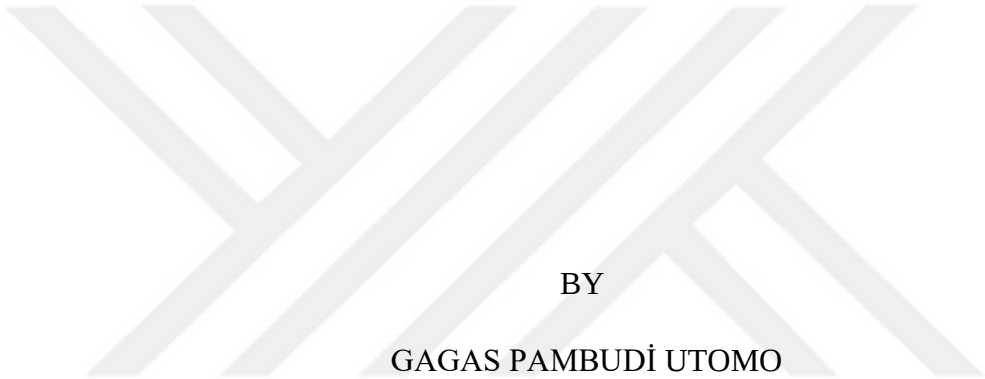


GEOCHEMICAL MODELING OF CO₂-WATER-ROCK INTERACTION IN
INDONESIAN GEOTHERMAL FIELDS FOR A POSSIBLE FUTURE CARBON
CAPTURE AND STORAGE PROJECT

A THESIS SUBMITTED TO
THE GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES
OF
MIDDLE EAST TECHNICAL UNIVERSITY



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GAGAS PAMBUDI UTOMO

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Approval of the thesis:

**GEOCHEMICAL MODELING OF CO₂-WATER-ROCK INTERACTION IN
INDONESIAN GEOTHERMAL FIELDS FOR A POSSIBLE FUTURE
CARBON CAPTURE AND STORAGE PROJECT**

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ABSTRACT

GEOCHEMICAL MODELING OF CO₂-WATER-ROCK INTERACTION IN INDONESIAN GEOTHERMAL FIELDS FOR A POSSIBLE FUTURE CARBON CAPTURE AND STORAGE PROJECT

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The rise of CO₂ concentration in Earth's atmosphere from anthropogenic emissions is the main cause of global warming and climate change. Carbon Capture and Storage (CCS) is considered as an effective method to reduce such emission. CCS can be performed in various sites including geothermal reservoirs. This study is concerned with geochemical modeling of CO₂-water-rock interaction for a possible future CCS project in Indonesian geothermal fields, namely Ungaran, Baturaden, Dieng and Awibengkok. The modeling is performed using PHREEQC program and the data published in mainstream journals, and attempts to examine the effect of CO₂ injection on the rock and water composition of the geothermal reservoirs. Modeling assumes a single stage CO₂ injection at constant pressure and temperature. The study consists of equilibrium and kinetic modeling.

Equilibrium modeling reveal: 1) potential for mineral trapping via the formation of carbonates, 2) increasing pH in Ungaran and Baturraden, 3) decreasing pH in Dieng and Awibengkok and 4) decreasing porosity for all fields except Ungaran. Kinetic modeling suggests that solubility trapping existed immediately after CO₂ injection and is followed by complete or partial replacement of mineral trapping as suggested by

the drop in dissolved CO₂ concentration. The modeling identified reactions involving the formation of new carbonates: i) anorthite dissolution to calcite in Ungaran, ii) diopside dissolution to dolomite in Baturraden and Dieng and iii) calcite dissolution and dolomite dissolution to magnesite in Awibengkok. Equilibrium state is reached in 10 years for Ungaran and Baturraden, 10 hours for Dieng and 10000 years for Awibengkok.

Keywords: CO₂ storage, geothermal reservoir, equilibrium modeling, kinetic modeling, PHREEQC



ÖZ

OLASI BİR KARBON YAKALAMA VE DEPOLAMA PROJESİ İÇİN ENDONEZYA JEOTERMAL SAHALARINDA CO₂-SU-KAYAÇ ETKİLEŞİMİNİN JEOKİMYASAL MODELLEMESİ

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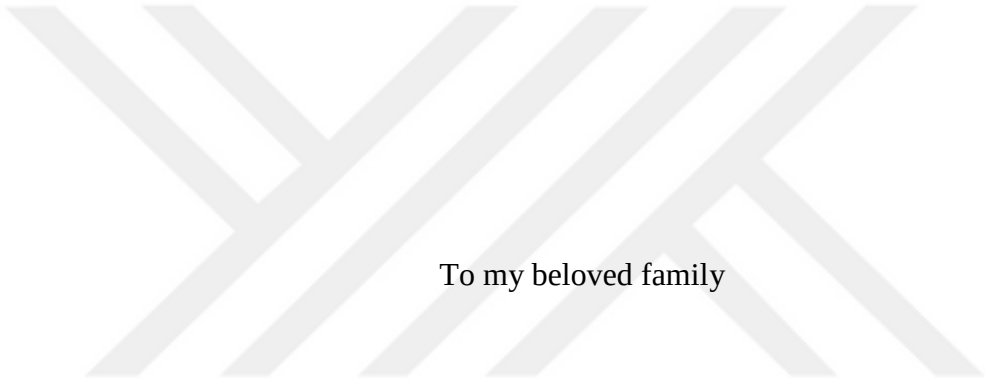
Haziran 2019, 210 sayfa

Dünya atmosferindeki CO₂ derişiminin antropojenik kaynaklı emisyonlar sonucu yükselmesi küresel ısınma ve iklim değışikliği sorununun başlıca nedenidir. Karbon Yakalama ve Depolama (CCS), bu tür emisyonların azaltılmasında etkili bir yöntem olarak kabul edilmektedir. CCS, jeotermal rezervuarlar dahil çeşitli jeolojik oluşumlarda gerçekleştirilebilir. Bu çalışma, Endonezyada bulunan Ungaran, Baturaden, Dieng ve Awibengkok jeotermal sahalarında olası bir CCS projesi için, CO₂-su-kayaç etkileşiminin jeokimyasal modellemesine ilişkindir. Modelleme, PHREEQC programı ve anaakım dergilerde yayınlanan veriler kullanılarak CO₂'in jeotermal rezervuarlarda kayaç ve su kimyasına etkisini incelemeye yöneliktir ve sabit basınç ve sıcaklıkta tek kademeli bir CO₂ enjeksiyonunu baz almaktadır. Çalışma, denge ve kinetik modellemeye dayanmaktadır.

Denge modellemesi şunları ortaya koymaktadır: 1) karbonat oluşumu yoluyla mineral kapanlanması potansiyeli, 2) Ungaran ve Baturraden sahalarında pH artışı, 3) Dieng ve Awibengkok sahalarında pH düşüşü ve 4) Ungaran dışındaki tüm sahalarda porozite azalması. Kinetik modelleme, çözünürlük kapanlanmasının CO₂ enjeksiyonundan hemen sonra gerçekleştiğini ve ardından, çözünmüş CO₂ derişimindeki düşüşün işaret ettiği üzere, kısmen veya tümüyle mineral kapanlanması

tarafından takip edildiğini göstermektedir. Modelleme yeni karbonatların oluşumunu içeren reaksiyonları şu şekilde tanımlamaktadır: i) Ungaran sahasında anortit çözünümü ile kalsit oluşumu, ii) Baturraden ve Dieng sahaslarında diyopsit çözünümü ile dolomit oluşumu ve iii) Awibengkoc sahasında kalsit ve dolomit çözünümü ile manyezit oluşumu. Denge durumuna, Ungaran ve Baturraden sahaslarında 10 yıl, Dieng sahasında 10 saat ve Awibengkoc sahasında da 10000 yılda ulaşılmaktadır..

