5
  V3O5             -9.83     -8.00    1.84  V3O5
  V4O7            -12.32     -5.14    7.19  V4O7
  V6O13            -6.80    -67.66  -60.86  V6O13
  Valentinite      -0.66     -9.14   -8.48  Sb2O3
  VCl2            -42.86    -23.98   18.87  VCl2
  VCl3            -47.10    -23.67   23.43  VCl3
  Vmetal          -68.64    -24.61   44.03  V
  VO              -22.78     -8.03   14.76  VO
  VO(OH)2          -2.61      2.54    5.15  VO(OH)2
  VO2Cl           -16.57    -13.73    2.84  VO2Cl
  VOCl            -18.86     -7.71   11.15  VOCl
  VOCl2           -25.85    -13.09   12.76  VOCl2
  VOSO4           -10.93     -7.32    3.61  VOSO4
  Witherite        -2.21    -10.78   -8.57  BaCO3

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


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Beginning of batch-reaction calculations.
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Reaction step 1.

Using solution 3.     Solution after simulation 1.
Using pure phase assemblage 5.

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

                                                      Moles in assemblage
Phase               SI  log IAP  log K(T, P)   Initial       Final       Delta

Al2O3            -5.90    13.75     19.65    0.000e+00           0   0.000e+00
Anhydrite        -0.82    -5.18     -4.36    0.000e+00           0   0.000e+00
Anilite          -8.92   -40.80    -31.88    0.000e+00           0   0.000e+00
Aragonite        -1.33    -9.63     -8.30    0.000e+00           0   0.000e+00
Artinite         -3.69     5.91      9.60    0.000e+00           0   0.000e+00
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Ba3(AsO4)2       -0.00    -8.91     -8.91    0.000e+00   8.173e-05   8.173e-05
Barite           -2.13   -12.11     -9.98    0.000e+00           0   0.000e+00
Boehmite         -1.71     6.87      8.58    0.000e+00           0   0.000e+00
Brucite          -3.45    13.40     16.84    0.000e+00           0   0.000e+00
CaMoO4            0.00    -7.95     -7.95    0.000e+00   5.047e-04   5.047e-04
Calcite          -1.15    -9.63     -8.48    0.000e+00           0   0.000e+00
Celestite         0.00    -6.62     -6.62    0.000e+00   1.363e-02   1.363e-02
Chalcedony       -0.45    -4.00     -3.55    0.000e+00           0   0.000e+00
Chalcocite       -8.53   -43.45    -34.92    0.000e+00           0   0.000e+00
Chrysotile       -0.00    32.20     32.20    0.000e+00   1.087e-02   1.087e-02
Cr(OH)3(am)      -0.44    -1.19     -0.75    0.000e+00           0   0.000e+00
Cr2O3             0.00    -2.36     -2.36    0.000e+00   7.138e-08   7.138e-08
Cristobalite     -0.65    -4.00     -3.35    0.000e+00           0   0.000e+00
Cu2Sb:3H2O      -20.67   -55.55    -34.88    0.000e+00           0   0.000e+00
Cu3Sb           -23.53   -66.13    -42.59    0.000e+00           0   0.000e+00
Cumetal          -4.53   -13.29     -8.76    0.000e+00           0   0.000e+00
Cupricferrite   -13.22    -7.24      5.99    0.000e+00           0   0.000e+00
Cuprite         -13.80   -15.21     -1.41    0.000e+00           0   0.000e+00
Cuprousferrite   -0.00    -8.92     -8.92    0.000e+00   1.561e-05   1.561e-05
Diaspore         -0.00     6.87      6.87    0.000e+00   2.348e-03   2.348e-03
Djurleite        -8.83   -42.75    -33.92    0.000e+00           0   0.000e+00
Dolomite(disordered)   -0.55   -17.09    -16.54    0.000e+00           0
0.000e+00
Dolomite(ordered)    0.00   -17.09    -17.09    0.000e+00   2.173e-01   2.173e-01
Fe(OH)2          -7.54     6.02     13.56    0.000e+00           0   0.000e+00
Fe(OH)2.7Cl.3    -1.70    -4.74     -3.04    0.000e+00           0   0.000e+00
Fe3(OH)8        -16.85     3.37     20.22    0.000e+00           0   0.000e+00
FeCr2O4          -3.53     3.67      7.20    0.000e+00           0   0.000e+00
FeMoO4           -3.06   -13.15    -10.09    0.000e+00           0   0.000e+00
Ferrihydrite     -4.52    -1.33      3.19    0.000e+00           0   0.000e+00
Gibbsite         -1.43     6.87      8.29    0.000e+00           0   0.000e+00
Goethite         -1.81    -1.32      0.49    0.000e+00           0   0.000e+00
Greenalite      -10.73    10.08     20.81    0.000e+00           0   0.000e+00
Gypsum           -0.59    -5.20     -4.61    0.000e+00           0   0.000e+00
Halloysite       -3.84     5.74      9.57    0.000e+00           0   0.000e+00
Hematite         -1.21    -2.63     -1.42    0.000e+00           0   0.000e+00
Hercynite        -3.11    19.79     22.89    0.000e+00           0   0.000e+00
Huntite          -2.04   -32.01    -29.97    0.000e+00           0   0.000e+00
Hydromagnesite   -7.71   -16.47     -8.77    0.000e+00           0   0.000e+00
K-Jarosite      -15.79   -30.59    -14.80    0.000e+00           0   0.000e+00
Kaolinite        -1.70     5.74      7.43    0.000e+00           0   0.000e+00
Lepidocrocite    -2.69    -1.32      1.37    0.000e+00           0   0.000e+00
Maghemite        -9.01    -2.63      6.39    0.000e+00           0   0.000e+00
Magnesioferrite   -6.08    10.78     16.86    0.000e+00           0   0.000e+00
Magnesite         0.00    -7.46     -7.46    0.000e+00   2.148e-01   2.148e-01
Magnetite        -0.00     3.40      3.40    0.000e+00   6.965e-04   6.965e-04
MgCr2O4          -5.15    11.05     16.20    0.000e+00           0   0.000e+00
Na-Jarosite     -18.58   -29.78    -11.20    0.000e+00           0   0.000e+00
Nesquehonite     -2.81    -7.48     -4.67    0.000e+00           0   0.000e+00
Quartz            0.00    -4.00     -4.00    0.000e+00   2.481e-01   2.481e-01
Rhodochrosite    -2.65   -13.23    -10.58    0.000e+00           0   0.000e+00
Sb(OH)3          -2.10    -9.21     -7.11    0.000e+00           0   0.000e+00
SbO2              0.00   -27.82    -27.82    0.000e+00   6.204e-05   6.204e-05
Senarmontite     -6.04   -18.40    -12.37    0.000e+00           0   0.000e+00
Sepiolite        -0.98    14.78     15.76    0.000e+00           0   0.000e+00
Sepiolite(A)     -4.00    14.78     18.78    0.000e+00           0   0.000e+00
SiO2(am-gel)     -1.29    -4.00     -2.71    0.000e+00           0   0.000e+00
SiO2(am-ppt)     -1.26    -4.00     -2.74    0.000e+00           0   0.000e+00
Siderite         -4.59   -14.83    -10.24    0.000e+00           0   0.000e+00
Spinel           -9.69    27.16     36.85    0.000e+00           0   0.000e+00
Strontianite     -1.80   -11.07     -9.27    0.000e+00           0   0.000e+00
Witherite        -7.99   -16.56     -8.57    0.000e+00           0   0.000e+00

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

       Elements           Molality       Moles

       Al                6.664e-09   1.045e-08
       As                7.551e-04   1.184e-03
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       Ba                8.044e-11   1.261e-10
       C                 1.916e-03   3.005e-03
       Ca                2.198e-03   3.446e-03
       Cl                1.505e-04   2.361e-04
       Cr                1.101e-08   1.727e-08
       Cu                2.567e-15   4.026e-15
       Fe                8.678e-08   1.361e-07
       K                 9.354e-02   1.467e-01
       Li                1.289e-02   2.021e-02
       Mg                2.787e-01   4.370e-01
       Mn                3.356e-06   5.262e-06
       Mo                1.595e-04   2.501e-04
       Na                5.792e-01   9.082e-01
       Pb                3.086e-05   4.839e-05
       S                 3.825e-01   5.999e-01
       Sb                1.228e-09   1.926e-09
       Si                8.205e-05   1.287e-04
       Sr                7.264e-05   1.139e-04
       V                 6.637e-04   1.041e-03

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

                                        pH  =   7.452      Charge balance
                                        pe  =  -1.762      Adjusted to redox
equilibrium
                         Activity of water  =   0.982
                  Ionic strength (mol/kgw)  =   7.346e-01
                        Mass of water (kg)  =   1.568e+00
                  Total alkalinity (eq/kg)  =   2.261e-03
                        Total CO2 (mol/kg)  =   1.916e-03
                          Temperature (°C)  =  25.00
                   Electrical balance (eq)  =   7.518e-01
  Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  44.47
                                Iterations  =  19
                                   Total H  = 1.740922e+02
                                   Total O  = 8.945881e+01