Anahtar Kelimeler: CO₂ depolama, jeotermal rezervuar, denge modellemesi, kinetik modelleme, PHREEQC



To my beloved family

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CHAPTER 1

INTRODUCTION

The amount of CO₂ emitted to Earth's atmosphere as a product of fossil fuel burning and industrial facilities has been increasing since the start of 1880s and consequently caused global warming. The global annual temperature has increased at an average rate of 0.07°C per decade since 1880 and at an average rate of 0.17°C per decade since 1970 (NOAA, 2017). Global temperature across the world's land and ocean surfaces in September 2018 was recorded 0.78°C above the 20th century average of 15.0°C (CO₂-Earth, 2018). One of the methods to reduce CO₂ emission is by performing CO₂ Capture and Storage (CCS) which involves capturing CO₂ produced at large industrial facilities and power plants and storing it in deep underground rock formations (Capturready, 2018).

CCS can be applied in un-mineable coal seams, depleted oil and gas fields and deep saline aquifers. CCS was initially developed for enhanced oil recovery in USA during the early 1970s. Sleipner project in 1996 is the first commercial example of CO₂ storage in a deep saline aquifer operated by Statoil, Norway's largest oil company. There are currently around 136 industrial and 62 research projects related to CCS worldwide (Capturready, 2018). In recent years, geothermal fields started to draw attention as possible storage sites for CO₂. One example of CCS in a geothermal reservoir is done in Hellisheidi field in Iceland under The CarbFix Project which started in 2014. This project reported that over 95% of CO₂ captured and injected at site was mineralized within two years (CarbFix, 2018).

The two mechanisms of CO₂ fixation are physical and geochemical trapping (Bachu et al., 2007). Physical trapping consists of static (structural and stratigraphic), hydrodynamic and residual gas trapping. Geochemical trapping is divided into

solubility and mineral trapping. Physical trapping is controlled by the integrity of the cap rock and it occurs immediately after injection. Geochemical trapping is dependent on brine and rock chemistry and it takes place some time after injection as CO₂-brine-rock interaction proceeds (Steel et al., 2018; Liu et al., 2019). Among the two mechanisms, CO₂ fixation through geochemical (solubility and mineral) trapping are considered to be the safest processes in which the injected CO₂ is converted into aqueous and mineral phases.

Solubility and mineral trapping in CCS can be assessed by carrying out geochemical studies. Previous geochemical studies related to CO₂-brine-rock interaction play an important role in evaluating and predicting the outcome of CCS operations. Most of the studies concentrate on observing composition changes in brine and reservoir mineralogy, and also the change of porosity and permeability of the host rock due to CO₂ introduction (Wang et al., 2016; Steel et al., 2018). These studies generally include laboratory experiment for short term observation and numerical simulation for long term prediction.

The implementation of CCS in geothermal fields makes Indonesia a potential host for such technology. Indonesia is the world's second largest geothermal energy producer with Java Island being its most prolific region consisting of 27 geothermal fields, in which 6 of them actively producing electricity (ESDM, 2016). These geothermal fields have a potential to become possible future CO₂ storage sites. In this respect, the potential of these geothermal fields to be developed as possible CCS sites must be supported with adequate study before the method can later be applicable. Long-term safety of CO₂ fixation is considered to be the main aspect in determining the success of CCS (Snaebjornsdottir et al., 2018). Therefore, it is important to perform preliminary investigation on how CO₂ will be trapped once it is injected into the geologic formation.

1.1. Purpose and Scope

This study attempts to perform a preliminary investigation on predicting the long-term effect of CO₂ injection in four selected geothermal fields namely Ungaran, Baturaden, Dieng and Awibengkok in Java Island, Indonesia for a possible carbon capture and storage operation. This is achieved by modeling CO₂-brine-reservoir rock interaction. Modeling study includes equilibrium and kinetic modeling in static environment. Reactive mass transport modeling is outside the scope of this study. Equilibrium modeling is done to understand the change in mineral composition, brine chemistry and the change in rock porosity after equilibrium is achieved among CO₂-brine-reservoir rocks. Kinetic modeling is done to understand how chemical reactions among the three components proceed from the start of CO₂ injection until equilibrium is achieved.

1.2. Material and Method

Geochemical modeling study is done using PHREEQC program and the data available in four geothermal fields in Java Island, Indonesia. The data used include both reservoir rock properties and brine chemistry of the fields. Reservoir properties include rock mineralogy, estimated reservoir depth and rock porosity. Mineralogy of reservoir rock is defined by computing the published major elements chemistry from four selected geothermal fields into CIPW Norms. CIPW Norm calculation is a procedure for transferring the chemical composition of a rock into a hypothetical assemblage of water-free standard minerals (Best, 2003). The alteration minerals reported in the published papers is also added to the reservoir rock mineralogy. Reservoir temperature is taken from published well bottom measurements where available, or is estimated via geothermometry applications. Brine chemistry is compiled from published work and visualized by plotting its major ions constituent into Schoeller diagram.

Equilibrium and Kinetic modeling are carried out by the assistance of PHREEQC program. PHREEQC performs a wide variety of aqueous geochemical calculations and is used for modeling reactions and processes, including (1) speciation and saturation-index calculations, and (2) batch-reaction (Parkhurst and Appelo, 2013). Modeling assumes a single stage CO₂ injection under static environment at a constant temperature and pressure.

1.3. Layout of Thesis

This thesis is divided into six chapters with the following content:

Chapter 1 gives a brief summary of the study, the scope and method that is used in the study.

Chapter 2 is a literature review which describes Carbon Capture and Storage and concise information about existing CCS operation and physico-chemical processes involved in CO₂ storage.

Chapter 3 gives detailed information about the four geothermal fields studied in this thesis. The information includes the geology, reservoir rock property and brine chemistry of the fields.

Chapter 4 describes in detail how equilibrium and kinetic modeling is done.

Chapter 5 compares and discusses the modeling results.

Chapter 6 gives the conclusions obtained from this thesis study and the recommendations for future studies

CHAPTER 2

CARBON CAPTURE AND STORAGE

Carbon Capture and Storage (CCS) involves three major steps: i) capturing CO₂ by separating it from other gases produced at large industrial process facilities such as coal and natural gas power plants, steel mills and cement plants (Figure 2.1), ii) transporting the separated CO₂ to a suitable site for geological storage and iii) storing the CO₂ by injecting it into underground rock formations at depths of one kilometer or more (GlobalCCSI, 2018).

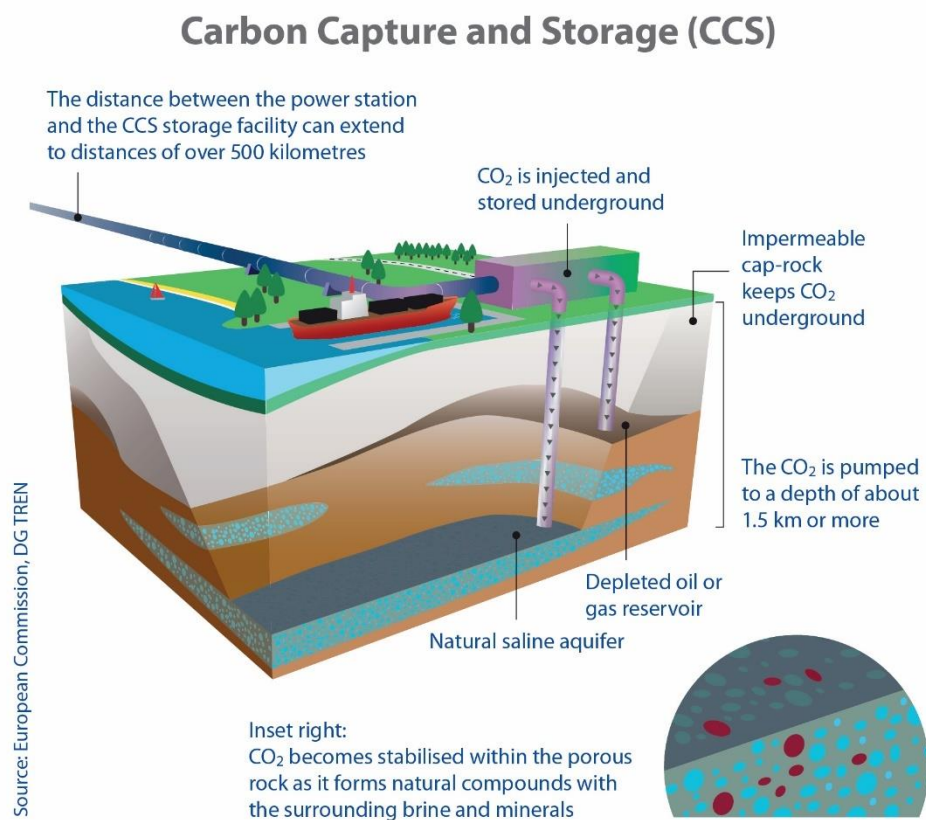


Figure 2.1. Carbon capture and storage diagram (EU, 2019).

2.1. CO₂ Capture

Separation of carbon dioxide from other gases from point source can be performed in three different ways: pre-combustion capture, post-combustion capture and oxy-fuel combustion. The most common method used in CCS is the post-combustion capture which involves capturing CO₂ gas from the exhaust chamber of a combustion process. This is done by absorbing CO₂ into a suitable solvent. The absorbed CO₂ is released from the solvent and is compressed for transportation and storage (CCSA, 2018).

2.2. CO₂ Storage and Sites

Geological storage of CO₂ can be performed at various geological sites such as depleted oil and gas fields, deep coal seams and deep saline aquifers (IPCC, 2014). The storage site needs to be at sufficient depth and have an impenetrable cap rock layer above it to prevent any upward movement of CO₂ (Global CCS Institute, 2014). Deep saline aquifers have the largest storage capacity compared to other optional geologic sites. However, the usage of depleted oil/gas reservoirs for CCS is considered preferable since the reservoir is generally already being well studied and the presence of existing wells makes depleted oil/gas reservoir more advantageous for such operation. Another alternative site that can be utilized for CCS are geothermal reservoirs. Generally geothermal powerplants produces naturally occurring CO₂ gas. These gases can be captured and injected back to the geothermal reservoir to both reduce CO₂ emission and maintain reservoir pressure (Buscheck et al., 2014). The following are some of the example of CCS operation around the world.

Sleipner – Norway

Sleipner is the first offshore carbon capture and storage site currently operated by Equinor. The company initiated the project to reduce the concentration of CO₂ inside the produced natural gas from 9% to 2.5 % as regulated by the Norwegian government. According to Kvamme and Aromada (2018) the Sleipner CCS operation has been

injecting approximately one million tonnes of CO₂ yearly since the start of its operation in 1996. The storage site is within the Utsira (deep saline) formation located 800 to 1000 m beneath the sea bed. It is estimated that the formation has a storage capacity of 600 billion tonnes of CO₂ (Torp, 2011).

In Salah – Algeria

In Salah carbon capture and storage project in Algeria is operated by BP, Sontrach and Equinor. The operation started in 2004 and was suspended in 2011 (MIT, 2016). In this project, CO₂ separated and captured from several gas field was combined and transported to the storage site in Krechba field. During this period approximately 3.8 million tonnes of CO₂ have been stored in the Carboniferous sandstone unit located at the depth of 1900 meters (Ringrose et al., 2013).

Weyburn and Midale – Canada

The Weyburn-Midale CO₂ Monitoring and Storage Project is operated in Weyburn and Midale oil fields, Saskatchewan, Canada. The project is conducted to enhance oil production in a depleted oil field. The operation in Weyburn and Midale started in 2000 and 2005 respectively. It is reported that over 18 million tonnes of CO₂ had been injected into both fields by 2010 (Whittaker et al., 2011). The source of CO₂ that is injected to both fields comes from the Dakota Gasification plant in North Dakota and is transported 320 km to the CCS sites (Gilfillan et al., 2017).

Hellisheidi- Iceland

Carbon capture and storage in Hellisheidi geothermal is operated under The CarbFix project. The project started in 2014 and by the end of 2018, approximately 66,000 tonnes of sour gases comprising 2/3rd CO₂ and 1/3rd H₂S produced from the power plant has been captured and stored in the site (CarbFix, 2018). Captured CO₂ is injected into basaltic rock formation with 25% weight of calcium, magnesium and iron oxides. This makes this type of rock more reactive to CO₂ and thus allowing mineral

carbonation can occur at a faster time scale compared to other type of rocks (Gislason and Oelkers, 2014).

2.3. Physical and Chemical Process

CO₂ can be injected from the surface as gaseous/supercritical CO₂ or as a dissolved aqueous CO₂. In the first case, injected CO₂ will be stored in three different phases: 1) free CO₂ in supercritical phase, 2) dissolved CO₂ in aqueous phase, 3) precipitated CO₂ in mineral phase (Blackford et al., 2017). CO₂ injected into a geologic formation will move up to the top of formation because of its density difference to formation water. Once gathered in the upper part of the formation, CO₂ will not be able to migrate further upward, and it will start to move outwards away from injection point and form a plume (CCP, 2015). At the center of this plume, CO₂ is present inside the pore spaces in the form of supercritical phase. At the outer boundary of the plume, CO₂ start to dissolve in formation water in aqueous phase. Addition of dissolved CO₂ increase the saturation index of liquid with respect to CO₂ and eventually promote precipitation of dissolved aqueous CO₂ into mineral phase in the form of carbonate minerals (CCP, 2015).

In the second case, CO₂ is dissolved into a water during injection. This method allows the gas to be stored directly as aqueous phase once it reaches the storage site. This is achieved by controlling the mol amount of injected CO₂ gas bellow the CO₂ solubility of the formation water in the storage site. Dissolved CO₂ will make the water in the injection site denser than the surrounding formation water. Consequently, the CO₂ saturated water will tend to sink to the base of formation making it less likely to escape upwards. The time required for mineral trapping, in which injected CO₂ is transformed into mineral phase, is lowered compared to the injection as gas or supercritical form. This is due to the earlier presence of dissolved CO₂ (Figure 2.2) (Sigfussona et al., 2015).

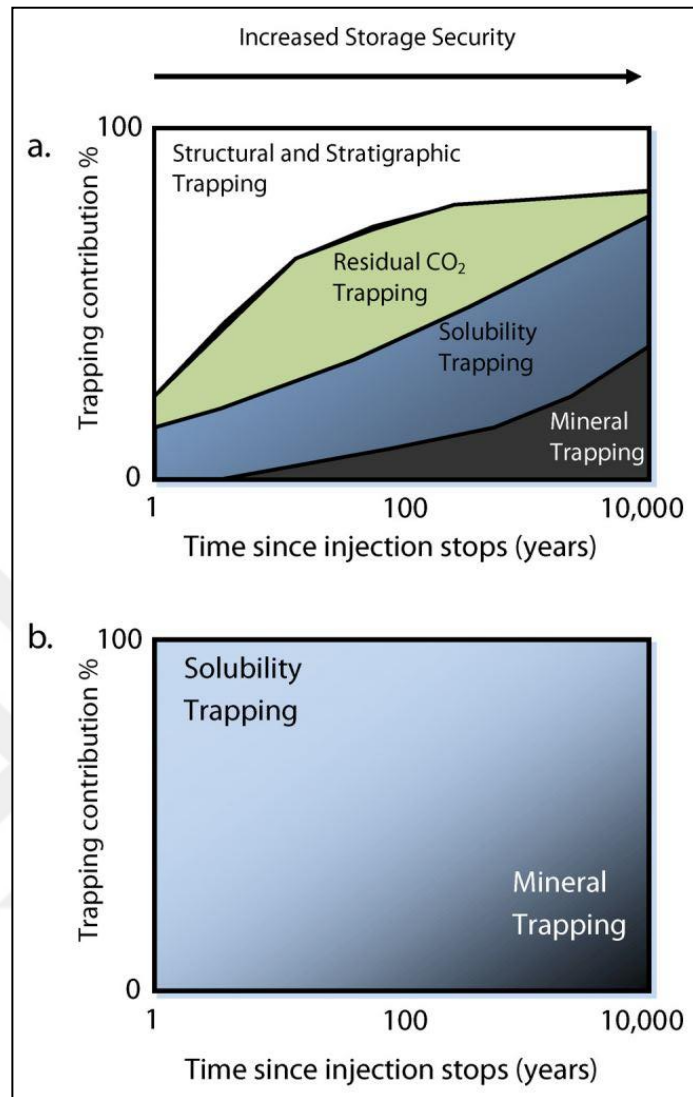
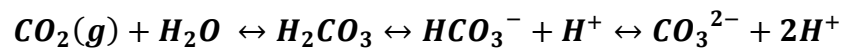