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

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

   OH-             4.646e-07   2.798e-07    -6.333    -6.553    -0.220     (0)  
   H+              4.690e-08   3.533e-08    -7.329    -7.452    -0.123      0.00
   H2O             5.551e+01   9.819e-01     1.744    -0.008     0.000     18.07
Al            6.664e-09
   Al(OH)4-        6.514e-09   4.178e-09    -8.186    -8.379    -0.193     (0)  
   Al(OH)3         1.186e-10   1.186e-10    -9.926    -9.926     0.000     (0)  
   Al(OH)2+        3.167e-11   2.124e-11   -10.499   -10.673    -0.173     (0)  
   AlOH+2          4.721e-13   9.555e-14   -12.326   -13.020    -0.694     (0)  
   AlSO4+          1.250e-13   8.016e-14   -12.903   -13.096    -0.193     (0)  
   Al(SO4)2-       4.050e-14   2.598e-14   -13.393   -13.585    -0.193     (0)  
   Al+3            4.368e-15   3.415e-16   -14.360   -15.467    -1.107     (0)  
   AlMo6O21-3      1.085e-27   1.263e-31   -26.964   -30.899    -3.934     (0)  
As(3)         4.112e-04
   H3AsO3          3.955e-04   3.955e-04    -3.403    -3.403     0.000     (0)  
   H2AsO3-         1.571e-05   5.741e-06    -4.804    -5.241    -0.437     (0)  
   HAsO3-2         8.305e-09   1.482e-10    -8.081    -9.829    -1.748     (0)  
   H4AsO3+         1.894e-11   6.923e-12   -10.723   -11.160    -0.437     (0)  
   AsO3-3          1.389e-12   1.617e-16   -11.857   -15.791    -3.934     (0)  
As(5)         3.439e-04
   HAsO4-2         3.341e-04   5.961e-06    -3.476    -5.225    -1.748     (0)  
   H2AsO4-         5.256e-06   1.921e-06    -5.279    -5.716    -0.437     (0)  
   AsO4-3          4.585e-06   5.336e-10    -5.339    -9.273    -3.934     (0)  
   H3AsO4          9.959e-12   1.179e-11   -11.002   -10.928     0.073     (0)  
Ba            8.044e-11
   Ba+2            8.014e-11   2.582e-11   -10.096   -10.588    -0.492     (0)  
   BaHCO3+         2.898e-13   1.993e-13   -12.538   -12.700    -0.163     (0)  
   BaCO3           1.420e-14   1.420e-14   -13.848   -13.848     0.000     (0)  
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   BaOH+           4.790e-17   3.153e-17   -16.320   -16.501    -0.182     (0)
C(4)          1.916e-03
   HCO3-           1.205e-03   8.084e-04    -2.919    -3.092    -0.173     (0)
   MgHCO3+         4.293e-04   2.674e-04    -3.367    -3.573    -0.206     (0)
   NaHCO3          1.677e-04   1.677e-04    -3.775    -3.775     0.000     (0)
   H2CO3           6.424e-05   6.424e-05    -4.192    -4.192     0.000     (0)
   MgCO3           2.884e-05   2.884e-05    -4.540    -4.540     0.000     (0)
   NaCO3-          1.099e-05   7.368e-06    -4.959    -5.133    -0.173     (0)
   CaHCO3+         4.783e-06   3.290e-06    -5.320    -5.483    -0.163     (0)
   CO3-2           3.330e-06   1.073e-06    -5.478    -5.970    -0.492     (0)
   PbCO3           5.634e-07   5.634e-07    -6.249    -6.249     0.000     (0)
   CaCO3           3.715e-07   3.715e-07    -6.430    -6.430     0.000     (0)
   PbHCO3+         2.872e-07   1.050e-07    -6.542    -6.979    -0.437     (0)
   SrHCO3+         1.512e-07   1.040e-07    -6.820    -6.983    -0.163     (0)
   Pb(CO3)2-2      9.768e-08   1.743e-09    -7.010    -8.759    -1.748     (0)
   SrCO3           5.493e-09   5.493e-09    -8.260    -8.260     0.000     (0)
   MnHCO3+         1.338e-09   8.809e-10    -8.874    -9.055    -0.182     (0)
   FeHCO3+         2.022e-11   1.391e-11   -10.694   -10.857    -0.163     (0)
   BaHCO3+         2.898e-13   1.993e-13   -12.538   -12.700    -0.163     (0)
   BaCO3           1.420e-14   1.420e-14   -13.848   -13.848     0.000     (0)
   CuCO3           1.987e-19   1.987e-19   -18.702   -18.702     0.000     (0)
   Cu(CO3)2-2      3.215e-20   5.737e-22   -19.493   -21.241    -1.748     (0)
   CuHCO3+         4.390e-21   1.605e-21   -20.358   -20.795    -0.437     (0)
Ca            2.198e-03
   CaSO4           1.514e-03   1.514e-03    -2.820    -2.820     0.000     (0)
   Ca+2            6.784e-04   2.185e-04    -3.169    -3.660    -0.492     (0)
   CaHCO3+         4.783e-06   3.290e-06    -5.320    -5.483    -0.163     (0)
   CaCO3           3.715e-07   3.715e-07    -6.430    -6.430     0.000     (0)
   CaOH+           1.774e-09   1.220e-09    -8.751    -8.914    -0.163     (0)
Cl            1.505e-04
   Cl-             1.505e-04   1.134e-04    -3.822    -3.945    -0.123     (0)
   PbCl+           1.924e-09   7.031e-10    -8.716    -9.153    -0.437     (0)
   MnCl+           1.184e-11   7.798e-12   -10.926   -11.108    -0.182     (0)
   PbCl2           3.562e-13   3.562e-13   -12.448   -12.448     0.000     (0)
   MnCl2           1.249e-15   1.249e-15   -14.903   -14.903     0.000     (0)
   CuCl            1.271e-16   1.271e-16   -15.896   -15.896     0.000     (0)
   CrCl+2          9.152e-17   1.633e-18   -16.038   -17.787    -1.748     (0)
   PbCl3-          4.400e-17   1.608e-17   -16.357   -16.794    -0.437     (0)
   CuCl2-          4.833e-18   3.011e-18   -17.316   -17.521    -0.206     (0)
   VOCl+           8.963e-19   3.276e-19   -18.048   -18.485    -0.437     (0)
   MnCl3-          5.927e-20   3.902e-20   -19.227   -19.409    -0.182     (0)
   PbCl4-2         4.672e-20   8.337e-22   -19.330   -21.079    -1.748     (0)
   CrOHCl2         9.852e-22   9.852e-22   -21.006   -21.006     0.000     (0)
   CuCl3-2         3.886e-22   7.300e-23   -21.410   -22.137    -0.726     (0)
   CrCl2+          4.809e-23   1.757e-23   -22.318   -22.755    -0.437     (0)
   CuCl+           9.078e-24   5.654e-24   -23.042   -23.248    -0.206     (0)
   FeCl+2          4.008e-26   7.529e-27   -25.397   -26.123    -0.726     (0)
   CuCl2           2.224e-28   2.224e-28   -27.653   -27.653     0.000     (0)
   FeCl2+          5.793e-30   3.814e-30   -29.237   -29.419    -0.182     (0)
   CuCl3-          3.778e-34   2.353e-34   -33.423   -33.628    -0.206     (0)
   FeCl3           4.326e-35   4.326e-35   -34.364   -34.364     0.000     (0)
   CuCl4-2         7.122e-40   1.338e-40   -39.147   -39.874    -0.726     (0)
   CrO3Cl-         0.000e+00   0.000e+00   -47.696   -48.133    -0.437     (0)
Cr(2)         8.604e-18
   Cr+2            8.604e-18   1.535e-19   -17.065   -18.814    -1.748     (0)
Cr(3)         1.101e-08
   Cr(OH)2+        6.346e-09   2.320e-09    -8.197    -8.635    -0.437     (0)
   Cr(OH)+2        3.818e-09   6.812e-11    -8.418   -10.167    -1.748     (0)
   CrOHSO4         4.889e-10   4.889e-10    -9.311    -9.311     0.000     (0)
   Cr(OH)3         2.438e-10   2.438e-10    -9.613    -9.613     0.000     (0)
   Cr+3            9.561e-11   1.113e-14   -10.020   -13.954    -3.934     (0)
   CrO2-           9.133e-12   3.338e-12   -11.039   -11.477    -0.437     (0)
   Cr(OH)4-        7.433e-12   2.717e-12   -11.129   -11.566    -0.437     (0)
   CrSO4+          2.150e-12   7.858e-13   -11.668   -12.105    -0.437     (0)
   Cr2(OH)2SO4+2   1.687e-16   3.010e-18   -15.773   -17.521    -1.748     (0)
   CrCl+2          9.152e-17   1.633e-18   -16.038   -17.787    -1.748     (0)
   Cr2(OH)2(SO4)2   5.408e-18   5.408e-18   -17.267   -17.267     0.000      (0)
   CrOHCl2         9.852e-22   9.852e-22   -21.006   -21.006     0.000     (0)
   CrCl2+          4.809e-23   1.757e-23   -22.318   -22.755    -0.437     (0)
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Cr(6)           2.262e-36
   NaCrO4-         1.259e-36   4.602e-37   -35.900   -36.337    -0.437     (0)
   CrO4-2          7.793e-37   2.510e-37   -36.108   -36.600    -0.492     (0)
   KCrO4-          1.450e-37   5.299e-38   -36.839   -37.276    -0.437     (0)
   HCrO4-          7.853e-38   2.870e-38   -37.105   -37.542    -0.437     (0)
   CrO3SO4-2       0.000e+00   0.000e+00   -42.273   -44.022    -1.748     (0)
   H2CrO4          0.000e+00   0.000e+00   -45.085   -45.085     0.000     (0)
   CrO3Cl-         0.000e+00   0.000e+00   -47.696   -48.133    -0.437     (0)
   Cr2O7-2         0.000e+00   0.000e+00   -71.788   -73.536    -1.748     (0)
Cu(1)           2.567e-15
   Cu+             2.435e-15   8.899e-16   -14.614   -15.051    -0.437     (0)
   CuCl            1.271e-16   1.271e-16   -15.896   -15.896     0.000     (0)
   CuCl2-          4.833e-18   3.011e-18   -17.316   -17.521    -0.206     (0)
   CuCl3-2         3.886e-22   7.300e-23   -21.410   -22.137    -0.726     (0)
   Cu(S4)2-3       1.468e-38   4.370e-39   -37.833   -38.360    -0.526     (0)
   CuS4S5-3        2.511e-39   8.136e-40   -38.600   -39.090    -0.489     (0)
Cu(2)           5.971e-19
   CuSO4           2.179e-19   2.179e-19   -18.662   -18.662     0.000     (0)
   CuCO3           1.987e-19   1.987e-19   -18.702   -18.702     0.000     (0)
   Cu+2            9.765e-20   3.146e-20   -19.010   -19.502    -0.492     (0)
   CuOH+           4.469e-20   2.784e-20   -19.350   -19.555    -0.206     (0)
   Cu(CO3)2-2      3.215e-20   5.737e-22   -19.493   -21.241    -1.748     (0)
   CuHCO3+         4.390e-21   1.605e-21   -20.358   -20.795    -0.437     (0)
   Cu(OH)2         1.554e-21   1.554e-21   -20.808   -20.808     0.000     (0)
   CuCl+           9.078e-24   5.654e-24   -23.042   -23.248    -0.206     (0)
   Cu(OH)3-        2.441e-24   8.922e-25   -23.612   -24.050    -0.437     (0)
   CuCl2           2.224e-28   2.224e-28   -27.653   -27.653     0.000     (0)
   Cu(OH)4-2       1.101e-28   1.965e-30   -27.958   -29.707    -1.748     (0)
   Cu2(OH)2+2      1.091e-33   1.947e-35   -32.962   -34.711    -1.748     (0)
   CuCl3-          3.778e-34   2.353e-34   -33.423   -33.628    -0.206     (0)
   CuCl4-2         7.122e-40   1.338e-40   -39.147   -39.874    -0.726     (0)
   Cu(HS)3-        0.000e+00   0.000e+00   -55.570   -56.007    -0.437     (0)
Fe(2)           8.678e-08
   Fe+2            7.659e-08   1.367e-09    -7.116    -8.864    -1.748     (0)
   FeSO4           1.015e-08   1.015e-08    -7.994    -7.994     0.000     (0)
   FeOH+           2.313e-11   1.523e-11   -10.636   -10.817    -0.182     (0)
   FeHCO3+         2.022e-11   1.391e-11   -10.694   -10.857    -0.163     (0)
   Fe(OH)2         3.385e-15   3.385e-15   -14.470   -14.470     0.000     (0)
   Fe(OH)3-        4.550e-16   2.995e-16   -15.342   -15.524    -0.182     (0)
   Fe(HS)2         0.000e+00   0.000e+00   -41.517   -41.517     0.000     (0)
   Fe(HS)3-        0.000e+00   0.000e+00   -59.844   -60.281    -0.437     (0)
Fe(3)           7.797e-14
   Fe(OH)2+        6.447e-14   4.324e-14   -13.191   -13.364    -0.173     (0)
   Fe(OH)3         1.300e-14   1.300e-14   -13.886   -13.886     0.000     (0)
   Fe(OH)4-        5.048e-16   3.386e-16   -15.297   -15.470    -0.173     (0)
   FeOH+2          2.114e-18   3.972e-19   -17.675   -18.401    -0.726     (0)
   Fe(SO4)2-       1.320e-21   4.823e-22   -20.880   -21.317    -0.437     (0)
   FeSO4+          1.133e-21   7.459e-22   -20.946   -21.127    -0.182     (0)
   Fe+3            2.812e-23   2.198e-24   -22.551   -23.658    -1.107     (0)
   FeCl+2          4.008e-26   7.529e-27   -25.397   -26.123    -0.726     (0)
   Fe2(OH)2+4      5.152e-29   5.223e-36   -28.288   -35.282    -6.994     (0)
   FeCl2+          5.793e-30   3.814e-30   -29.237   -29.419    -0.182     (0)
   FeCl3           4.326e-35   4.326e-35   -34.364   -34.364     0.000     (0)
   Fe3(OH)4+5      2.767e-37   0.000e+00   -36.558   -47.486   -10.928     (0)
H(0)            4.979e-15
   H2              2.489e-15   2.948e-15   -14.604   -14.530     0.073     (0)
K               9.354e-02
   K+              7.541e-02   5.681e-02    -1.123    -1.246    -0.123     (0)
   KSO4-           1.813e-02   1.216e-02    -1.741    -1.915    -0.173     (0)
   KCrO4-          1.450e-37   5.299e-38   -36.839   -37.276    -0.437     (0)
Li              1.289e-02
   Li+             1.119e-02   8.433e-03    -1.951    -2.074    -0.123     (0)
   LiSO4-          1.691e-03   1.113e-03    -2.772    -2.953    -0.182     (0)
Mg              2.787e-01
   MgSO4           1.779e-01   1.779e-01    -0.750    -0.750     0.000     (0)
   Mg+2            1.003e-01   3.232e-02    -0.999    -1.490    -0.492     (0)
   MgHCO3+         4.293e-04   2.674e-04    -3.367    -3.573    -0.206     (0)
   MgCO3           2.884e-05   2.884e-05    -4.540    -4.540     0.000     (0)
   MgOH+           5.139e-06   3.601e-06    -5.289    -5.444    -0.154     (0)
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Mn(2)          3.356e-06
   Mn+2             3.061e-06   5.461e-08    -5.514    -7.263    -1.748     (0)
   MnSO4            2.937e-07   2.937e-07    -6.532    -6.532     0.000     (0)
   MnHCO3+          1.338e-09   8.809e-10    -8.874    -9.055    -0.182     (0)
   MnOH+            5.831e-11   3.839e-11   -10.234   -10.416    -0.182     (0)
   MnCl+            1.184e-11   7.798e-12   -10.926   -11.108    -0.182     (0)
   MnCl2            1.249e-15   1.249e-15   -14.903   -14.903     0.000     (0)
   MnCl3-           5.927e-20   3.902e-20   -19.227   -19.409    -0.182     (0)
   Mn(OH)3-         2.822e-20   1.858e-20   -19.549   -19.731    -0.182     (0)
   Mn(OH)4-2        8.937e-26   1.679e-26   -25.049   -25.775    -0.726     (0)
Mn(3)          5.403e-34
   Mn+3             5.403e-34   4.224e-35   -33.267   -34.374    -1.107     (0)
Mn(6)          0.000e+00
   MnO4-2           0.000e+00   0.000e+00   -72.422   -73.148    -0.726     (0)
Mn(7)          0.000e+00
   MnO4-            0.000e+00   0.000e+00   -84.045   -84.282    -0.237     (0)
Mo             1.595e-04
   MoO4-2           1.594e-04   5.134e-05    -3.798    -4.290    -0.492     (0)
   HMoO4-           9.875e-08   3.609e-08    -7.005    -7.443    -0.437     (0)
   H2MoO4           9.341e-12   9.341e-12   -11.030   -11.030     0.000     (0)
   Mo7O24-6         1.308e-21   2.400e-37   -20.883   -36.620   -15.736     (0)
   HMo7O24-5        1.751e-27   2.067e-38   -26.757   -37.685   -10.928     (0)
   AlMo6O21-3       1.085e-27   1.263e-31   -26.964   -30.899    -3.934     (0)
   H2Mo7O24-4       4.361e-34   0.000e+00   -33.360   -40.354    -6.994     (0)
   H3Mo7O24-3       0.000e+00   0.000e+00   -40.626   -44.560    -3.934     (0)
Na             5.792e-01
   Na+              4.897e-01   3.689e-01    -0.310    -0.433    -0.123     (0)
   NaSO4-           8.933e-02   5.992e-02    -1.049    -1.222    -0.173     (0)
   NaHCO3           1.677e-04   1.677e-04    -3.775    -3.775     0.000     (0)
   NaCO3-           1.099e-05   7.368e-06    -4.959    -5.133    -0.173     (0)
   NaCrO4-          1.259e-36   4.602e-37   -35.900   -36.337    -0.437     (0)
O(0)           0.000e+00
   O2               0.000e+00   0.000e+00   -63.323   -63.250     0.073     (0)
Pb             3.086e-05
   Pb(SO4)2-2       2.643e-05   4.717e-07    -4.578    -6.326    -1.748     (0)
   PbSO4            2.588e-06   2.588e-06    -5.587    -5.587     0.000     (0)
   PbCO3            5.634e-07   5.634e-07    -6.249    -6.249     0.000     (0)
   Pb+2             5.424e-07   1.747e-07    -6.266    -6.758    -0.492     (0)
   PbOH+            3.361e-07   1.228e-07    -6.474    -6.911    -0.437     (0)
   PbHCO3+          2.872e-07   1.050e-07    -6.542    -6.979    -0.437     (0)
   Pb(CO3)2-2       9.768e-08   1.743e-09    -7.010    -8.759    -1.748     (0)
   Pb2OH+3          2.923e-09   3.402e-13    -8.534   -12.468    -3.934     (0)
   PbCl+            1.924e-09   7.031e-10    -8.716    -9.153    -0.437     (0)
   Pb(OH)2          1.087e-09   1.087e-09    -8.964    -8.964     0.000     (0)
   Pb4(OH)4+4       5.639e-11   5.717e-18   -10.249   -17.243    -6.994     (0)
   Pb(OH)3-         8.322e-13   3.042e-13   -12.080   -12.517    -0.437     (0)
   PbCl2            3.562e-13   3.562e-13   -12.448   -12.448     0.000     (0)
   Pb3(OH)4+2       2.308e-13   4.119e-15   -12.637   -14.385    -1.748     (0)
   Pb(OH)4-2        1.168e-15   2.085e-17   -14.932   -16.681    -1.748     (0)
   PbCl3-           4.400e-17   1.608e-17   -16.357   -16.794    -0.437     (0)
   PbCl4-2          4.672e-20   8.337e-22   -19.330   -21.079    -1.748     (0)
   Pb(HS)2          8.125e-34   8.125e-34   -33.090   -33.090     0.000     (0)
   Pb(HS)3-         0.000e+00   0.000e+00   -52.154   -52.591    -0.437     (0)
S(-2)          6.640e-21
   HS-              4.323e-21   1.580e-21   -20.364   -20.801    -0.437     (0)
   S5-2             1.081e-21   1.930e-23   -20.966   -22.715    -1.748     (0)
   H2S              5.846e-22   5.846e-22   -21.233   -21.233     0.000     (0)
   S6-2             3.296e-22   5.882e-24   -21.482   -23.230    -1.748     (0)
   S4-2             2.743e-22   4.895e-24   -21.562   -23.310    -1.748     (0)
   S3-2             4.289e-23   7.653e-25   -22.368   -24.116    -1.748     (0)
   S2-2             4.133e-24   7.375e-26   -23.384   -25.132    -1.748     (0)
   S-2              1.193e-30   2.242e-31   -29.923   -30.649    -0.726     (0)
   Pb(HS)2          8.125e-34   8.125e-34   -33.090   -33.090     0.000     (0)
   Cu(S4)2-3        1.468e-38   4.370e-39   -37.833   -38.360    -0.526     (0)
   CuS4S5-3         2.511e-39   8.136e-40   -38.600   -39.090    -0.489     (0)
   Fe(HS)2          0.000e+00   0.000e+00   -41.517   -41.517     0.000     (0)
   Pb(HS)3-         0.000e+00   0.000e+00   -52.154   -52.591    -0.437     (0)
   Cu(HS)3-         0.000e+00   0.000e+00   -55.570   -56.007    -0.437     (0)
   Fe(HS)3-         0.000e+00   0.000e+00   -59.844   -60.281    -0.437     (0)
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   Sb2S4-2         0.000e+00   0.000e+00   -65.349   -67.097     -1.748     (0)
S(6)          3.825e-01
   MgSO4           1.779e-01   1.779e-01    -0.750    -0.750      0.000     (0)
   SO4-2           9.389e-02   3.024e-02    -1.027    -1.519     -0.492     (0)
   NaSO4-          8.933e-02   5.992e-02    -1.049    -1.222     -0.173     (0)
   KSO4-           1.813e-02   1.216e-02    -1.741    -1.915     -0.173     (0)
   LiSO4-          1.691e-03   1.113e-03    -2.772    -2.953     -0.182     (0)
   CaSO4           1.514e-03   1.514e-03    -2.820    -2.820      0.000     (0)
   SrSO4           4.786e-05   4.786e-05    -4.320    -4.320      0.000     (0)
   Pb(SO4)2-2      2.643e-05   4.717e-07    -4.578    -6.326     -1.748     (0)
   PbSO4           2.588e-06   2.588e-06    -5.587    -5.587      0.000     (0)
   MnSO4           2.937e-07   2.937e-07    -6.532    -6.532      0.000     (0)
   HSO4-           1.628e-07   1.044e-07    -6.788    -6.981     -0.193     (0)
   FeSO4           1.015e-08   1.015e-08    -7.994    -7.994      0.000     (0)
   CrOHSO4         4.889e-10   4.889e-10    -9.311    -9.311      0.000     (0)
   CrSO4+          2.150e-12   7.858e-13   -11.668   -12.105     -0.437     (0)
   AlSO4+          1.250e-13   8.016e-14   -12.903   -13.096     -0.193     (0)
   Al(SO4)2-       4.050e-14   2.598e-14   -13.393   -13.585     -0.193     (0)
   VOSO4           8.577e-15   8.577e-15   -14.067   -14.067      0.000     (0)
   Cr2(OH)2SO4+2   1.687e-16   3.010e-18   -15.773   -17.521     -1.748     (0)
   Cr2(OH)2(SO4)2   5.408e-18   5.408e-18   -17.267   -17.267      0.000     (0)
   VO2SO4-         3.464e-19   1.266e-19   -18.460   -18.898     -0.437     (0)
   CuSO4           2.179e-19   2.179e-19   -18.662   -18.662      0.000     (0)
   VSO4+           1.467e-21   5.360e-22   -20.834   -21.271     -0.437     (0)
   Fe(SO4)2-       1.320e-21   4.823e-22   -20.880   -21.317     -0.437     (0)
   FeSO4+          1.133e-21   7.459e-22   -20.946   -21.127     -0.182     (0)
   CrO3SO4-2       0.000e+00   0.000e+00   -42.273   -44.022     -1.748     (0)
Sb(3)         1.223e-09
   Sb(OH)3         6.134e-10   6.134e-10    -9.212    -9.212      0.000     (0)
   HSbO2           6.098e-10   6.098e-10    -9.215    -9.215      0.000     (0)
   SbO2-           7.648e-14   2.795e-14   -13.116   -13.554     -0.437     (0)
   Sb(OH)4-        4.226e-14   1.544e-14   -13.374   -13.811     -0.437     (0)
   Sb(OH)2+        1.466e-15   5.360e-16   -14.834   -15.271     -0.437     (0)
   SbO+            5.149e-16   1.882e-16   -15.288   -15.725     -0.437     (0)
   Sb2S4-2         0.000e+00   0.000e+00   -65.349   -67.097     -1.748     (0)
Sb(5)         4.779e-12
   SbO3-           4.776e-12   1.746e-12   -11.321   -11.758     -0.437     (0)
   Sb(OH)6-        2.566e-15   1.933e-15   -14.591   -14.714     -0.123     (0)
   SbO2+           1.741e-27   6.365e-28   -26.759   -27.196     -0.437     (0)
Si            8.205e-05
   H4SiO4          8.141e-05   9.642e-05    -4.089    -4.016      0.073     (0)
   H3SiO4-         6.333e-07   3.944e-07    -6.198    -6.404     -0.206     (0)
   H2SiO4-2        3.480e-12   7.044e-13   -11.458   -12.152     -0.694     (0)
Sr            7.264e-05
   SrSO4           4.786e-05   4.786e-05    -4.320    -4.320      0.000     (0)
   Sr+2            2.462e-05   7.932e-06    -4.609    -5.101     -0.492     (0)
   SrHCO3+         1.512e-07   1.040e-07    -6.820    -6.983     -0.163     (0)
   SrCO3           5.493e-09   5.493e-09    -8.260    -8.260      0.000     (0)
   SrOH+           2.228e-11   1.466e-11   -10.652   -10.834     -0.182     (0)
V(2)          8.584e-24
   V+2             5.952e-24   1.062e-25   -23.225   -24.974     -1.748     (0)
   VOH+            2.632e-24   9.618e-25   -23.580   -24.017     -0.437     (0)
V(3)          6.637e-04
   V(OH)3          6.637e-04   6.637e-04    -3.178    -3.178      0.000     (0)
   V(OH)2+         4.222e-14   1.543e-14   -13.374   -13.812     -0.437     (0)
   VOH+2           2.951e-16   5.266e-18   -15.530   -17.279     -1.748     (0)
   V+3             3.226e-19   3.754e-23   -18.491   -22.425     -3.934     (0)
   VSO4+           1.467e-21   5.360e-22   -20.834   -21.271     -0.437     (0)
   V2(OH)2+4       1.726e-27   1.750e-34   -26.763   -33.757     -6.994     (0)
   V2(OH)3+3       1.976e-29   2.300e-33   -28.704   -32.638     -3.934     (0)
V(4)          2.207e-13
   V(OH)3+         1.545e-13   5.645e-14   -12.811   -13.248     -0.437     (0)
   VO+2            5.770e-14   1.030e-15   -13.239   -14.987     -1.748     (0)
   VOSO4           8.577e-15   8.577e-15   -14.067   -14.067      0.000     (0)
   VOCl+           8.963e-19   3.276e-19   -18.048   -18.485     -0.437     (0)
   H2V2O4+2        9.283e-21   1.657e-22   -20.032   -21.781     -1.748     (0)
V(5)          4.561e-11
   HVO4-2          2.704e-11   4.825e-13   -10.568   -12.317     -1.748     (0)
   H2VO4-          1.857e-11   6.787e-12   -10.731   -11.168     -0.437     (0)
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   H3VO4          2.398e-15   2.398e-15   -14.620   -14.620     0.000     (0)
   VO4-3          5.881e-16   6.844e-20   -15.231   -19.165    -3.934     (0)
   HV2O7-3        9.709e-18   1.130e-21   -17.013   -20.947    -3.934     (0)
   V2O7-4         8.490e-18   8.608e-25   -17.071   -24.065    -6.994     (0)
   VO2SO4-        3.464e-19   1.266e-19   -18.460   -18.898    -0.437     (0)
   H3V2O7-        2.928e-19   1.070e-19   -18.533   -18.971    -0.437     (0)
   VO2+           2.327e-19   1.753e-19   -18.633   -18.756    -0.123     (0)
   V3O9-3         2.971e-24   3.457e-28   -23.527   -27.461    -3.934     (0)
   V4O12-4        9.824e-30   9.961e-37   -29.008   -36.002    -6.994     (0)
   V10O28-6       0.000e+00   0.000e+00   -76.754   -92.490   -15.736     (0)
   HV10O28-5      0.000e+00   0.000e+00   -80.827   -91.755   -10.928     (0)
   H2V10O28-4     0.000e+00   0.000e+00   -87.005   -93.999    -6.994     (0)

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

  Phase               SI** log IAP   log K(298 K,   1 atm)

  Al(OH)3(am)      -3.93      6.87   10.80  Al(OH)3
  Al2(MoO4)3      -46.17    -43.80    2.37  Al2(MoO4)3
  Al2O3            -5.90     13.75   19.65  Al2O3
  Al4(OH)10SO4    -11.65     11.05   22.70  Al4(OH)10SO4
  AlAsO4:2H2O      -8.86     -4.06    4.80  AlAsO4:2H2O
  AlOHSO4          -6.31     -9.54   -3.23  AlOHSO4
  AlSb           -102.07    -36.44   65.62  AlSb
  Alunite          -4.62     -6.02   -1.40  KAl3(SO4)2(OH)6
  Anglesite        -0.49     -8.28   -7.79  PbSO4
  Anhydrite        -0.82     -5.18   -4.36  CaSO4
  Anilite          -8.92    -40.80  -31.88  Cu0.25Cu1.5S
  Antlerite       -39.04    -30.25    8.79  Cu3(OH)4SO4
  Aragonite        -1.33     -9.63   -8.30  CaCO3
  Arsenolite      -10.80    -13.56   -2.76  As4O6
  Artinite         -3.69      5.91    9.60  MgCO3:Mg(OH)2:3H2O
  As2O5           -28.54    -21.83    6.71  As2O5
  Atacamite       -28.01    -20.62    7.39  Cu2(OH)3Cl
  Azurite         -38.65    -55.56  -16.91  Cu3(OH)2(CO3)2
  Ba(OH)2:8H2O    -20.16      4.24   24.39  Ba(OH)2:8H2O
  Ba2V2O7:2H2O    -29.89    -14.02   15.87  Ba2V2O7:2H2O
  Ba3(AsO4)2       -0.00     -8.91   -8.91  Ba3(AsO4)2
  Ba3(VO4)2:4H2O  -42.67     -9.73   32.94  Ba3(VO4)2:4H2O
  BaCrO4          -37.52    -47.19   -9.67  BaCrO4
  BaMoO4           -7.92    -14.88   -6.96  BaMoO4
  Barite           -2.13    -12.11   -9.98  BaSO4
  BaS             -40.12    -23.94   16.18  BaS
  Birnessite      -24.44     -6.34   18.09  MnO2
  Bixbyite        -23.42    -24.06   -0.64  Mn2O3
  BlaubleiI        -9.75    -33.91  -24.16  Cu0.9Cu0.2S
  BlaubleiII       -9.81    -37.09  -27.28  Cu0.6Cu0.8S
  Boehmite         -1.71      6.87    8.58  AlOOH
  Brochantite     -50.09    -34.86   15.22  Cu4(OH)6SO4
  Brucite          -3.45     13.40   16.84  Mg(OH)2
  Ca(VO3)2        -17.04    -11.38    5.66  Ca(VO3)2
  Ca2V2O7         -17.65     -0.15   17.50  Ca2V2O7
  Ca2V2O7:2H2O    -21.71     -0.16   21.55  Ca2V2O7:2H2O
  Ca3(AsO4)2:4H2O -10.46     11.84   22.30  Ca3(AsO4)2:4H2O
  Ca3(VO4)2       -27.87     11.09   38.96  Ca3(VO4)2
  Ca3(VO4)2:4H2O  -28.80     11.06   39.86  Ca3(VO4)2:4H2O
  Ca3Sb2         -195.90    -52.93  142.97  Ca3Sb2
  CaCrO4          -38.00    -40.26   -2.27  CaCrO4
  Calcite          -1.15     -9.63   -8.48  CaCO3
  CaMoO4            0.00     -7.95   -7.95  CaMoO4
  Celestite         0.00     -6.62   -6.62  SrSO4
  Cerussite         0.40    -12.73  -13.13  PbCO3
  CH4(g)          -25.33    -66.37  -41.05  CH4
  Chalcanthite    -18.42    -21.06   -2.64  CuSO4:5H2O
  Chalcedony       -0.45     -4.00   -3.55  SiO2
  Chalcocite       -8.53    -43.45  -34.92  Cu2S
  Chalcopyrite    -19.80    -55.07  -35.27  CuFeS2
  Chrysotile       -0.00     32.20   32.20  Mg3Si2O5(OH)4
  Claudetite      -10.50    -13.56   -3.06  As4O6
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CO2(g)           -2.72    -20.87  -18.15  CO2
Cotunnite        -9.87    -14.65   -4.78  PbCl2
Covellite       -10.55    -32.85  -22.30  CuS
Cr(OH)2         -14.74     -3.93   10.82  Cr(OH)2
Cr(OH)3          -2.53     -1.19    1.34  Cr(OH)3
Cr(OH)3(am)      -0.44     -1.19   -0.75  Cr(OH)3
Cr2O3             0.00     -2.36   -2.36  Cr2O3
CrCl2           -40.80    -26.70   14.09  CrCl2
CrCl3           -50.47    -35.36   15.11  CrCl3
Cristobalite     -0.65     -4.00   -3.35  SiO2
Crmetal         -45.77    -15.29   30.48  Cr
CrO3            -48.29    -51.50   -3.21  CrO3
Cu(OH)2         -13.29     -4.61    8.67  Cu(OH)2
Cu(SbO3)2       -45.47     -0.26   45.21  Cu(SbO3)2
Cu2Sb:3H2O      -20.67    -55.55  -34.88  Cu2Sb:3H2O
Cu2SO4          -29.67    -31.62   -1.95  Cu2SO4
Cu3(AsO4)2:2H2O -41.77    -35.67    6.10  Cu3(AsO4)2:2H2O
Cu3Sb           -23.53    -66.13  -42.59  Cu3Sb
CuCO3           -13.97    -25.47  -11.50  CuCO3
CuCrO4          -50.66    -56.10   -5.44  CuCrO4
Cumetal          -4.53    -13.29   -8.76  Cu
CuMoO4          -10.72    -23.79  -13.08  CuMoO4
CuOCuSO4        -35.93    -25.63   10.30  CuOCuSO4
Cupricferrite   -13.22     -7.24    5.99  CuFe2O4
Cuprite         -13.80    -15.21   -1.41  Cu2O
Cuprousferrite   -0.00     -8.92   -8.92  CuFeO2
CuSO4           -23.96    -21.02    2.94  CuSO4
Diaspore         -0.00      6.87    6.87  AlOOH
Djurleite        -8.83    -42.75  -33.92  Cu0.066Cu1.868S
Dolomite(disordered)  -0.55    -17.09  -16.54  CaMg(CO3)2
Dolomite(ordered)   0.00    -17.09  -17.09  CaMg(CO3)2
Epsomite         -0.94     -3.07   -2.13  MgSO4:7H2O
Fe(OH)2          -7.54      6.02   13.56  Fe(OH)2
Fe(OH)2.7Cl.3    -1.70     -4.74   -3.04  Fe(OH)2.7Cl.3
Fe(VO3)2        -12.87    -16.59   -3.72  Fe(VO3)2
Fe2(SO4)3       -48.14    -51.87   -3.73  Fe2(SO4)3
Fe3(OH)8        -16.85      3.37   20.22  Fe3(OH)8
FeAsO4:2H2O     -12.65    -12.25    0.40  FeAsO4:2H2O
FeCr2O4          -3.53      3.67    7.20  FeCr2O4
FeMoO4           -3.06    -13.15  -10.09  FeMoO4
Ferrihydrite     -4.52     -1.33    3.19  Fe(OH)3
FeS(ppt)        -19.26    -22.21   -2.95  FeS
Galena           -6.14    -20.11  -13.97  PbS
Gibbsite         -1.43      6.87    8.29  Al(OH)3
Goethite         -1.81     -1.32    0.49  FeOOH
Greenalite      -10.73     10.08   20.81  Fe3Si2O5(OH)4
Greigite        -64.54   -109.58  -45.03  Fe3S4
Gypsum           -0.59     -5.20   -4.61  CaSO4:2H2O
H-Jarosite      -24.71    -36.81  -12.10  (H3O)Fe3(SO4)2(OH)6
H2MoO4           -6.32    -19.19  -12.88  H2MoO4
H2S(g)          -20.24    -28.25   -8.01  H2S
Halite           -5.98     -4.38    1.60  NaCl
Halloysite       -3.84      5.74    9.57  Al2Si2O5(OH)4
Hausmannite     -26.76     34.27   61.03  Mn3O4
Hematite         -1.21     -2.63   -1.42  Fe2O3
Hercynite        -3.11     19.79   22.89  FeAl2O4
Huntite          -2.04    -32.01  -29.97  CaMg3(CO3)4
Hydrocerussite    1.45    -17.32  -18.77  Pb3(OH)2(CO3)2
Hydromagnesite   -7.71    -16.47   -8.77  Mg5(CO3)4(OH)2:4H2O
K-Alum          -14.68    -19.85   -5.17  KAl(SO4)2:12H2O
K-Jarosite      -15.79    -30.59  -14.80  KFe3(SO4)2(OH)6
K2Cr2O7         -73.35    -90.59  -17.24  K2Cr2O7
K2CrO4          -38.58    -39.09   -0.51  K2CrO4
K2MoO4          -10.04     -6.78    3.26  K2MoO4
Kaolinite        -1.70      5.74    7.43  Al2Si2O5(OH)4
Langite         -52.36    -34.87   17.49  Cu4(OH)6SO4:H2O
Larnakite         0.30     -0.14   -0.43  PbO:PbSO4
Laurionite       -3.88     -3.26    0.62  PbOHCl
Lepidocrocite    -2.69     -1.32    1.37  FeOOH
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Li2CrO4         -45.61    -40.75    4.86  Li2CrO4
Li2MoO4         -10.88     -8.44    2.44  Li2MoO4
Lime            -21.46     11.24   32.70  CaO
Litharge         -4.56      8.14   12.69  PbO
Mackinawite     -18.61    -22.21   -3.60  FeS
Maghemite        -9.01     -2.63    6.39  Fe2O3
Magnesioferrite  -6.08     10.78   16.86  Fe2MgO4
Magnesite         0.00     -7.46   -7.46  MgCO3
Magnetite        -0.00      3.40    3.40  Fe3O4
Malachite       -24.78    -30.09   -5.31  Cu2(OH)2CO3
Manganite       -12.02     13.32   25.34  MnOOH
Massicot         -4.76      8.14   12.89  PbO
Melanothallite  -33.65    -27.39    6.26  CuCl2
Melanterite      -8.23    -10.44   -2.21  FeSO4:7H2O
Mg(OH)2(active)  -5.40     13.40   18.79  Mg(OH)2
Mg(VO3)2        -20.49     -9.21   11.28  Mg(VO3)2
Mg2Sb3         -149.40    -74.71   74.68  Mg2Sb3
Mg2V2O7         -22.17      4.19   26.36  Mg2V2O7
MgCr2O4          -5.15     11.05   16.20  MgCr2O4
MgCrO4          -43.47    -38.09    5.38  MgCrO4
MgMoO4           -3.93     -5.78   -1.85  MgMoO4
Minium          -37.73     35.79   73.52  Pb3O4
Mirabilite       -1.35     -2.46   -1.11  Na2SO4:10H2O
Mn(VO3)2        -19.88    -14.98    4.90  Mn(VO3)2
Mn2(SO4)3       -67.60    -73.31   -5.71  Mn2(SO4)3
Mn2Sb           -94.82    -33.74   61.08  Mn2Sb
Mn3(AsO4)2:8H2O -11.50      1.00   12.50  Mn3(AsO4)2:8H2O
MnCl2:4H2O      -17.90    -15.19    2.72  MnCl2:4H2O
MnS(grn)        -20.78    -20.61    0.17  MnS
MnS(pnk)        -23.95    -20.61    3.34  MnS
MnSb            -52.44    -55.35   -2.91  MnSb
MnSO4           -11.37     -8.78    2.58  MnSO4
MoO3            -11.19    -19.19   -8.00  MoO3
MoS2            -16.79    -87.05  -70.26  MoS2
Na-Jarosite     -18.58    -29.78  -11.20  NaFe3(SO4)2(OH)6
Na2Cr2O7        -79.07    -88.96   -9.90  Na2Cr2O7
Na2CrO4         -40.40    -37.47    2.93  Na2CrO4
Na2Mo2O7         -7.74    -24.34  -16.60  Na2Mo2O7
Na2MoO4          -6.65     -5.16    1.49  Na2MoO4
Na2MoO4:2H2O     -6.40     -5.17    1.22  Na2MoO4:2H2O
Na3Sb          -116.73    -22.27   94.45  Na3Sb
Na3VO4          -26.95      9.74   36.68  Na3VO4
Na4V2O7         -31.96      5.44   37.40  Na4V2O7
Nantokite       -12.27    -19.00   -6.73  CuCl
NaSb            -48.10    -24.93   23.17  NaSb
Natron           -5.60     -6.91   -1.31  Na2CO3:10H2O
NaVO3            -8.15     -4.29    3.86  NaVO3
Nesquehonite     -2.81     -7.48   -4.67  MgCO3:3H2O
Nsutite         -23.85     -6.34   17.50  MnO2
O2(g)           -60.34     22.75   83.09  O2
Orpiment        -30.45    -91.52  -61.07  As2S3
Pb(OH)2          -0.02      8.13    8.15  Pb(OH)2
Pb10(OH)6O(CO3)6 -35.07     -43.83   -8.76  Pb10(OH)6O(CO3)6
Pb2(OH)3Cl       -3.92      4.87    8.79  Pb2(OH)3Cl
Pb2O(OH)2        -9.92     16.27   26.19  Pb2O(OH)2
Pb2O3           -33.39     27.65   61.04  Pb2O3
Pb2OCO3          -4.03     -4.59   -0.56  Pb2OCO3
Pb2V2O7          -4.44     -6.34   -1.90  Pb2V2O7
Pb3(AsO4)2       -3.22      2.58    5.80  Pb3(AsO4)2
Pb3(VO4)2        -4.34      1.80    6.14  Pb3(VO4)2
Pb3O2CO3         -7.47      3.55   11.02  Pb3O2CO3
Pb3O2SO4         -2.69      8.00   10.69  Pb3O2SO4
Pb4(OH)6SO4      -4.99     16.11   21.10  Pb4(OH)6SO4
Pb4O3SO4         -5.74     16.14   21.88  Pb4O3SO4
PbCrO4          -30.76    -43.36  -12.60  PbCrO4
Pbmetal          -7.48     -3.23    4.25  Pb
PbMoO4            4.57    -11.05  -15.62  PbMoO4
PbO:0.3H2O       -4.84      8.14   12.98  PbO:0.33H2O
Periclase        -8.18     13.41   21.58  MgO
```