Figure 2.2. Contribution of trapping mechanism to CO₂ fixation, [a] represents the injection of CO₂ as gaseous or supercritical phase, [b] depicts the injection of CO₂ in dissolved phase (Sigfussona et al., 2015)

2.3.1. CO₂-water interaction

The injection of CO₂ into water promotes formation of weak carbonic acid (H₂CO₃). This process is followed by dissociation of carbonic acid to form bicarbonate (HCO₃⁻) and succeeded by bicarbonate dissociation into carbonate (CO₃²⁻):



The solubility of CO₂ in brine generally increases with increasing pressure and decreases with increasing temperature and salinity (Duan and Sun, 2003; Duan et al., 2006). (Figure 2.3, Figure 2.4.) Once CO₂ is dissolved and fluid is oversaturated with respect to CO₂, precipitation of carbonate minerals occurs, and mineral trapping takes place.

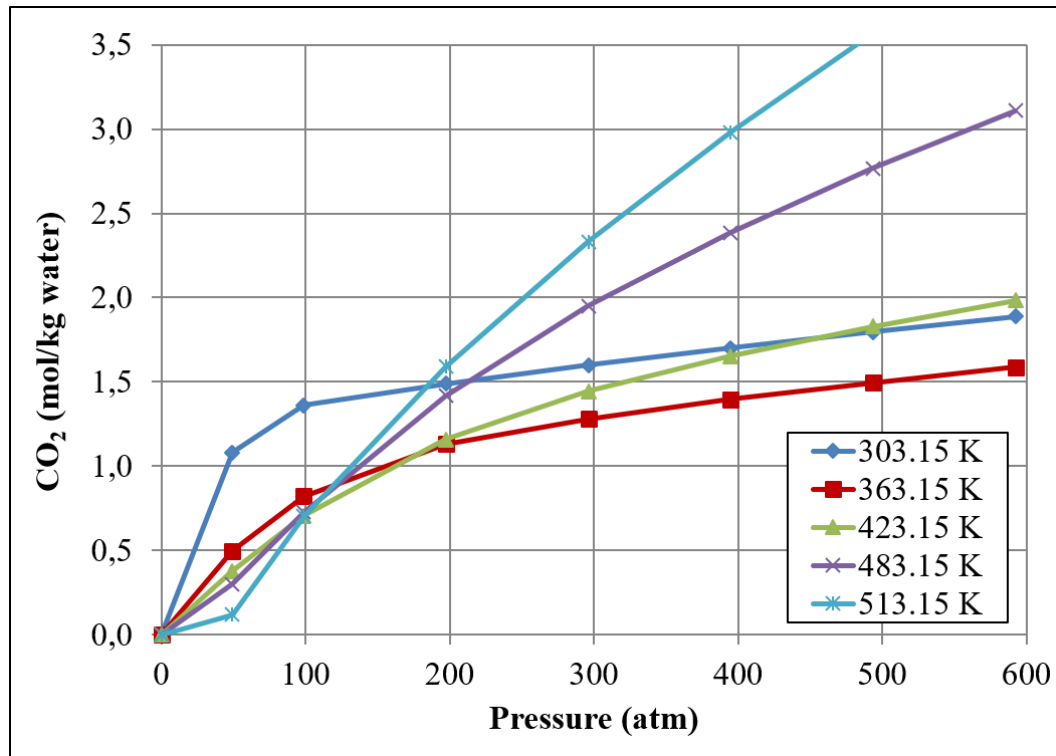


Figure 2.3. Solubility of CO₂ in a pure water at various pressure and temperature (Duan and Sun, 2003).

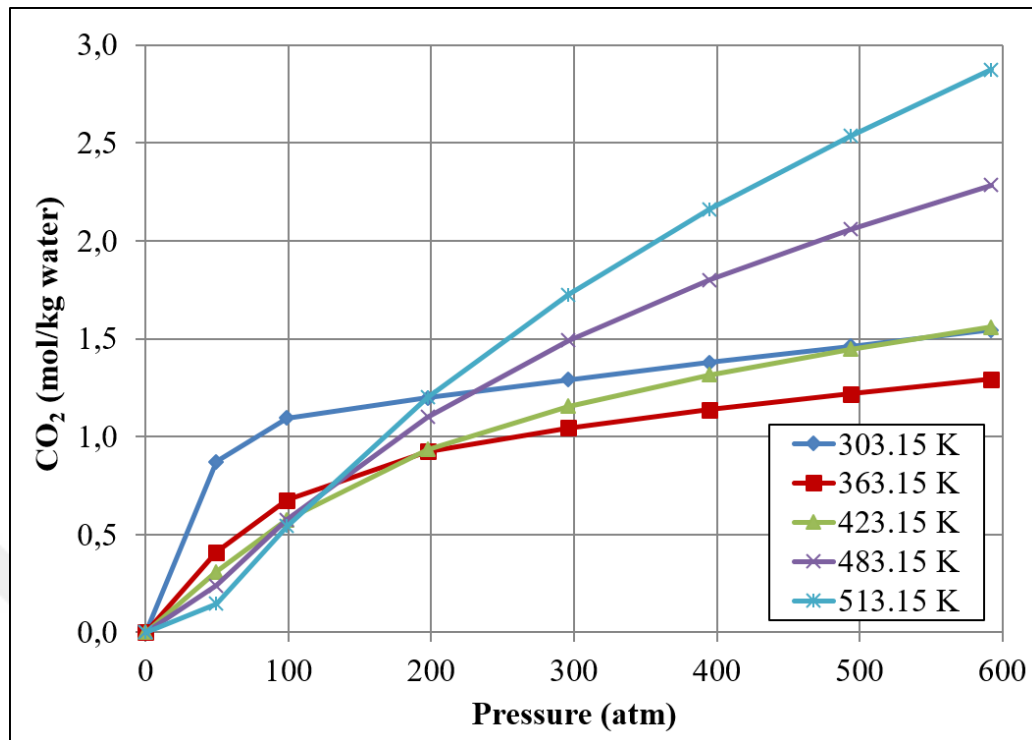


Figure 2.4. Solubility of CO₂ in 1m NaCl saturated water at various pressure and temperature (Duan and Sun, 2003).

2.3.2. CO₂-water-rock interaction

The pH drop of brine due to CO₂ introduction promotes the dissolution of alkali earth metals such as calcium and magnesium. These metals react with the dissolved carbon bearing species such as bicarbonate or carbonate which result in the precipitation of carbonate minerals such as calcite and dolomite. As an example, the reaction between carbonate and calcium leads to the precipitation of calcite. Interaction among CO₂-brine-rock produces a complex series of reactions that varies depending on the chemical composition of the fluid and the mineralogy of the rock. (Rosenbauer et al., 2005). CO₂-brine-rock interaction generally promotes the change in porosity of reservoir. Excess dissolution of reservoir rock mineral will lead to porosity increase which is desirable since it increases the CO₂ storage capacity of a reservoir. When precipitation of new or existing mineral is dominant, porosity decrease will be observed.