```
  Phosgenite       -7.57    -27.38  -19.81  PbCl2:PbCO3
  Plattnerite     -30.09     19.51   49.60  PbO2
  Portlandite     -11.58     11.23   22.80  Ca(OH)2
  Pyrite          -20.58    -39.09  -18.51  FeS2
  Pyrochroite      -7.57      7.63   15.19  Mn(OH)2
  Pyrolusite      -22.37     19.01   41.38  MnO2
  Quartz            0.00     -4.00   -4.00  SiO2
  Realgar         -17.58    -37.32  -19.75  AsS
  Rhodochrosite    -2.65    -13.23  -10.58  MnCO3
  Sb(OH)3          -2.10     -9.21   -7.11  Sb(OH)3
  Sb2O4           -10.43     -7.03    3.40  Sb2O4
  Sb2O5           -34.61    -44.28   -9.67  Sb2O5
  Sb4O6(cubic)    -18.54    -36.80  -18.26  Sb4O6
  Sb4O6(orth)     -18.90    -36.80  -17.90  Sb4O6
  SbCl3           -43.95    -43.38    0.57  SbCl3
  Sbmetal         -14.57    -26.26  -11.69  Sb
  SbO2              0.00    -27.82  -27.82  SbO2
  Senarmontite     -6.04    -18.40  -12.37  Sb2O3
  Sepiolite        -0.98     14.78   15.76  Mg2Si3O7.5OH:3H2O
  Sepiolite(A)     -4.00     14.78   18.78  Mg2Si3O7.5OH:3H2O
  Siderite         -4.59    -14.83  -10.24  FeCO3
  SiO2(am-gel)     -1.29     -4.00   -2.71  SiO2
  SiO2(am-ppt)     -1.26     -4.00   -2.74  SiO2
  Spinel           -9.69     27.16   36.85  MgAl2O4
  SrCrO4          -37.05    -41.70   -4.65  SrCrO4
  Stibnite        -52.68   -103.14  -50.46  Sb2S3
  Strontianite     -1.80    -11.07   -9.27  SrCO3
  Sulfur          -14.73    -16.87   -2.14  S
  Tenorite        -12.25     -4.61    7.64  CuO
  Thenardite       -2.71     -2.39    0.32  Na2SO4
  Thermonatrite    -7.48     -6.84    0.64  Na2CO3:H2O
  V(OH)3           -7.68     -0.09    7.59  V(OH)3
  V2O5            -21.26    -22.62   -1.36  V2O5
  V3O5            -13.48    -11.65    1.84  V3O5
  V4O7            -18.93    -11.74    7.19  V4O7
  V6O13           -29.73    -90.59  -60.86  V6O13
  Valentinite      -9.92    -18.40   -8.48  Sb2O3
  VCl2            -47.43    -28.55   18.87  VCl2
  VCl3            -57.69    -34.26   23.43  VCl3
  Vmetal          -61.17    -17.14   44.03  V
  VO              -20.52     -5.77   14.76  VO
  VO(OH)2          -5.25     -0.10    5.15  VO(OH)2
  VO2Cl           -25.54    -22.70    2.84  VO2Cl
  VOCl            -22.63    -11.48   11.15  VOCl
  VOCl2           -35.64    -22.88   12.76  VOCl2
  VOSO4           -20.12    -16.51    3.61  VOSO4
  Witherite        -7.99    -16.56   -8.57  BaCO3

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

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End of simulation.
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Reading input data for simulation 6.
------------------------------------

       USE  SOLUTION 4
       EQUILIBRIUM_PHASES 6
       Al2O3  0      0
       Anhydrite     0      0
       Anilite 0     0
       Aragonite     0      0
       Artinite      0      0
       Ba3(AsO4)2    0      0
       Barite  0     0
       BlaubleiII    0      0
```

```
       Boehmite       0       0
       Brucite 0      0
       Calcite 0      0
       CaMoO4  0      0
       Chrysotile     0       0
       Chalcocite     0       0
       Chalcedony     0       0
       Celestite      0       0
       Cr(OH)3(am)    0       0
       Cr2O3   0      0
       Cristobalite   0       0
       Cu2Sb:3H2O     0       0
       Cuprousferrite 0       0
       Cuprite 0      0
       Cupricferrite  0       0
       Cumetal 0      0
       Cu3Sb   0      0
       Diaspore       0       0
       Djurleite      0       0
       Dolomite(disordered)   0      0
       Dolomite(ordered)      0      0
       Fe(OH)2 0      0
       Fe(OH)2.7Cl.3  0       0
       Greenalite     0       0
       Goethite       0       0
       Gibbsite       0       0
       Ferrihydrite   0       0
       FeMoO4  0      0
       FeCr2O4 0      0
       Fe3(OH)8       0       0
       Gypsum  0      0
       Halloysite     0       0
       Hematite       0       0
       Hercynite      0       0
       Huntite 0      0
       Hydromagnesite 0       0
       MgCr2O4 0      0
       Magnetite      0       0
       Magnesite         0       0
       Magnesioferrite        0      0
       Maghemite      0       0
       Kaolinite      0       0
       K-Jarosite     0       0
       Lepidocrocite  0       0
       Nesquehonite   0       0
       Quartz  0      0
       PbMoO4  0      0
       SiO2(am-gel)   0       0
       Siderite       0       0
       SiO2(am-ppt)   0       0
       Sepiolite(A)   0       0
       Sepiolite      0       0
       Senarmontite   0       0
       Rhodochrosite  0       0
       Sb(OH)3 0      0
       SbO2    0      0
       Strontianite   0       0
       Spinel  0      0
       Witherite      0       0
       SAVE SOLUTION 4
       END
-----------------------------------------
Beginning of batch-reaction calculations.
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Reaction step 1.

Using solution 4.     Solution after simulation 2.
Using pure phase assemblage 6.
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```
-------------------------------Phase assemblage--------------------------------

                                                      Moles in assemblage
Phase               SI  log IAP  log K(T, P)   Initial       Final       Delta

Al2O3            -5.90    13.75     19.65   0.000e+00           0   0.000e+00
Anhydrite        -0.75    -5.11     -4.36   0.000e+00           0   0.000e+00
Anilite          -8.78   -40.66    -31.88   0.000e+00           0   0.000e+00
Aragonite        -1.33    -9.63     -8.30   0.000e+00           0   0.000e+00
Artinite         -3.69     5.91      9.60   0.000e+00           0   0.000e+00
Ba3(AsO4)2        0.00    -8.91     -8.91   0.000e+00   8.173e-05   8.173e-05
Barite           -2.08   -12.06     -9.98   0.000e+00           0   0.000e+00
BlaubleiII       -9.68   -36.96    -27.28   0.000e+00           0   0.000e+00
Boehmite         -1.70     6.87      8.58   0.000e+00           0   0.000e+00
Brucite          -3.45    13.40     16.84   0.000e+00           0   0.000e+00
CaMoO4           -0.00    -7.95     -7.95   0.000e+00   5.246e-04   5.246e-04
Calcite          -1.15    -9.63     -8.48   0.000e+00           0   0.000e+00
Celestite         0.00    -6.62     -6.62   0.000e+00   1.363e-02   1.363e-02
Chalcedony       -0.45    -4.00     -3.55   0.000e+00           0   0.000e+00
Chalcocite       -8.39   -43.31    -34.92   0.000e+00           0   0.000e+00
Chrysotile        0.00    32.20     32.20   0.000e+00   1.090e-02   1.090e-02
Cr(OH)3(am)      -0.44    -1.19     -0.75   0.000e+00           0   0.000e+00
Cr2O3             0.00    -2.36     -2.36   0.000e+00   6.943e-08   6.943e-08
Cristobalite     -0.65    -4.00     -3.35   0.000e+00           0   0.000e+00
Cu2Sb:3H2O      -20.61   -55.49    -34.88   0.000e+00           0   0.000e+00
Cu3Sb           -23.46   -66.06    -42.59   0.000e+00           0   0.000e+00
Cumetal          -4.52   -13.28     -8.76   0.000e+00           0   0.000e+00
Cupricferrite   -13.23    -7.25      5.99   0.000e+00           0   0.000e+00
Cuprite         -13.79   -15.20     -1.41   0.000e+00           0   0.000e+00
Cuprousferrite    0.00    -8.92     -8.92   0.000e+00   1.561e-05   1.561e-05
Diaspore          0.00     6.87      6.87   0.000e+00   2.348e-03   2.348e-03
Djurleite        -8.69   -42.61    -33.92   0.000e+00           0   0.000e+00
Dolomite(disordered)   -0.55   -17.09    -16.54   0.000e+00           0
0.000e+00
Dolomite(ordered)    0.00   -17.09    -17.09    0.000e+00   2.167e-01   2.167e-01
Fe(OH)2          -7.54     6.03     13.56   0.000e+00           0   0.000e+00
Fe(OH)2.7Cl.3    -1.68    -4.72     -3.04   0.000e+00           0   0.000e+00
Fe3(OH)8        -16.85     3.37     20.22   0.000e+00           0   0.000e+00
FeCr2O4          -3.52     3.68      7.20   0.000e+00           0   0.000e+00
FeMoO4           -3.06   -13.15    -10.09   0.000e+00           0   0.000e+00
Ferrihydrite     -4.52    -1.33      3.19   0.000e+00           0   0.000e+00
Gibbsite         -1.43     6.86      8.29   0.000e+00           0   0.000e+00
Goethite         -1.81    -1.32      0.49   0.000e+00           0   0.000e+00
Greenalite      -10.72    10.09     20.81   0.000e+00           0   0.000e+00
Gypsum           -0.52    -5.13     -4.61   0.000e+00           0   0.000e+00
Halloysite       -3.84     5.74      9.57   0.000e+00           0   0.000e+00
Hematite         -1.22    -2.63     -1.42   0.000e+00           0   0.000e+00
Hercynite        -3.10    19.79     22.89   0.000e+00           0   0.000e+00
Huntite          -2.04   -32.01    -29.97   0.000e+00           0   0.000e+00
Hydromagnesite   -7.71   -16.48     -8.77   0.000e+00           0   0.000e+00
K-Jarosite      -15.70   -30.50    -14.80   0.000e+00           0   0.000e+00
Kaolinite        -1.70     5.74      7.43   0.000e+00           0   0.000e+00
Lepidocrocite    -2.69    -1.32      1.37   0.000e+00           0   0.000e+00
Maghemite        -9.02    -2.63      6.39   0.000e+00           0   0.000e+00
Magnesioferrite   -6.09    10.77     16.86    0.000e+00           0   0.000e+00
Magnesite         0.00    -7.46     -7.46   0.000e+00   1.446e-01   1.446e-01
Magnetite         0.00     3.40      3.40   0.000e+00   6.965e-04   6.965e-04
MgCr2O4          -5.15    11.05     16.20   0.000e+00           0   0.000e+00
Nesquehonite     -2.82    -7.49     -4.67   0.000e+00           0   0.000e+00
PbMoO4           -0.00   -15.62    -15.62   0.000e+00   4.839e-05   4.839e-05
Quartz            0.00    -4.00     -4.00   0.000e+00   2.481e-01   2.481e-01
Rhodochrosite    -2.79   -13.37    -10.58   0.000e+00           0   0.000e+00
Sb(OH)3          -2.09    -9.20     -7.11   0.000e+00           0   0.000e+00
SbO2              0.00   -27.82    -27.82   0.000e+00   6.204e-05   6.204e-05
Senarmontite     -6.02   -18.38    -12.37   0.000e+00           0   0.000e+00
Sepiolite        -0.98    14.78     15.76   0.000e+00           0   0.000e+00
Sepiolite(A)     -4.00    14.78     18.78   0.000e+00           0   0.000e+00
SiO2(am-gel)     -1.29    -4.00     -2.71   0.000e+00           0   0.000e+00
```

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SiO2(am-ppt)     -1.26    -4.00     -2.74    0.000e+00           0   0.000e+00
Siderite         -4.59   -14.83    -10.24    0.000e+00           0   0.000e+00
Spinel           -9.69    27.16     36.85    0.000e+00           0   0.000e+00
Strontianite     -1.87   -11.14     -9.27    0.000e+00           0   0.000e+00
Witherite        -8.01   -16.58     -8.57    0.000e+00           0   0.000e+00

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

       Elements           Molality       Moles

       Al                5.898e-09   8.950e-09
       As                7.804e-04   1.184e-03
       Ba                9.642e-11   1.463e-10
       C                 1.819e-03   2.760e-03
       Ca                2.627e-03   3.987e-03
       Cl                1.556e-04   2.361e-04
       Cr                1.395e-08   2.118e-08
       Cu                3.027e-15   4.593e-15
       Fe                1.244e-07   1.888e-07
       K                 9.667e-02   1.467e-01
       Li                1.332e-02   2.021e-02
       Mg                3.346e-01   5.078e-01
       Mn                3.468e-06   5.262e-06
       Mo                1.198e-04   1.818e-04
       Na                5.985e-01   9.082e-01
       Pb                9.630e-10   1.461e-09
       S                 3.953e-01   5.999e-01
       Sb                1.251e-09   1.898e-09
       Si                8.102e-05   1.229e-04
       Sr                7.471e-05   1.134e-04
       V                 6.859e-04   1.041e-03

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

                                       pH  =   7.396      Charge balance
                                       pe  =  -1.714      Adjusted to redox
equilibrium
                        Activity of water  =   0.981
                 Ionic strength (mol/kgw)  =   7.756e-01
                       Mass of water (kg)  =   1.517e+00
                 Total alkalinity (eq/kg)  =   2.138e-03
                       Total CO2 (mol/kg)  =   1.819e-03
                         Temperature (°C)  =  25.00
                  Electrical balance (eq)  =   8.947e-01
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  52.15
                               Iterations  =  21
                                  Total H  = 1.684662e+02
                                  Total O  = 8.664483e+01

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

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

   OH-             4.108e-07   2.457e-07    -6.386    -6.610    -0.223     (0)
   H+              5.301e-08   4.020e-08    -7.276    -7.396    -0.120      0.00
   H2O             5.551e+01   9.808e-01     1.744    -0.008     0.000     18.07
Al            5.898e-09
   Al(OH)4-        5.742e-09   3.664e-09    -8.241    -8.436    -0.195     (0)
   Al(OH)3         1.185e-10   1.185e-10    -9.926    -9.926     0.000     (0)
   Al(OH)2+        3.618e-11   2.416e-11   -10.442   -10.617    -0.175     (0)
   AlOH+2          6.223e-13   1.238e-13   -12.206   -12.907    -0.701     (0)
   AlSO4+          1.666e-13   1.063e-13   -12.778   -12.973    -0.195     (0)
   Al(SO4)2-       4.853e-14   3.096e-14   -13.314   -13.509    -0.195     (0)
   Al+3            6.079e-15   5.040e-16   -14.216   -15.298    -1.081     (0)
   AlMo6O21-3      9.407e-28   8.527e-32   -27.027   -31.069    -4.043     (0)
As(3)         4.599e-04
   H3AsO3          4.439e-04   4.439e-04    -3.353    -3.353     0.000     (0)
   H2AsO3-         1.593e-05   5.664e-06    -4.798    -5.247    -0.449     (0)
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   HAsO3-2         8.048e-09   1.285e-10    -8.094    -9.891    -1.797     (0)
   H4AsO3+         2.487e-11   8.841e-12   -10.604   -11.054    -0.449     (0)
   AsO3-3          1.360e-12   1.232e-16   -11.867   -15.909    -4.043     (0)
As(5)         3.205e-04
   HAsO4-2         3.111e-04   4.967e-06    -3.507    -5.304    -1.797     (0)
   H2AsO4-         5.123e-06   1.821e-06    -5.291    -5.740    -0.449     (0)
   AsO4-3          4.311e-06   3.908e-10    -5.365    -9.408    -4.043     (0)
   H3AsO4          1.064e-11   1.272e-11   -10.973   -10.896     0.078     (0)
Ba            9.642e-11
   Ba+2            9.609e-11   3.177e-11   -10.017   -10.498    -0.481     (0)
   BaHCO3+         3.140e-13   2.152e-13   -12.503   -12.667    -0.164     (0)
   BaCO3           1.348e-14   1.348e-14   -13.870   -13.870     0.000     (0)
   BaOH+           5.200e-17   3.407e-17   -16.284   -16.468    -0.184     (0)
C(4)          1.819e-03
   HCO3-           1.062e-03   7.092e-04    -2.974    -3.149    -0.175     (0)
   MgHCO3+         4.914e-04   3.042e-04    -3.309    -3.517    -0.208     (0)
   NaHCO3          1.552e-04   1.552e-04    -3.809    -3.809     0.000     (0)
   H2CO3           6.411e-05   6.411e-05    -4.193    -4.193     0.000     (0)
   MgCO3           2.884e-05   2.884e-05    -4.540    -4.540     0.000     (0)
   NaCO3-          8.976e-06   5.995e-06    -5.047    -5.222    -0.175     (0)
   CaHCO3+         5.462e-06   3.743e-06    -5.263    -5.427    -0.164     (0)
   CO3-2           2.502e-06   8.272e-07    -5.602    -6.082    -0.481     (0)
   CaCO3           3.715e-07   3.715e-07    -6.430    -6.430     0.000     (0)
   SrHCO3+         1.482e-07   1.015e-07    -6.829    -6.993    -0.164     (0)
   SrCO3           4.714e-09   4.714e-09    -8.327    -8.327     0.000     (0)
   MnHCO3+         1.110e-09   7.272e-10    -8.955    -9.138    -0.184     (0)
   FeHCO3+         2.339e-11   1.602e-11   -10.631   -10.795    -0.164     (0)
   PbCO3           1.507e-11   1.507e-11   -10.822   -10.822     0.000     (0)
   PbHCO3+         8.982e-12   3.193e-12   -11.047   -11.496    -0.449     (0)
   Pb(CO3)2-2      2.251e-12   3.594e-14   -11.648   -13.444    -1.797     (0)
   BaHCO3+         3.140e-13   2.152e-13   -12.503   -12.667    -0.164     (0)
   BaCO3           1.348e-14   1.348e-14   -13.870   -13.870     0.000     (0)
   CuCO3           1.959e-19   1.959e-19   -18.708   -18.708     0.000     (0)
   Cu(CO3)2-2      2.731e-20   4.362e-22   -19.564   -21.360    -1.797     (0)
   CuHCO3+         5.063e-21   1.800e-21   -20.296   -20.745    -0.449     (0)
Ca            2.627e-03
   CaSO4           1.765e-03   1.765e-03    -2.753    -2.753     0.000     (0)
   Ca+2            8.571e-04   2.834e-04    -3.067    -3.548    -0.481     (0)
   CaHCO3+         5.462e-06   3.743e-06    -5.263    -5.427    -0.164     (0)
   CaCO3           3.715e-07   3.715e-07    -6.430    -6.430     0.000     (0)
   CaOH+           2.028e-09   1.389e-09    -8.693    -8.857    -0.164     (0)
Cl            1.556e-04
   Cl-             1.556e-04   1.180e-04    -3.808    -3.928    -0.120     (0)
   MnCl+           1.165e-11   7.632e-12   -10.934   -11.117    -0.184     (0)
   PbCl+           7.134e-14   2.536e-14   -13.147   -13.596    -0.449     (0)
   MnCl2           1.272e-15   1.272e-15   -14.896   -14.896     0.000     (0)
   CrCl+2          1.569e-16   2.506e-18   -15.804   -17.601    -1.797     (0)
   CuCl            1.514e-16   1.514e-16   -15.820   -15.820     0.000     (0)
   PbCl2           1.336e-17   1.336e-17   -16.874   -16.874     0.000     (0)
   CuCl2-          6.029e-18   3.733e-18   -17.220   -17.428    -0.208     (0)
   VOCl+           1.260e-18   4.481e-19   -17.899   -18.349    -0.449     (0)
   MnCl3-          6.307e-20   4.132e-20   -19.200   -19.384    -0.184     (0)
   PbCl3-          1.766e-21   6.276e-22   -20.753   -21.202    -0.449     (0)
   CrOHCl2         1.380e-21   1.380e-21   -20.860   -20.860     0.000     (0)
   CuCl3-2         5.107e-22   9.415e-23   -21.292   -22.026    -0.734     (0)