2.4. Trapping Mechanisms

Injected CO₂ is trapped inside the geologic formation in two trapping mechanisms namely physical and geochemical trapping (Bachu et al., 2007). Physical trapping comprises of three mechanisms namely static (structural and stratigraphic), hydrodynamic and residual gas trapping. Geochemical trapping is further divided into solubility and mineral trapping.

Physical trapping is controlled by the integrity of the cap rock and it generally occurs immediately after injection. In static trapping, injected CO₂ which is more buoyant than the formation brine migrates upwards until it reaches the top of the formation where it is trapped by an impermeable layer of cap-rock. In hydrodynamic and residual trapping, CO₂ that is injected into the formation displaces formation brine as it moves through the porous spaces. The CO₂ continues to migrate, and formation brine later replaces the pore space left by the moving CO₂. Some of the CO₂ will be left behind as immobile residual droplets (CCP, 2015).

Geochemical trapping is dependent on brine and rock chemistry and it generally takes place some time after injection as CO₂-water-rock interaction proceeds (Steel et al., 2018; Liu et al., 2019). Solubility trapping occurs when injected CO₂ turns permanently into aqueous phase due to CO₂ dissolution in water. Mineral trapping takes place when dissolved carbon bearing species is converted into permanent mineral phases as a result of CO₂-water-rock interaction. Mineral trapping of CO₂ generally depends on the mineralogy of host rock. The significance of reservoir rock mineralogy in determining mineral trapping mechanism has been shown in various works: Chlorite and hematite dissolution give way to the formation of siderite and ankerite, whereas oligoclase dissolution is followed by dawsonite precipitation (Xu et al., 2005). Chlorite and anorthite dissolution result in precipitation of kaolinite and ankerite (Yang, 2014). According to Cui et. al. (2017) precipitation of plagioclase is observed at the expense of ankerite and clay mineral dissolution in sandstone

reservoir, and the precipitation of ankerite and calcite observed together with dolomite dissolution in carbonate reservoir.

2.5. Monitoring CCS

Monitoring of injected CO₂ in a storage site has three main purposes: to see how CO₂ is kept securely in the reservoir, to confirm the prediction made by preliminary modeling studies, and to support mitigation measures in case of CO₂ leakage (GlobalCCSI, 2018). Monitoring methods includes: 1) monitoring the migration of tracers added to the injected CO₂, 2) measurement of pressure and temperature in wells, 3) continuously recording of seismic activity and 4) performing borehole geophysical methods to determine the path of the CO₂ plume through the reservoir (GRREBS, 2018).

Risk assessment study is performed to determine and quantify the potential risks caused by CCS such as CO₂ leakage (IPCC, 2005). Stratigraphically or structurally trapped CO₂ has the potential to leak to the surface or contaminate nearby drinkable groundwater resources through existing pathways such as fractured zones and faults. CO₂ becomes dangerous to humans when its concentration in the air reached above 5%, in which headaches, dizziness and nausea can be triggered (GRREBS, 2018). CO₂ changes the chemical composition of water by making it more acidic in the case of its leak to drinkable groundwater. Risk assessments include the utilization of scenarios to identify, classify and describe possible condition of the storage site in the future as well as predicting events that might cause CO₂ leakage (IPCC, 2005).

CHAPTER 3

GEOTHERMAL FIELDS IN JAVA ISLAND, INDONESIA

Java Island is located along a volcanic arc built through a convergent tectonic margin between the Indian-Australian plates and the Eurasian continental plate (Hamilton, 1979). The subduction takes place along the Java trench that reaches a maximum depth of about 6.75 km. The Indian-Australian oceanic crust is being subducted to the Sunda volcanic arc at a rate of about 6-7 cm/yr (Hamilton, 1979; Simandjuntak and Barber, 1996) (see Figure 3.1). The subduction produced three volcanic belts on Java Island, the Paleogene, the Neogene and the active Quaternary volcanic belts (Bemmelen, 1949; Hall, 2002). The tectonic setting of Java Island is dominated by four main faults, namely the E–W backarc-thrust of Barabis–Kendeng, the NE–SW strike-slip fault of Cimandiri, the SE–NW Citandui fault in West Java and the NE–SW Central Java Fault (Hoffmann-Rothe et al., 2001) (see Figure 3.2). Geologic features of Java Island cause the area to be rich in geothermal resources.

The volcanoes and faults on Java Island host to at least 62 geothermal fields (Setiadji, 2010). Geothermal fields can be divided into volcano-hosted and fault hosted geothermal systems based on their geologic association (Alam et al., 2010). The volcano-hosted geothermal systems are distributed in the Quaternary volcanic complex, stretched E–W direction in the middle part of the island, including 7 developed geothermal fields (Awibengkok, Dieng, Darajat, Kamojang, Patuha, Karaha-Bodas and Wayang-Windu) (Purnomo and Pichler, 2014). The fault-hosted systems are located in the Tertiary volcanic belt, in the southern part of the island (Purnomo et al., 2016).

This study attempts to simulate interaction between CO₂-brine-reservoir rock from four geothermal fields in Java Island namely: Ungaran, Baturaden, Dieng and Awibengkok (Figure 3.3). The selection of the fields is based on the availability of

data on hydrogeochemistry and reservoir rock characteristics. Ungaran and Baturraden fields are still under exploration stage. Dieng and Awibengkok fields are currently producing combined 437 MW electricity (ESDM, 2016). The geographic setting, geology, hydro geochemistry and reservoir rock properties of each field are described in the following sections.