   CrCl2+          7.890e-23   2.805e-23   -22.103   -22.552    -0.449     (0)
   CuCl+           1.215e-23   7.520e-24   -22.916   -23.124    -0.208     (0)
   PbCl4-2         2.119e-24   3.384e-26   -23.674   -25.471    -1.797     (0)
   FeCl+2          6.225e-26   1.147e-26   -25.206   -25.940    -0.734     (0)
   CuCl2           3.076e-28   3.076e-28   -27.512   -27.512     0.000     (0)
   FeCl2+          9.228e-30   6.047e-30   -29.035   -29.218    -0.184     (0)
   CuCl3-          5.470e-34   3.387e-34   -33.262   -33.470    -0.208     (0)
   FeCl3           7.133e-35   7.133e-35   -34.147   -34.147     0.000     (0)
   CuCl4-2         1.086e-39   2.002e-40   -38.964   -39.698    -0.734     (0)
   CrO3Cl-         0.000e+00   0.000e+00   -47.692   -48.142    -0.449     (0)
Cr(2)         1.271e-17
   Cr+2            1.271e-17   2.030e-19   -16.896   -18.693    -1.797     (0)
Cr(3)         1.395e-08
   Cr(OH)2+        7.419e-09   2.637e-09    -8.130    -8.579    -0.449     (0)
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   Cr(OH)+2        5.525e-09   8.822e-11    -8.258   -10.054    -1.797      (0)
   CrOHSO4         5.690e-10   5.690e-10    -9.245    -9.245     0.000      (0)
   Cr(OH)3         2.434e-10   2.434e-10    -9.614    -9.614     0.000      (0)
   Cr+3            1.811e-10   1.641e-14    -9.742   -13.785    -4.043      (0)
   CrO2-           8.249e-12   2.932e-12   -11.084   -11.533    -0.449      (0)
   Cr(OH)4-        6.698e-12   2.381e-12   -11.174   -11.623    -0.449      (0)
   CrSO4+          2.930e-12   1.042e-12   -11.533   -11.982    -0.449      (0)
   Cr2(OH)2SO4+2   2.841e-16   4.537e-18   -15.547   -17.343    -1.797      (0)
   CrCl+2          1.569e-16   2.506e-18   -15.804   -17.601    -1.797      (0)
   Cr2(OH)2(SO4)2   7.325e-18   7.325e-18   -17.135   -17.135     0.000      (0)
   CrOHCl2         1.380e-21   1.380e-21   -20.860   -20.860     0.000      (0)
   CrCl2+          7.890e-23   2.805e-23   -22.103   -22.552    -0.449      (0)
Cr(6)         1.726e-36
   NaCrO4-         9.928e-37   3.529e-37   -36.003   -36.452    -0.449      (0)
   CrO4-2          5.518e-37   1.825e-37   -36.258   -36.739    -0.481      (0)
   KCrO4-          1.147e-37   4.078e-38   -36.940   -37.390    -0.449      (0)
   HCrO4-          6.676e-38   2.373e-38   -37.175   -37.625    -0.449      (0)
   CrO3SO4-2       0.000e+00   0.000e+00   -42.297   -44.094    -1.797      (0)
   H2CrO4          0.000e+00   0.000e+00   -45.112   -45.112     0.000      (0)
   CrO3Cl-         0.000e+00   0.000e+00   -47.692   -48.142    -0.449      (0)
   Cr2O7-2         0.000e+00   0.000e+00   -71.904   -73.701    -1.797      (0)
Cu(1)         3.026e-15
   Cu+             2.869e-15   1.020e-15   -14.542   -14.992    -0.449      (0)
   CuCl            1.514e-16   1.514e-16   -15.820   -15.820     0.000      (0)
   CuCl2-          6.029e-18   3.733e-18   -17.220   -17.428    -0.208      (0)
   CuCl3-2         5.107e-22   9.415e-23   -21.292   -22.026    -0.734      (0)
   Cu(S4)2-3       1.878e-38   5.566e-39   -37.726   -38.254    -0.528      (0)
   CuS4S5-3        3.211e-39   1.036e-39   -38.493   -38.984    -0.491      (0)
Cu(2)         6.524e-19
   CuSO4           2.504e-19   2.504e-19   -18.601   -18.601     0.000      (0)
   CuCO3           1.959e-19   1.959e-19   -18.708   -18.708     0.000      (0)
   Cu+2            1.216e-19   4.022e-20   -18.915   -19.396    -0.481      (0)
   CuOH+           5.048e-20   3.125e-20   -19.297   -19.505    -0.208      (0)
   Cu(CO3)2-2      2.731e-20   4.362e-22   -19.564   -21.360    -1.797      (0)
   CuHCO3+         5.063e-21   1.800e-21   -20.296   -20.745    -0.449      (0)
   Cu(OH)2         1.532e-21   1.532e-21   -20.815   -20.815     0.000      (0)
   CuCl+           1.215e-23   7.520e-24   -22.916   -23.124    -0.208      (0)
   Cu(OH)3-        2.172e-24   7.721e-25   -23.663   -24.112    -0.449      (0)
   CuCl2           3.076e-28   3.076e-28   -27.512   -27.512     0.000      (0)
   Cu(OH)4-2       9.349e-29   1.493e-30   -28.029   -29.826    -1.797      (0)
   Cu2(OH)2+2      1.536e-33   2.453e-35   -32.814   -34.610    -1.797      (0)
   CuCl3-          5.470e-34   3.387e-34   -33.262   -33.470    -0.208      (0)
   CuCl4-2         1.086e-39   2.002e-40   -38.964   -39.698    -0.734      (0)
   Cu(HS)3-        0.000e+00   0.000e+00   -55.214   -55.663    -0.449      (0)
Fe(2)         1.244e-07
   Fe+2            1.124e-07   1.795e-09    -6.949    -8.746    -1.797      (0)
   FeSO4           1.197e-08   1.197e-08    -7.922    -7.922     0.000      (0)
   FeOH+           2.679e-11   1.755e-11   -10.572   -10.756    -0.184      (0)
   FeHCO3+         2.339e-11   1.602e-11   -10.631   -10.795    -0.164      (0)
   Fe(OH)2         3.426e-15   3.426e-15   -14.465   -14.465     0.000      (0)
   Fe(OH)3-        4.062e-16   2.662e-16   -15.391   -15.575    -0.184      (0)
   Fe(HS)2         0.000e+00   0.000e+00   -41.241   -41.241     0.000      (0)
   Fe(HS)3-        0.000e+00   0.000e+00   -59.477   -59.926    -0.449      (0)
Fe(3)         8.646e-14
   Fe(OH)2+        7.313e-14   4.884e-14   -13.136   -13.311    -0.175      (0)
   Fe(OH)3         1.289e-14   1.289e-14   -13.890   -13.890     0.000      (0)
   Fe(OH)4-        4.414e-16   2.948e-16   -15.355   -15.530    -0.175      (0)
   FeOH+2          2.772e-18   5.109e-19   -17.557   -18.292    -0.734      (0)
   Fe(SO4)2-       1.605e-21   5.707e-22   -20.794   -21.244    -0.449      (0)
   FeSO4+          1.499e-21   9.822e-22   -20.824   -21.008    -0.184      (0)
   Fe+3            3.885e-23   3.221e-24   -22.411   -23.492    -1.081      (0)
   FeCl+2          6.225e-26   1.147e-26   -25.206   -25.940    -0.734      (0)
   Fe2(OH)2+4      1.329e-28   8.644e-36   -27.876   -35.063    -7.187      (0)
   FeCl2+          9.228e-30   6.047e-30   -29.035   -29.218    -0.184      (0)
   FeCl3           7.133e-35   7.133e-35   -34.147   -34.147     0.000      (0)
   Fe3(OH)4+5      1.035e-36   0.000e+00   -35.985   -47.215   -11.230      (0)
H(0)          5.127e-15
   H2              2.563e-15   3.065e-15   -14.591   -14.514     0.078      (0)
K             9.667e-02
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   K+             7.934e-02   6.016e-02    -1.101    -1.221    -0.120     (0)
   KSO4-          1.733e-02   1.158e-02    -1.761    -1.936    -0.175     (0)
   KCrO4-         1.147e-37   4.078e-38   -36.940   -37.390    -0.449     (0)
Li             1.332e-02
   Li+            1.171e-02   8.878e-03    -1.932    -2.052    -0.120     (0)
   LiSO4-         1.607e-03   1.053e-03    -2.794    -2.977    -0.184     (0)
Mg             3.346e-01
   MgSO4          2.073e-01   2.073e-01    -0.683    -0.683     0.000     (0)
   Mg+2           1.268e-01   4.192e-02    -0.897    -1.378    -0.481     (0)
   MgHCO3+        4.914e-04   3.042e-04    -3.309    -3.517    -0.208     (0)
   MgCO3          2.884e-05   2.884e-05    -4.540    -4.540     0.000     (0)
   MgOH+          5.871e-06   4.100e-06    -5.231    -5.387    -0.156     (0)
Mn(2)          3.468e-06
   Mn+2           3.218e-06   5.139e-08    -5.492    -7.289    -1.797     (0)
   MnSO4          2.484e-07   2.484e-07    -6.605    -6.605     0.000     (0)
   MnHCO3+        1.110e-09   7.272e-10    -8.955    -9.138    -0.184     (0)
   MnOH+          4.840e-11   3.172e-11   -10.315   -10.499    -0.184     (0)
   MnCl+          1.165e-11   7.632e-12   -10.934   -11.117    -0.184     (0)
   MnCl2          1.272e-15   1.272e-15   -14.896   -14.896     0.000     (0)
   MnCl3-         6.307e-20   4.132e-20   -19.200   -19.384    -0.184     (0)
   Mn(OH)3-       1.806e-20   1.183e-20   -19.743   -19.927    -0.184     (0)
   Mn(OH)4-2      5.092e-26   9.385e-27   -25.293   -26.028    -0.734     (0)
Mn(3)          5.349e-34
   Mn+3           5.349e-34   4.435e-35   -33.272   -34.353    -1.081     (0)
Mn(6)          0.000e+00
   MnO4-2         0.000e+00   0.000e+00   -72.700   -73.434    -0.734     (0)
Mn(7)          0.000e+00
   MnO4-          0.000e+00   0.000e+00   -84.280   -84.520    -0.240     (0)
Mo             1.198e-04
   MoO4-2         1.197e-04   3.959e-05    -3.922    -4.402    -0.481     (0)
   HMoO4-         8.907e-08   3.166e-08    -7.050    -7.499    -0.449     (0)
   H2MoO4         9.323e-12   9.323e-12   -11.030   -11.030     0.000     (0)
   Mo7O24-6       1.625e-21   1.097e-37   -20.789   -36.960   -16.171     (0)
   HMo7O24-5      1.823e-27   1.075e-38   -26.739   -37.969   -11.230     (0)
   AlMo6O21-3     9.407e-28   8.527e-32   -27.027   -31.069    -4.043     (0)
   H2Mo7O24-4     4.023e-34   0.000e+00   -33.395   -40.582    -7.187     (0)
   H3Mo7O24-3     0.000e+00   0.000e+00   -40.690   -44.732    -4.043     (0)
Na             5.985e-01
   Na+            5.133e-01   3.892e-01    -0.290    -0.410    -0.120     (0)
   NaSO4-         8.506e-02   5.681e-02    -1.070    -1.246    -0.175     (0)
   NaHCO3         1.552e-04   1.552e-04    -3.809    -3.809     0.000     (0)
   NaCO3-         8.976e-06   5.995e-06    -5.047    -5.222    -0.175     (0)
   NaCrO4-        9.928e-37   3.529e-37   -36.003   -36.452    -0.449     (0)
O(0)           0.000e+00
   O2             0.000e+00   0.000e+00   -63.362   -63.285     0.078     (0)
Pb             9.630e-10
   Pb(SO4)2-2     8.272e-10   1.321e-11    -9.082   -10.879    -1.797     (0)
   PbSO4          8.066e-11   8.066e-11   -10.093   -10.093     0.000     (0)
   Pb+2           1.832e-11   6.059e-12   -10.737   -11.218    -0.481     (0)
   PbCO3          1.507e-11   1.507e-11   -10.822   -10.822     0.000     (0)
   PbOH+          1.052e-11   3.739e-12   -10.978   -11.427    -0.449     (0)
   PbHCO3+        8.982e-12   3.193e-12   -11.047   -11.496    -0.449     (0)
   Pb(CO3)2-2     2.251e-12   3.594e-14   -11.648   -13.444    -1.797     (0)
   PbCl+          7.134e-14   2.536e-14   -13.147   -13.596    -0.449     (0)
   Pb(OH)2        2.905e-14   2.905e-14   -13.537   -13.537     0.000     (0)
   Pb(OH)3-       2.008e-17   7.138e-18   -16.697   -17.146    -0.449     (0)
   PbCl2          1.336e-17   1.336e-17   -16.874   -16.874     0.000     (0)
   Pb2OH+3        3.961e-18   3.591e-22   -17.402   -21.445    -4.043     (0)
   Pb(OH)4-2      2.690e-20   4.295e-22   -19.570   -21.367    -1.797     (0)
   PbCl3-         1.766e-21   6.276e-22   -20.753   -21.202    -0.449     (0)
   PbCl4-2        2.119e-24   3.384e-26   -23.674   -25.471    -1.797     (0)
   Pb3(OH)4+2     6.390e-27   1.020e-28   -26.194   -27.991    -1.797     (0)
   Pb4(OH)4+4     7.553e-29   4.911e-36   -28.122   -35.309    -7.187     (0)
   Pb(HS)2        4.053e-38   4.053e-38   -37.392   -37.392     0.000     (0)
   Pb(HS)3-       0.000e+00   0.000e+00   -56.365   -56.814    -0.449     (0)
S(-2)          8.171e-21
   HS-            5.332e-21   1.895e-21   -20.273   -20.722    -0.449     (0)
   S5-2           1.274e-21   2.034e-23   -20.895   -22.692    -1.797     (0)
   H2S            7.978e-22   7.978e-22   -21.098   -21.098     0.000     (0)
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   S6-2            3.884e-22   6.202e-24   -21.411   -23.207    -1.797    (0)
   S4-2            3.232e-22   5.161e-24   -21.491   -23.287    -1.797    (0)
   S3-2            5.053e-23   8.069e-25   -22.296   -24.093    -1.797    (0)
   S2-2            4.869e-24   7.775e-26   -23.313   -25.109    -1.797    (0)
   S-2             1.282e-30   2.363e-31   -29.892   -30.626    -0.734    (0)
   Pb(HS)2         4.053e-38   4.053e-38   -37.392   -37.392     0.000    (0)
   Cu(S4)2-3       1.878e-38   5.566e-39   -37.726   -38.254    -0.528    (0)
   CuS4S5-3        3.211e-39   1.036e-39   -38.493   -38.984    -0.491    (0)
   Fe(HS)2         0.000e+00   0.000e+00   -41.241   -41.241     0.000    (0)
   Cu(HS)3-        0.000e+00   0.000e+00   -55.214   -55.663    -0.449    (0)
   Pb(HS)3-        0.000e+00   0.000e+00   -56.365   -56.814    -0.449    (0)
   Fe(HS)3-        0.000e+00   0.000e+00   -59.477   -59.926    -0.449    (0)
   Sb2S4-2         0.000e+00   0.000e+00   -64.854   -66.650    -1.797    (0)
S(6)          3.953e-01
   MgSO4           2.073e-01   2.073e-01    -0.683    -0.683     0.000    (0)
   NaSO4-          8.506e-02   5.681e-02    -1.070    -1.246    -0.175    (0)
   SO4-2           8.220e-02   2.718e-02    -1.085    -1.566    -0.481    (0)
   KSO4-           1.733e-02   1.158e-02    -1.761    -1.936    -0.175    (0)
   CaSO4           1.765e-03   1.765e-03    -2.753    -2.753     0.000    (0)