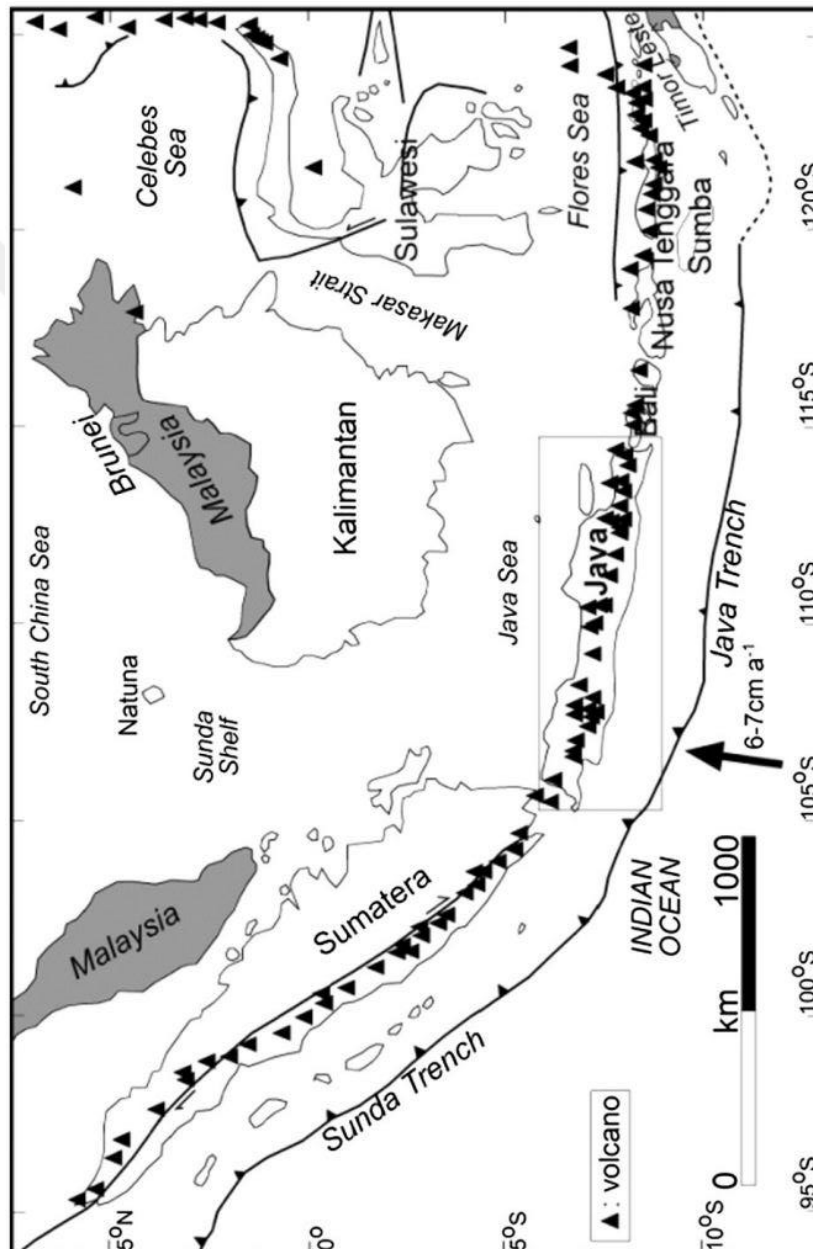


Figure 3.1. Geographic and tectonic map of Java Island in the Indonesian archipelago taken from Purnomo and Pichler (2014) modified after Hamilton, (1979) and Simandjuntak and Barber (1996).

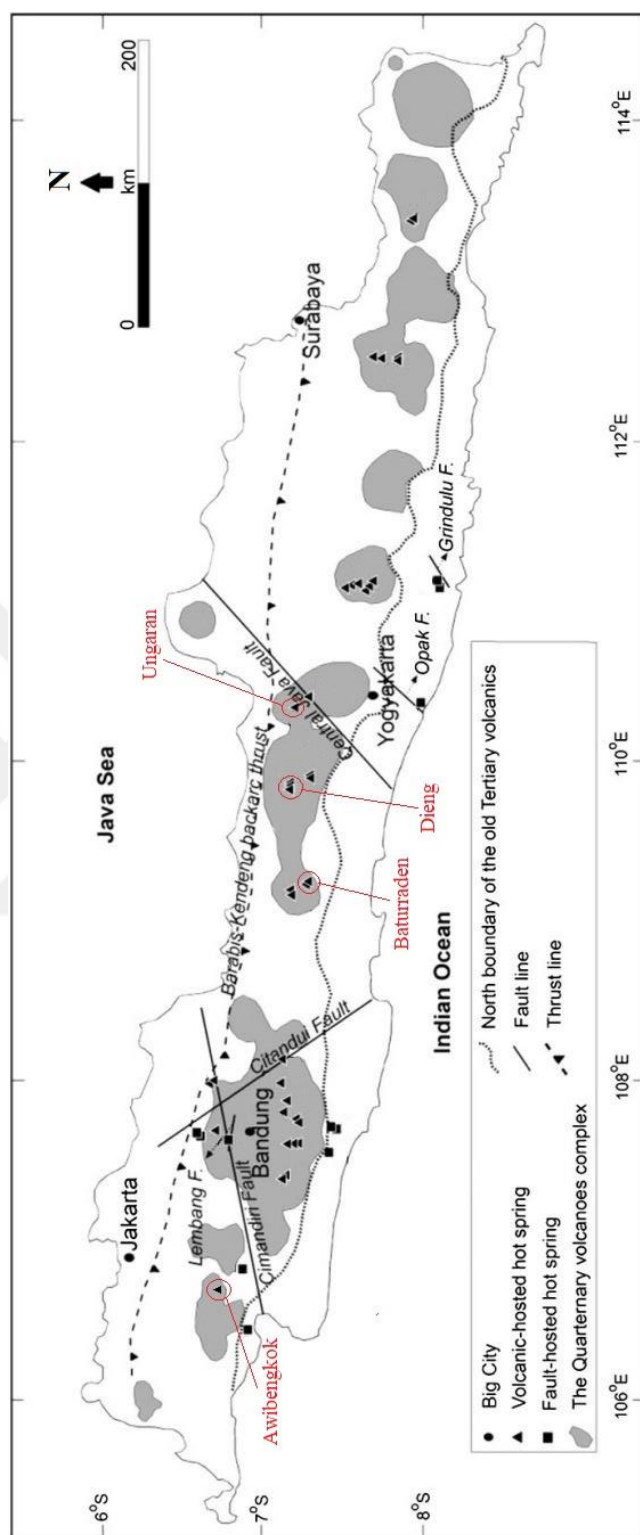


Figure 3.2. Tectonic map and the distribution of hot springs on Java island (from Purnomo and Pichler (2014), modified after Hamilton (1979) and Simandjuntak and Barber (1996)). The red circle indicates the study areas.



Figure 3.3. Geographic map of four selected geothermal fields located in Java Island, Indonesia.

3.1. Ungaran Geothermal Field

3.1.1. Geographic Setting and Geology

Ungaran geothermal field is situated in the southern flank of Ungaran volcano (Figure 3.4). This volcano has an elevation of 2050 m and is located 30 km south of Semarang city in Central Java province, Indonesia. Tertiary marine sediments comprising of Banyak, Kapung, Damar and Kalibeng formations is present at the base of Ungaran volcano. These units are overlain by Kaligetas formation formed during Early Pliocene which consists of lava flows, breccia, claystone and tuffaceous sandstone (Putranto and Rüde, 2016; Phuong et al., 2012). Ungaran volcano is characterized by three stages of growth: Oldest Ungaran, Old Ungaran and Young Ungaran. Oldest

Ungaran was formed from submarine activity during Early Pleistocene. Erosion of Oldest Ungaran produced five remnants hills with Munding hill (Figure 3.4) being the most elevated. Old Ungaran was formed during Middle Pleistocene (Claproth, 1989). Collapse of Old Ungaran formed a caldera and is followed by the growth several parasitic cones with Kendalisodo (Figure 3.4) being the most noticable (Thanden et al., 1975). Young Ungaran was formed during Late Pleistocene-Early Holocene and was built inside the caldera produced from subsidence of Old Ungaran (Claproth, 1989). Young Ungaran is characterized by andesitic lava, perlitic lava, and volcanic breccia (Claproth, 1989). Structural analysis of this area revealed that the Ungaran volcanic system is controlled primarily by the occurrence of the Ungaran collapse structure running from the northwest to the southeast. Fault systems trending northwest to southeast and northeast to southwest control the old volcanic rocks of the pre-caldera formation (Setyawan et al., 2009).

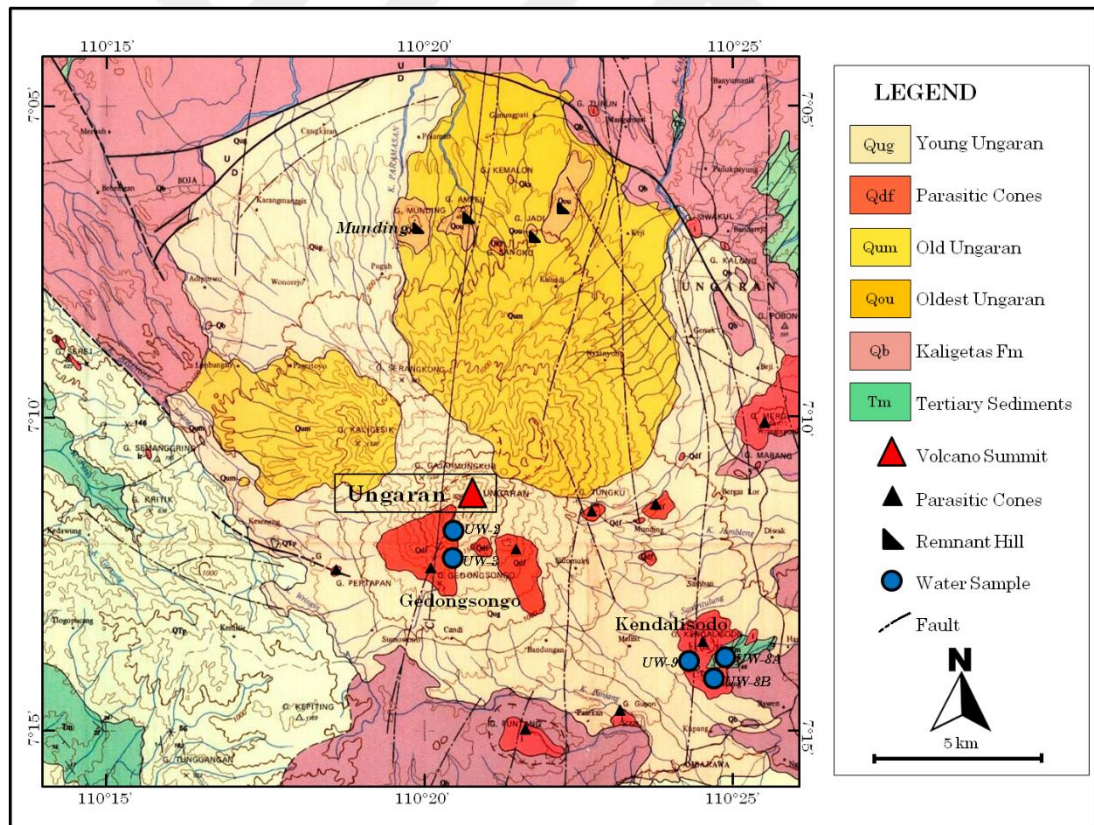


Figure 3.4. Geologic map of Ungaran volcano (Thanden et al., 1975; Putranto and Rde, 2016) showing the major volcanoes and the location of the geothermal manifestations.

3.1.2. Hydrogeochemistry

The Ungaran geothermal field is related with the recent Young Ungaran volcanism. Gedongsongo and Kendalisodo are the main manifestation sites located on the southern flank of the Ungaran volcano (Hochstein and Sudarman, 2015). According to Phuong et al. (2005), the composition of thermal spring waters at Ungaran geothermal field reveal the presence of two water types: the acid-sulfate water type which originates from steam heated meteoric water located near the volcano summit and neutral bicarbonate water type located at lower altitude. The chemical compositions of water samples in Ungaran geothermal field are given in Table 3.1. The water compositions are depicted in terms of a Schoeller diagram in Figure 3. 5. Of these waters, UW-2 and UW-3 are from the Gedongsongo region in southern flank of Ungaran volcano. The other three, UW-8A, UW-8B and UW-9 are located in Kendalisodo (See Figure 3.4). UW-2 is classified as calcium-sulphate (Ca-SO_4) water, UW-3 and UW-9 are calcium-bicarbonate (Ca-HCO_3) water, UW-8A and UW-8B are alkali-bicarbonate-chloride ($\text{Na+K-HCO}_3\text{-Cl}$) water type (Figure 3. 5).

Hydrogeochemical conceptual model of Ungaran field, as proposed by Phuong et al. (2012), is given in Figure 3. 6. Water sample UW-2 represents the upflow zone of the field (Phuong et al., 2012). Geothermal water coming from the source circulates through the fault and fracture zones. During its ascent to the surface, the water becomes enriched in sulfate from condensation of H_2S and CO_2 rich volcanic steam (UW-2). Some of the ascending water mix with shallow, bicarbonate rich groundwater of meteoric origin (UW-3) (Phuong et al., 2012).

Table 3.1. Chemical composition of Ungaran waters (in mg/L) (Phuong et al., 2012)

ID	T(°C)	pH	K ⁺	Na ⁺	Ca ²⁺	Mg ²⁺	SiO ₂	HCO ₃ ⁻	SO ₄ ²⁻	Cl ⁻	TDS
UW-2	40	5.4	8.6	25	33	10.3	109	59	136	1.2	383
UW-3	56	6.1	7.9	14	37	15.1	86	200	31.8	0.8	393.5
UW-8A	35.2	6.8	44	700	217	118	92	1732	0.2	998	3917
UW-8B	38.1	6.8	47	746	278	126	95	1824	0.1	1088	4224
UW-9	23.8	7.9	2.4	23	62.1	26.9	51	351	4.4	7.2	528

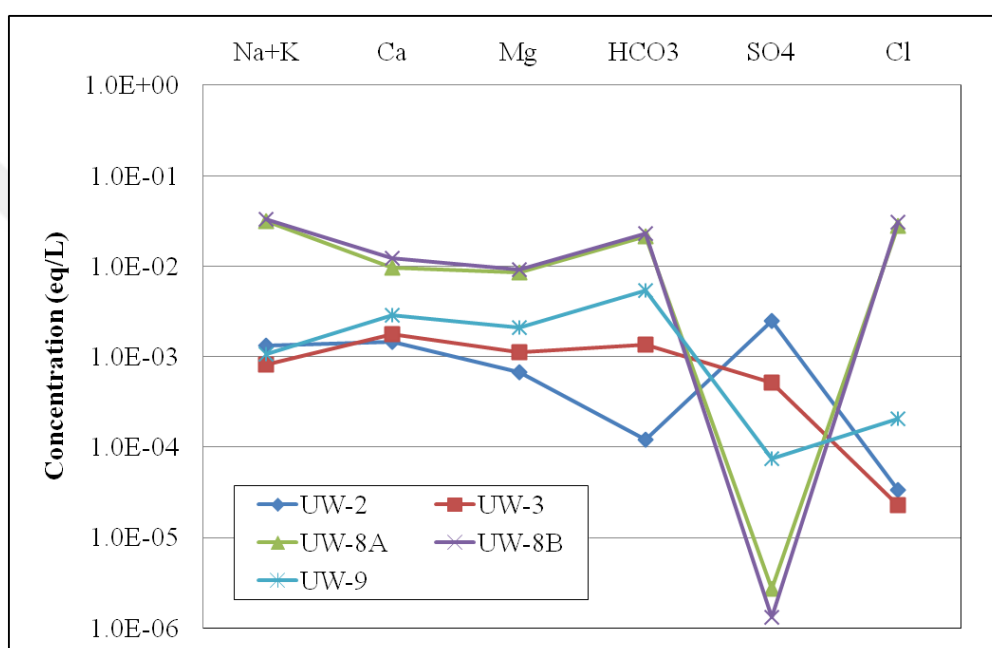


Figure 3.5. Schoeller diagram of Ungaran waters.