   LiSO4-          1.607e-03   1.053e-03    -2.794    -2.977    -0.184    (0)
   SrSO4           4.786e-05   4.786e-05    -4.320    -4.320     0.000    (0)
   MnSO4           2.484e-07   2.484e-07    -6.605    -6.605     0.000    (0)
   HSO4-           1.673e-07   1.068e-07    -6.776    -6.972    -0.195    (0)
   FeSO4           1.197e-08   1.197e-08    -7.922    -7.922     0.000    (0)
   Pb(SO4)2-2      8.272e-10   1.321e-11    -9.082   -10.879    -1.797    (0)
   CrOHSO4         5.690e-10   5.690e-10    -9.245    -9.245     0.000    (0)
   PbSO4           8.066e-11   8.066e-11   -10.093   -10.093     0.000    (0)
   CrSO4+          2.930e-12   1.042e-12   -11.533   -11.982    -0.449    (0)
   AlSO4+          1.666e-13   1.063e-13   -12.778   -12.973    -0.195    (0)
   Al(SO4)2-       4.853e-14   3.096e-14   -13.314   -13.509    -0.195    (0)
   VOSO4           1.013e-14   1.013e-14   -13.994   -13.994     0.000    (0)
   Cr2(OH)2SO4+2   2.841e-16   4.537e-18   -15.547   -17.343    -1.797    (0)
   Cr2(OH)2(SO4)2   7.325e-18   7.325e-18   -17.135   -17.135     0.000    (0)
   VO2SO4-         3.624e-19   1.288e-19   -18.441   -18.890    -0.449    (0)
   CuSO4           2.504e-19   2.504e-19   -18.601   -18.601     0.000    (0)
   VSO4+           2.069e-21   7.356e-22   -20.684   -21.133    -0.449    (0)
   Fe(SO4)2-       1.605e-21   5.707e-22   -20.794   -21.244    -0.449    (0)
   FeSO4+          1.499e-21   9.822e-22   -20.824   -21.008    -0.184    (0)
   CrO3SO4-2       0.000e+00   0.000e+00   -42.297   -44.094    -1.797    (0)
Sb(3)         1.247e-09
   Sb(OH)3         6.247e-10   6.247e-10    -9.204    -9.204     0.000    (0)
   HSbO2           6.217e-10   6.217e-10    -9.206    -9.206     0.000    (0)
   SbO2-           7.047e-14   2.505e-14   -13.152   -13.601    -0.449    (0)
   Sb(OH)4-        3.885e-14   1.381e-14   -13.411   -13.860    -0.449    (0)
   Sb(OH)2+        1.749e-15   6.217e-16   -14.757   -15.206    -0.449    (0)
   SbO+            6.147e-16   2.185e-16   -15.211   -15.660    -0.449    (0)
   Sb2S4-2         0.000e+00   0.000e+00   -64.854   -66.650    -1.797    (0)
Sb(5)         4.231e-12
   SbO3-           4.228e-12   1.503e-12   -11.374   -11.823    -0.449    (0)
   Sb(OH)6-        2.188e-15   1.659e-15   -14.660   -14.780    -0.120    (0)
   SbO2+           1.998e-27   7.102e-28   -26.699   -27.149    -0.449    (0)
Si            8.102e-05
   H4SiO4          8.046e-05   9.619e-05    -4.094    -4.017     0.078    (0)
   H3SiO4-         5.587e-07   3.459e-07    -6.253    -6.461    -0.208    (0)
   H2SiO4-2        2.729e-12   5.430e-13   -11.564   -12.265    -0.701    (0)
Sr            7.471e-05
   SrSO4           4.786e-05   4.786e-05    -4.320    -4.320     0.000    (0)
   Sr+2            2.669e-05   8.826e-06    -4.574    -5.054    -0.481    (0)
   SrHCO3+         1.482e-07   1.015e-07    -6.829    -6.993    -0.164    (0)
   SrCO3           4.714e-09   4.714e-09    -8.327    -8.327     0.000    (0)
   SrOH+           2.187e-11   1.433e-11   -10.660   -10.844    -0.184    (0)
V(2)          1.235e-23
   V+2             9.102e-24   1.453e-25   -23.041   -24.838    -1.797    (0)
   VOH+            3.251e-24   1.156e-24   -23.488   -23.937    -0.449    (0)
V(3)          6.859e-04
   V(OH)3          6.859e-04   6.859e-04    -3.164    -3.164     0.000    (0)
   V(OH)2+         5.109e-14   1.816e-14   -13.292   -13.741    -0.449    (0)
   VOH+2           4.421e-16   7.060e-18   -15.354   -17.151    -1.797    (0)
   V+3             6.325e-19   5.733e-23   -18.199   -22.242    -4.043    (0)
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   VSO4+           2.069e-21   7.356e-22   -20.684   -21.133    -0.449     (0)
   V2(OH)2+4       4.836e-27   3.145e-34   -26.316   -33.502    -7.187     (0)
   V2(OH)3+3       4.004e-29   3.630e-33   -28.398   -32.440    -4.043     (0)
V(4)          2.780e-13
   V(OH)3+         1.831e-13   6.509e-14   -12.737   -13.186    -0.449     (0)
   VO+2            8.478e-14   1.354e-15   -13.072   -14.868    -1.797     (0)
   VOSO4           1.013e-14   1.013e-14   -13.994   -13.994     0.000     (0)
   VOCl+           1.260e-18   4.481e-19   -17.899   -18.349    -0.449     (0)
   H2V2O4+2        1.383e-20   2.208e-22   -19.859   -21.656    -1.797     (0)
V(5)          3.985e-11
   HVO4-2          2.318e-11   3.702e-13   -10.635   -12.432    -1.797     (0)
   H2VO4-          1.666e-11   5.923e-12   -10.778   -11.227    -0.449     (0)
   H3VO4           2.381e-15   2.381e-15   -14.623   -14.623     0.000     (0)
   VO4-3           5.091e-16   4.615e-20   -15.293   -19.336    -4.043     (0)
   HV2O7-3         8.356e-18   7.575e-22   -17.078   -21.121    -4.043     (0)
   V2O7-4          7.800e-18   5.072e-25   -17.108   -24.295    -7.187     (0)
   VO2SO4-         3.624e-19   1.288e-19   -18.441   -18.890    -0.449     (0)
   VO2+            2.618e-19   1.985e-19   -18.582   -18.702    -0.120     (0)
   H3V2O7-         2.612e-19   9.284e-20   -18.583   -19.032    -0.449     (0)
   V3O9-3          2.545e-24   2.307e-28   -23.594   -27.637    -4.043     (0)
   V4O12-4         8.930e-30   5.807e-37   -29.049   -36.236    -7.187     (0)
   V10O28-6        0.000e+00   0.000e+00   -76.680   -92.851   -16.171     (0)
   HV10O28-5       0.000e+00   0.000e+00   -80.830   -92.060   -11.230     (0)
   H2V10O28-4      0.000e+00   0.000e+00   -87.061   -94.248    -7.187     (0)

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

  Phase               SI** log IAP   log K(298 K,   1 atm)

  Al(OH)3(am)      -3.94      6.86   10.80  Al(OH)3
  Al2(MoO4)3      -46.17    -43.80    2.37  Al2(MoO4)3
  Al2O3            -5.90     13.75   19.65  Al2O3
  Al4(OH)10SO4    -11.58     11.12   22.70  Al4(OH)10SO4
  AlAsO4:2H2O      -8.82     -4.02    4.80  AlAsO4:2H2O
  AlOHSO4          -6.25     -9.48   -3.23  AlOHSO4
  AlSb           -102.00    -36.38   65.62  AlSb
  Alunite          -4.52     -5.92   -1.40  KAl3(SO4)2(OH)6
  Anglesite        -4.99    -12.78   -7.79  PbSO4
  Anhydrite        -0.75     -5.11   -4.36  CaSO4
  Anilite          -8.78    -40.66  -31.88  Cu0.25Cu1.5S
  Antlerite       -38.99    -30.20    8.79  Cu3(OH)4SO4
  Aragonite        -1.33     -9.63   -8.30  CaCO3
  Arsenolite      -10.60    -13.36   -2.76  As4O6
  Artinite         -3.69      5.91    9.60  MgCO3:Mg(OH)2:3H2O
  As2O5           -28.47    -21.77    6.71  As2O5
  Atacamite       -27.95    -20.56    7.39  Cu2(OH)3Cl
  Azurite         -38.67    -55.58  -16.91  Cu3(OH)2(CO3)2
  Ba(OH)2:8H2O    -20.18      4.21   24.39  Ba(OH)2:8H2O
  Ba2V2O7:2H2O    -29.94    -14.07   15.87  Ba2V2O7:2H2O
  Ba3(AsO4)2        0.00     -8.91   -8.91  Ba3(AsO4)2
  Ba3(VO4)2:4H2O  -42.74     -9.80   32.94  Ba3(VO4)2:4H2O
  BaCrO4          -37.57    -47.24   -9.67  BaCrO4
  BaMoO4           -7.94    -14.90   -6.96  BaMoO4
  Barite           -2.08    -12.06   -9.98  BaSO4
  BaS             -40.00    -23.82   16.18  BaS
  Birnessite      -24.59     -6.50   18.09  MnO2
  Bixbyite        -23.71    -24.36   -0.64  Mn2O3
  BlaubleiI        -9.62    -33.78  -24.16  Cu0.9Cu0.2S
  BlaubleiII       -9.68    -36.96  -27.28  Cu0.6Cu0.8S
  Boehmite         -1.70      6.87    8.58  AlOOH
  Brochantite     -50.05    -34.82   15.22  Cu4(OH)6SO4
  Brucite          -3.45     13.40   16.84  Mg(OH)2
  Ca(VO3)2        -17.05    -11.39    5.66  Ca(VO3)2
  Ca2V2O7         -17.65     -0.15   17.50  Ca2V2O7
  Ca2V2O7:2H2O    -21.72     -0.17   21.55  Ca2V2O7:2H2O
  Ca3(AsO4)2:4H2O -10.39     11.91   22.30  Ca3(AsO4)2:4H2O
  Ca3(VO4)2       -27.87     11.09   38.96  Ca3(VO4)2
  Ca3(VO4)2:4H2O  -28.81     11.05   39.86  Ca3(VO4)2:4H2O
  Ca3Sb2         -195.78    -52.81  142.97  Ca3Sb2
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CaCrO4          -38.02    -40.29   -2.27  CaCrO4
Calcite          -1.15     -9.63   -8.48  CaCO3
CaMoO4           -0.00     -7.95   -7.95  CaMoO4
Celestite         0.00     -6.62   -6.62  SrSO4
Cerussite        -4.17    -17.30  -13.13  PbCO3
CH4(g)          -25.26    -66.30  -41.05  CH4
Chalcanthite    -18.36    -21.00   -2.64  CuSO4:5H2O
Chalcedony       -0.45     -4.00   -3.55  SiO2
Chalcocite       -8.39    -43.31  -34.92  Cu2S
Chalcopyrite    -19.52    -54.79  -35.27  CuFeS2
Chrysotile        0.00     32.20   32.20  Mg3Si2O5(OH)4
Claudetite      -10.30    -13.36   -3.06  As4O6
CO2(g)           -2.72    -20.87  -18.15  CO2
Cotunnite       -14.29    -19.07   -4.78  PbCl2
Covellite       -10.42    -32.72  -22.30  CuS
Cr(OH)2         -14.74     -3.92   10.82  Cr(OH)2
Cr(OH)3          -2.53     -1.19    1.34  Cr(OH)3
Cr(OH)3(am)      -0.44     -1.19   -0.75  Cr(OH)3
Cr2O3             0.00     -2.36   -2.36  Cr2O3
CrCl2           -40.64    -26.55   14.09  CrCl2
CrCl3           -50.25    -35.14   15.11  CrCl3
Cristobalite     -0.65     -4.00   -3.35  SiO2
Crmetal         -45.75    -15.26   30.48  Cr
CrO3            -48.31    -51.52   -3.21  CrO3
Cu(OH)2         -13.29     -4.62    8.67  Cu(OH)2
Cu(SbO3)2       -45.50     -0.29   45.21  Cu(SbO3)2
Cu2Sb:3H2O      -20.61    -55.49  -34.88  Cu2Sb:3H2O
Cu2SO4          -29.60    -31.55   -1.95  Cu2SO4
Cu3(AsO4)2:2H2O -41.72    -35.62    6.10  Cu3(AsO4)2:2H2O
Cu3Sb           -23.46    -66.06  -42.59  Cu3Sb
CuCO3           -13.98    -25.48  -11.50  CuCO3
CuCrO4          -50.69    -56.13   -5.44  CuCrO4
Cumetal          -4.52    -13.28   -8.76  Cu
CuMoO4          -10.72    -23.80  -13.08  CuMoO4
CuOCuSO4        -35.88    -25.57   10.30  CuOCuSO4
Cupricferrite   -13.23     -7.25    5.99  CuFe2O4
Cuprite         -13.79    -15.20   -1.41  Cu2O
Cuprousferrite    0.00     -8.92   -8.92  CuFeO2
CuSO4           -23.90    -20.96    2.94  CuSO4
Diaspore          0.00      6.87    6.87  AlOOH
Djurleite        -8.69    -42.61  -33.92  Cu0.066Cu1.868S
Dolomite(disordered)  -0.55    -17.09  -16.54  CaMg(CO3)2
Dolomite(ordered)   0.00    -17.09  -17.09  CaMg(CO3)2
Epsomite         -0.88     -3.00   -2.13  MgSO4:7H2O
Fe(OH)2          -7.54      6.03   13.56  Fe(OH)2
Fe(OH)2.7Cl.3    -1.68     -4.72   -3.04  Fe(OH)2.7Cl.3
Fe(VO3)2        -12.86    -16.58   -3.72  Fe(VO3)2
Fe2(SO4)3       -47.95    -51.68   -3.73  Fe2(SO4)3
Fe3(OH)8        -16.85      3.37   20.22  Fe3(OH)8
FeAsO4:2H2O     -12.62    -12.22    0.40  FeAsO4:2H2O
FeCr2O4          -3.52      3.68    7.20  FeCr2O4
FeMoO4           -3.06    -13.15  -10.09  FeMoO4
Ferrihydrite     -4.52     -1.33    3.19  Fe(OH)3
FeS(ppt)        -19.12    -22.07   -2.95  FeS
Galena          -10.57    -24.54  -13.97  PbS
Gibbsite         -1.43      6.86    8.29  Al(OH)3
Goethite         -1.81     -1.32    0.49  FeOOH
Greenalite      -10.72     10.09   20.81  Fe3Si2O5(OH)4
Greigite        -64.00   -109.04  -45.03  Fe3S4
Gypsum           -0.52     -5.13   -4.61  CaSO4:2H2O
H-Jarosite      -24.59    -36.69  -12.10  (H3O)Fe3(SO4)2(OH)6
H2MoO4           -6.32    -19.19  -12.88  H2MoO4
H2S(g)          -20.11    -28.12   -8.01  H2S
Halite           -5.94     -4.34    1.60  NaCl
Halloysite       -3.84      5.74    9.57  Al2Si2O5(OH)4
Hausmannite     -27.19     33.84   61.03  Mn3O4
Hematite         -1.22     -2.63   -1.42  Fe2O3
Hercynite        -3.10     19.79   22.89  FeAl2O4
Huntite          -2.04    -32.01  -29.97  CaMg3(CO3)4
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Hydrocerussite  -12.27    -31.04  -18.77  Pb3(OH)2(CO3)2
Hydromagnesite   -7.71    -16.48   -8.77  Mg5(CO3)4(OH)2:4H2O
K-Alum          -14.58    -19.75   -5.17  KAl(SO4)2:12H2O
K-Jarosite      -15.70    -30.50  -14.80  KFe3(SO4)2(OH)6
K2Cr2O7         -73.46    -90.70  -17.24  K2Cr2O7
K2CrO4          -38.67    -39.18   -0.51  K2CrO4
K2MoO4          -10.11     -6.84    3.26  K2MoO4
Kaolinite        -1.70      5.74    7.43  Al2Si2O5(OH)4
Langite         -52.32    -34.83   17.49  Cu4(OH)6SO4:H2O
Larnakite        -8.78     -9.22   -0.43  PbO:PbSO4
Laurionite       -8.38     -7.76    0.62  PbOHCl
Lepidocrocite    -2.69     -1.32    1.37  FeOOH
Li2CrO4         -45.70    -40.84    4.86  Li2CrO4
Li2MoO4         -10.95     -8.51    2.44  Li2MoO4
Lime            -21.46     11.24   32.70  CaO
Litharge         -9.13      3.57   12.69  PbO
Mackinawite     -18.47    -22.07   -3.60  FeS
Maghemite        -9.02     -2.63    6.39  Fe2O3
Magnesioferrite  -6.09     10.77   16.86  Fe2MgO4
Magnesite         0.00     -7.46   -7.46  MgCO3
Magnetite         0.00      3.40    3.40  Fe3O4
Malachite       -24.79    -30.10   -5.31  Cu2(OH)2CO3
Manganite       -12.17     13.17   25.34  MnOOH
Massicot         -9.33      3.57   12.89  PbO
Melanothallite  -33.51    -27.25    6.26  CuCl2
Melanterite      -8.16    -10.37   -2.21  FeSO4:7H2O
Mg(OH)2(active)  -5.40     13.40   18.79  Mg(OH)2
Mg(VO3)2        -20.50     -9.22   11.28  Mg(VO3)2
Mg2Sb3         -149.26    -74.57   74.68  Mg2Sb3
Mg2V2O7         -22.17      4.19   26.36  Mg2V2O7
MgCr2O4          -5.15     11.05   16.20  MgCr2O4
MgCrO4          -43.50    -38.12    5.38  MgCrO4
MgMoO4           -3.93     -5.78   -1.85  MgMoO4
Minium          -51.47     22.05   73.52  Pb3O4
Mirabilite       -1.36     -2.47   -1.11  Na2SO4:10H2O
Mn(VO3)2        -20.03    -15.13    4.90  Mn(VO3)2
Mn2(SO4)3       -67.69    -73.40   -5.71  Mn2(SO4)3
Mn2Sb           -95.03    -33.95   61.08  Mn2Sb
Mn3(AsO4)2:8H2O -11.85      0.65   12.50  Mn3(AsO4)2:8H2O
MnCl2:4H2O      -17.89    -15.18    2.72  MnCl2:4H2O
MnS(grn)        -20.79    -20.62    0.17  MnS
MnS(pnk)        -23.96    -20.62    3.34  MnS
MnSb            -52.53    -55.44   -2.91  MnSb
MnSO4           -11.44     -8.85    2.58  MnSO4
MoO3            -11.19    -19.19   -8.00  MoO3
MoS2            -16.50    -86.76  -70.26  MoS2
Na-Jarosite     -18.49    -29.69  -11.20  NaFe3(SO4)2(OH)6
Na2Cr2O7        -79.19    -89.08   -9.90  Na2Cr2O7
Na2CrO4         -40.49    -37.56    2.93  Na2CrO4
Na2Mo2O7         -7.81    -24.41  -16.60  Na2Mo2O7
Na2MoO4          -6.71     -5.22    1.49  Na2MoO4
Na2MoO4:2H2O     -6.46     -5.24    1.22  Na2MoO4:2H2O
Na3Sb          -116.76    -22.31   94.45  Na3Sb
Na3VO4          -27.05      9.63   36.68  Na3VO4
Na4V2O7         -32.09      5.31   37.40  Na4V2O7
Nantokite       -12.19    -18.92   -6.73  CuCl
NaSb            -48.09    -24.92   23.17  NaSb
Natron           -5.68     -6.99   -1.31  Na2CO3:10H2O
NaVO3            -8.19     -4.33    3.86  NaVO3
Nesquehonite     -2.82     -7.49   -4.67  MgCO3:3H2O
Nsutite         -24.00     -6.50   17.50  MnO2
O2(g)           -60.38     22.71   83.09  O2
Orpiment        -29.94    -91.01  -61.07  As2S3
Pb(OH)2          -4.59      3.56    8.15  Pb(OH)2
Pb10(OH)6O(CO3)6 -80.80    -89.56   -8.76  Pb10(OH)6O(CO3)6
Pb2(OH)3Cl      -12.99     -4.20    8.79  Pb2(OH)3Cl
Pb2O(OH)2       -19.07      7.12   26.19  Pb2O(OH)2
Pb2O3           -42.55     18.49   61.04  Pb2O3
Pb2OCO3         -13.18    -13.73   -0.56  Pb2OCO3
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  Pb2V2O7         -13.59    -15.49   -1.90  Pb2V2O7
  Pb3(AsO4)2      -16.87    -11.07    5.80  Pb3(AsO4)2
  Pb3(VO4)2       -18.06    -11.92    6.14  Pb3(VO4)2
  Pb3O2CO3        -21.19    -10.17   11.02  Pb3O2CO3
  Pb3O2SO4        -16.34     -5.65   10.69  Pb3O2SO4
  Pb4(OH)6SO4     -23.21     -2.11   21.10  Pb4(OH)6SO4
  Pb4O3SO4        -23.96     -2.09   21.88  Pb4O3SO4
  PbCrO4          -35.36    -47.96  -12.60  PbCrO4
  Pbmetal         -12.04     -7.79    4.25  Pb
  PbMoO4           -0.00    -15.62  -15.62  PbMoO4
  PbO:0.3H2O       -9.42      3.56   12.98  PbO:0.33H2O
  Periclase        -8.18     13.41   21.58  MgO
  Phosgenite      -16.56    -36.37  -19.81  PbCl2:PbCO3
  Plattnerite     -34.68     14.92   49.60  PbO2
  Portlandite     -11.58     11.23   22.80  Ca(OH)2
  Pyrite          -20.32    -38.83  -18.51  FeS2
  Pyrochroite      -7.71      7.49   15.19  Mn(OH)2
  Pyrolusite      -22.53     18.85   41.38  MnO2
  Quartz            0.00     -4.00   -4.00  SiO2
  Realgar         -17.38    -37.13  -19.75  AsS
  Rhodochrosite    -2.79    -13.37  -10.58  MnCO3
  Sb(OH)3          -2.09     -9.20   -7.11  Sb(OH)3
  Sb2O4           -10.43     -7.03    3.40  Sb2O4
  Sb2O5           -34.63    -44.29   -9.67  Sb2O5
  Sb4O6(cubic)    -18.51    -36.77  -18.26  Sb4O6
  Sb4O6(orth)     -18.87    -36.77  -17.90  Sb4O6
  SbCl3           -43.72    -43.15    0.57  SbCl3
  Sbmetal         -14.54    -26.22  -11.69  Sb
  SbO2              0.00    -27.82  -27.82  SbO2
  Senarmontite     -6.02    -18.38  -12.37  Sb2O3
  Sepiolite        -0.98     14.78   15.76  Mg2Si3O7.5OH:3H2O
  Sepiolite(A)     -4.00     14.78   18.78  Mg2Si3O7.5OH:3H2O
  Siderite         -4.59    -14.83  -10.24  FeCO3
  SiO2(am-gel)     -1.29     -4.00   -2.71  SiO2
  SiO2(am-ppt)     -1.26     -4.00   -2.74  SiO2
  Spinel           -9.69     27.16   36.85  MgAl2O4
  SrCrO4          -37.14    -41.79   -4.65  SrCrO4
  Stibnite        -52.25   -102.71  -50.46  Sb2S3
  Strontianite     -1.87    -11.14   -9.27  SrCO3
  Sulfur          -14.61    -16.75   -2.14  S
  Tenorite        -12.26     -4.61    7.64  CuO
  Thenardite       -2.71     -2.39    0.32  Na2SO4
  Thermonatrite    -7.55     -6.91    0.64  Na2CO3:H2O
  V(OH)3           -7.67     -0.08    7.59  V(OH)3
  V2O5            -21.26    -22.62   -1.36  V2O5
  V3O5            -13.45    -11.61    1.84  V3O5
  V4O7            -18.88    -11.70    7.19  V4O7
  V6O13           -29.71    -90.57  -60.86  V6O13
  Valentinite      -9.90    -18.38   -8.48  Sb2O3
  VCl2            -47.26    -28.38   18.87  VCl2
  VCl3            -57.46    -34.03   23.43  VCl3
  Vmetal          -61.12    -17.10   44.03  V
  VO              -20.50     -5.74   14.76  VO
  VO(OH)2          -5.24     -0.09    5.15  VO(OH)2
  VO2Cl           -25.47    -22.63    2.84  VO2Cl
  VOCl            -22.54    -11.39   11.15  VOCl
  VOCl2           -35.49    -22.72   12.76  VOCl2
  VOSO4           -20.04    -16.43    3.61  VOSO4
  Witherite        -8.01    -16.58   -8.57  BaCO3

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

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End of simulation.
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Reading input data for simulation 7.
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End of Run after 0.532 Seconds.
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APPENDIX-F Previous Study Groundwater Analyses

Table F-1. Previous study groundwater analyses (Yazıcıgil et. al, 2015)

Sample Name	**PW-2**			**PW7**			**PW9**	**CEL35**		**CEL44**	**CEL51**
Date	Sep.13	July.14	Oct.14	Dec.13	July.14	Oct.14	Mar.15	Sep.13	Sep.14	Oct.13	Oct.13
Ag(d)	<0.00005	<0.00005	<0.00005	<0.00001	<0.00001	<0.00001	<0.00001	<0.00001	<0.00001	<0.00001	<0.00001
Ag(t)	<0.00005	<0.0001	<0.00005	<0.00001	<0.00001	<0.00001	<0.00001	<0.00001	<0.00001	<0.00001	<0.00001
Al(d)	0.084	<0.015	0.04	<0.003	<0.003	0.0033	0.0118	0.0082	0.0058	0.0035	0.0069
Al(t)	1.05	0.099	0.314	0.276	0.0088	0.038	0.0313	0.0088	0.0093	0.541	0.521
Alk.(t)	327	267	256	322	315	353	237	451	473	377	380
As(d)	0.133	0.0752	0.0638	0.0317	0.033	0.0336	0.0418	0.0056	0.00654	0.00094	0.00144
As(t)	0.138	0.0806	0.0668	0.0352	0.0333	0.0342	0.0422	0.00546	0.00643	0.00153	0.00256
B(d)	22.3	25.6	23.9	0.256	0.275	0.24	0.197	0.241	0.203	0.173	0.277
B(t)	22.8	22.8	25.1	0.285	0.298	0.264	0.198	0.281	0.216	0.195	0.282
Ba(d)	0.0567	0.0676	0.0829	0.0257	0.0171	0.0136	0.0547	0.201	0.154	0.106	0.14
Ba(t)	0.0758	0.0684	0.0884	0.0276	0.0167	0.0136	0.0558	0.206	0.15	0.22	0.144
Be(d)	<0.0025	<0.0025	<0.0025	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005
Be(t)	<0.0025	<0.005	<0.0025	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005
Bi(d)	<0.0025	<0.0025	<0.0025	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005
Bi(t)	<0.0025	<0.005	<0.0025	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005	<0.0005
Ca(d)	17.9	12.9	8.47	92	92.9	92.6	40.9	6.41	6.24	7.29	4.06
Ca(t)	28.1	15.2	12.2	89.8	91.9	90.7	41.4	6.47	6.23	9.95	8.79
Cd(d)	<0.00025	<0.00025	<0.00025	<0.00005	<0.00005	<0.00005	<0.00005	<0.00005	<0.00005	<0.00005	<0.00005
Cd(t)	<0.00025	<0.0005	<0.00025	<0.00005	<0.00005	<0.00005	<0.00005	<0.00005	<0.00005	<0.00005	<0.00005
Cl	882	1250	1330	45.8	43.4	45	15.5	<5	<5	7.1	7.9
CN	-	-	-	0.00024	0.00022	0.00028	<0.0001	<0.0001	<0.0001	<0.0001	0.00015
Co(d)	0.00082	0.00139	0.00146	0.00029	0.00024	0.00032	<0.0001	<0.0001	<0.0001	0.00031	0.00045
Co(t)	0.00128	0.0014	0.00163	<2	<2	<2	<2	19.4	<2	29.6	39.2
CO3	256	253	123	<20	<20	<20	<20	<20	<20	<20	<20
COD	147	202	198	804	812	813	491	819	820	770	755
EClab	3270	4160	4310	<0.0005	<0.0005	<0.0005	0.00102	<0.0005	<0.0005	0.00128	0.00153
Cr(d)	0.0164	<0.0025	<0.0025	0.00084	<0.0005	0.00067	0.00112	<0.0005	<0.0005	0.00862	0.0105
Cr(t)	0.0617	0.0092	0.0153	<0.0005	0.00083	0.00105	0.00066	<0.0005	<0.0005	<0.0005	<0.0005
Cu(d)	<0.0025	<0.0025	<0.0025	0.00055	0.00111	0.0024	0.00081	0.0015	0.00756	0.00134	0.00146
Cu(t)	0.0034	<0.005	<0.0025	0.41	0.38	0.24	0.316	0.30	0.35	0.44	0.33
F	0.52	0.92	0.61	<0.03	<0.03	<0.03	<0.03	0.16	0.09	0.03	<0.03
Fe(d)	<0.03	<0.03	0.04	0.312	<0.03	0.114	0.032	0.096	0.099	0.515	0.426
Fe(t)	0.941	0.077	0.316	413	419	422	235	325	331	321	324
Hard.(t)	44.7	34.7	28.4	322.0	315	353.0	237	432.0	473.0	347	341
HCO3	<1	13.5	133.0	<0.00005	<0.00005	<0.00005	<0.00005	<0.00001	<0.00005	<0.00005	<0.00005
Hg(d)	<0.00001	<0.00005	<0.00005	<0.00005	<0.00005	<0.00005	<0.00005	<0.00001	<0.00005	<0.00005	<0.00005
Hg(t)	<0.00001	<0.00005	<0.00005	5.7	5.4	5.7	3.2	7.2	6.9	10.3	8.6
K(d)	33	19.6	15.7	5.6	5.3	5.4	3.3	7.2	7	9.7	7.9
K(t)	31.6	20	15.7	0.105	0.0949	0.0966	0.102	0.71	0.596	0.377	0.949
Li(d)	1.02	1.42	1.59	0.106	0.0969	0.0987	0.098	0.739	0.591	0.38	0.916
Li(t)	1.05	1.39	1.63	44.6	45.4	46.3	32.2	75	76.5	73.5	76.3
Mg(d)	<0.1	0.63	1.76	46.5	44.9	45	33	75.6	77	69.3	71
Mg(t)	5.36	0.95	2.86	0.00993	0.00318	0.00353	0.00506	0.128	0.0633	0.0548	0.0713

Table F-2. Cont'd

Sample Name	**PW-2**			**PW7**			**PW9**	**CEL35**		**CEL44**	**CEL51**
Date	Sep.13	July.14	Oct.14	Dec.13	July.14	Oct.14	Mar.15	Sep.13	Sep.14	Oct.13	Oct.13
Mn(d)	0.00044	0.00609	0.0267	0.0137	0.00351	0.00376	0.00554	0.135	0.0625	0.0682	0.0875
Mn(t)	0.0479	0.011	0.0415	0.00375	0.00337	0.00332	0.0132	0.000772	0.000891	0.00156	0.000998
Mo(d)	0.0299	0.0238	0.0206	0.00395	0.0033	0.00343	0.0137	0.000872	0.000962	0.00176	0.00115
Mo(t)	0.0293	0.0225	0.0208	<0.05	<0.05	<0.05	0.188	0.61	0.597	1.06	1.19
N(Kjel)	5.94	4.66	4.83	<0.06	<0.06	<0.06	0.114	<0.08	<0.08	0.406	0.309
N(Org)	0.71	1.98	2.35	24.4	23.2	22.9	25.2	82.6	74.4	64.6	62.1
Na(d)	766	891	927	23.5	22.7	22.1	26.4	82.6	76.4	60.9	52.6
Na(t)	753	890	929	0.001	0.00098	0.001	0.00061	0.001	0.005	<0.0005	0.00054
Ni(d)	0.003	0.0049	0.005	0.00121	0.00092	0.00082	0.00061	<0.0005	0.00736	0.0015	0.00202
Ni(t)	0.006	0.0052	0.0051	<0.01	<0.01	0.011	0.0471	<0.01	<0.01	0.019	<0.01
N-NO2	<0.02	<0.02	<0.02	0.0174	0.0124	0.0058	0.0746	0.569	0.538	0.651	0.885
N-NH3	5.23	2.69	2.47	8.44	10.6	8.69	1.19	<0.05	<0.05	<0.05	<0.05
N-NO3	<0.1	<0.1	<0.1	<2	<2	<2	<2	<1	<2	<1	<1
OH	70.9	<1	<1	0.0524	-	-	0.0678	0.114	-	0.066	0.216
OrthoP)	0.0799	-	-	0.0716	0.0268	0.0298	0.0175	0.137	0.126	0.0814	0.273
P(t)	0.156	0.0618	0.216	7.84	8.09	7.94	7.99	8.52	8.27	8.48	8.64
pHlab	10.18	9.51	9.07	<0.00005	<0.00005	0.000392	0.000187	0.000061	0.000188	0.000127	<0.00005
Pb(d)	<0.00025	<0.00025	0.00108	0.000348	0.000426	0.0009	0.00023	0.000117	0.000159	0.0102	0.015
Pb(t)	0.00156	<0.0005	0.00149	0.0001	<0.0001	0.00011	0.00016	<0.0001	<0.0001	<0.0001	<0.0001
Sb(d)	0.0007	0.00054	<0.0005	0.00012	<0.0001	<0.0001	0.0002	<0.0001	<0.0001	0.00039	0.00032
Sb(t)	0.00055	<0.001	<0.0005	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
Se(d)	<0.005	<0.005	<0.005	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
Se(t)	<0.005	<0.01	<0.005	29.4	28.6	29.4	18	14.5	14.7	20.1	13.6
Si(d)	41.2	21.8	18.1	29.9	27.9	28.8	18.3	14.7	14.9	21.2	14.6
Si(t)	46.3	21.5	19.9	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	0.00012
Sn(d)	<0.0005	<0.0005	<0.0005	<0.0001	<0.0001	0.000	<0.0001	<0.0001	<0.0001	0.0002	0.00044
Sn(t)	<0.0005	<0.001	<0.0005	37.1	37.7	38.5	21.8	43.2	46.8	76.5	65.9
SO4	45	26	17	1.02	0.977	0.965	0.506	0.585	0.616	0.886	0.894
Sr(d)	0.562	0.466	0.427	1.02	0.974	0.973	0.528	0.596	0.621	0.887	0.915
Sr(t)	0.636	0.453	0.463	555	591	538	304	474	457	454	426
TDS	2060	2610	2630	<0.01	<0.01	0.011	<0.01	<0.01	<0.01	<0.01	<0.01
Ti(d)	<0.01	<0.01	<0.01	<0.01	<0.01	0.012	<0.01	<0.01	<0.01	0.015	0.015
Ti(t)	0.03	<0.01	<0.01	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
Tl(d)	<0.0005	<0.0005	<0.0005	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
Tl(t)	<0.0005	<0.001	<0.0005	1.36	1.02	1.21	1.35	1.39	1.59	3.97	3.99
TOC	34.5	43.7	49.6	7.4	6.4	<3	<3	<3	<3	12.2	17.5
TSS	121	11.4	19.4	0.00551	0.00596	0.00615	0.00228	0.000022	0.000024	0.000022	0.000068
U(d)	<0.00005	0.00031	0.000305	0.00611	0.00588	0.00618	0.00236	0.000025	0.000032	0.000061	0.000148
U(t)	0.000145	0.00032	0.000319	0.0094	0.0097	0.01	0.0075	<0.001	<0.001	<0.001	<0.001
V(d)	0.0652	0.0113	<0.005	0.0102	0.0098	0.0101	0.0079	<0.001	<0.001	0.0015	0.0022
V(t)	0.0717	0.013	<0.005	0.0038	<0.003	0.0042	0.0412	0.0054	0.0037	0.004	<0.003
Zn(d)	<0.015	<0.015	0.111	0.0034	0.0038	0.0037	0.046	<0.003	0.0118	0.138	0.164
Zn(t)	0.053	<0.03	0.246								