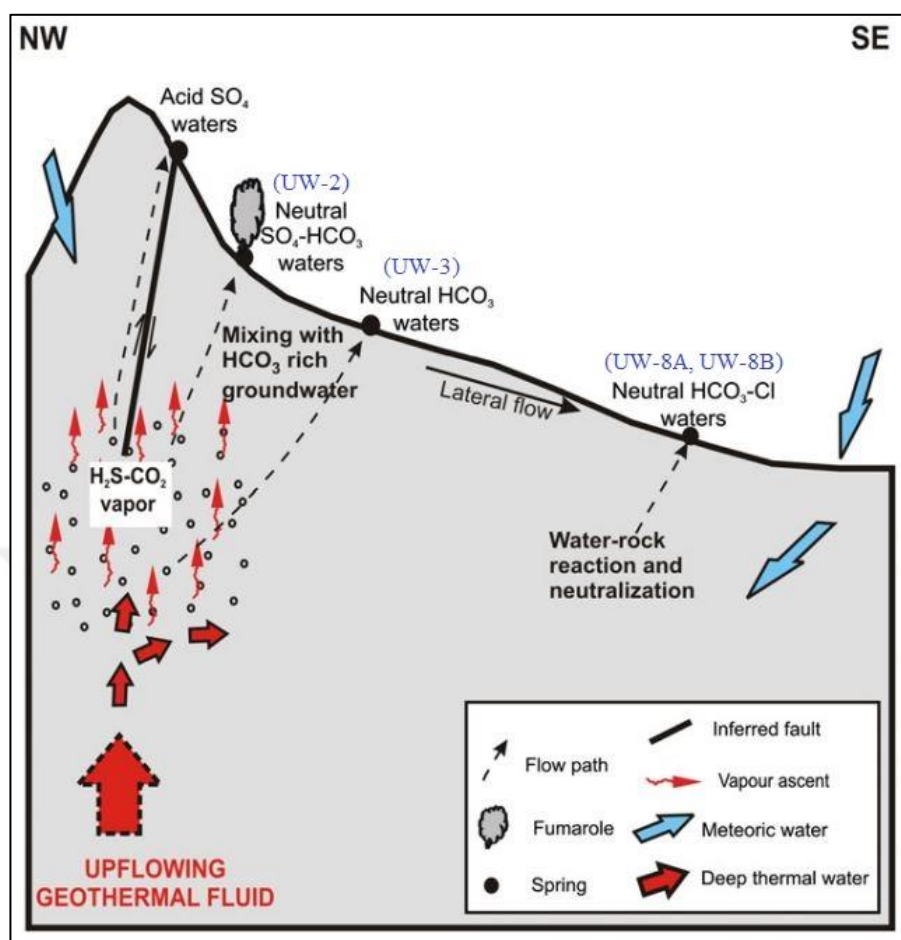


Figure 3.6. Conceptual model of hydrogeochemistry of Ungaran waters (Phuong et al., 2012).

3.1.3. Reservoir Rock Properties

A low resistivity anomaly of 30 Ωm , associated with a deep geothermal reservoir was reported to occur beneath the Ungaran summit (Phuong et al., 2005). Pre-caldera volcanics and the Tertiary marine sedimentary rocks are considered to be the main geothermal reservoir rocks of Ungaran geothermal field (Phuong et al., 2012). From geophysical study conducted by Setyawan et al. (2009) the depth of reservoir is estimated to be between 1000 to 3500 meters below surface. An average rock density of 2.64 g/cm³ of Old Ungaran volcanics is also obtained from the same study. Quartz, halloysite and alunite are the main secondary minerals reported in the hydrothermal alteration zones of the field (Phuong et al., 2012).

3.2. Baturaden Geothermal Field

3.2.1. Geographic Setting and Geology

Baturraden field is located in the southern flank of Slamet volcano (Figure 3. 7) having an elevation of 3428 meter above sea level (Djuri et al., 1996). The growth of Slamet volcano can be divided into two stages, Old Slamet and Young Slamet (Vukadinovic and Sutawidjaja, 1995). Slamet Volcano stands on Tertiary sedimentary rocks which consists of Rambatan, Halang, Tapak and Kaliglagah Formation (Harijoko and Juhri, 2017). Rambatan formation is composed of shale, marl, calcareous sandstone and conglomerate and is overlain by Halang Formation consisting of andesite sandstone, tuffaceous conglomerate and marl interbedded with sandstone (Djuri et al., 1996). This unit is overlain unconformably by Tapak formation comprising of coarse-grained sandstone and andesitic breccia deposited unconformably beneath Kaliglagah Formation which is made up of claystone, marl, sandstone and conglomerate (Djuri et al., 1996; Harijoko and Juhri, 2017). These sedimentary units are overlain unconformably by Slamet volcanics consisting of Old and Young Slamet. Old Slamet has andesitic composition formed during mid-Quaternary (Sutawidjaja and Sukhyar, 2009). This unit consist of volcanic breccia, lava and tuff and is deposited in the western part of Slamet volcano (Djuri et al., 1996). This area is dominated by normal faults with NW-SE and NE-SW trends (Harijoko and Juhri, 2017) (Figure 3. 7). Young Slamet formed from relatively recent eruption and has an andesitic to basaltic composition. This unit is composed of mainly andesitic lavas and is deposited in the eastern part of Slamet volcano (Djuri et al., 1996). The growth of Young Slamet is accompanied by the formation of approximately 35 scoria cones distributed in the northeastern part of the main volcano (Sutawidjaja and Sukhyar, 2009). The youngest unit in the area is the Lahar deposit which comprise of andesitic-basaltic volcanic boulders distributed in the western part of the area (Djuhari et. al., 1996) (Figure 3. 7).

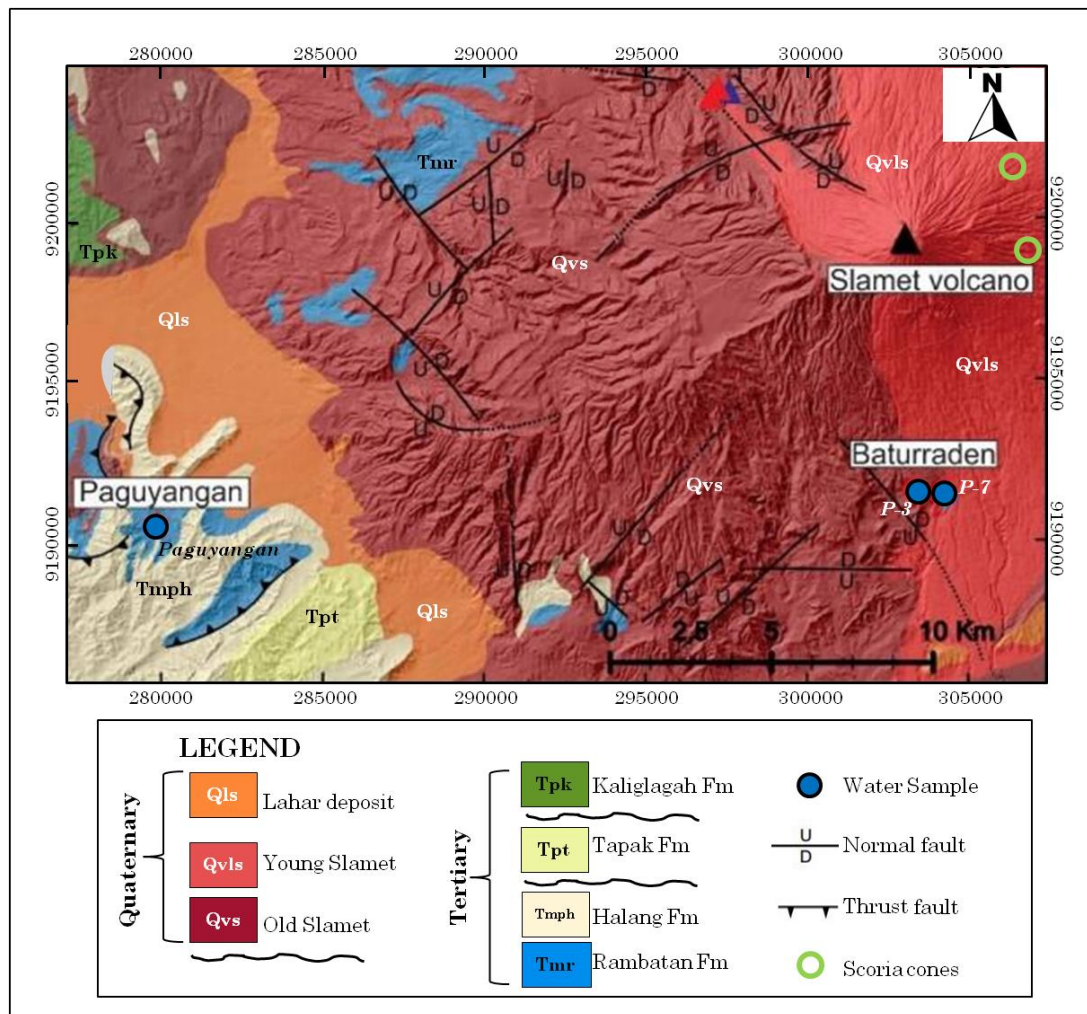


Figure 3.7. Geologic map of Baturaden volcano (Harijoko and Juhri, 2017) showing the scoria cones and the location of the water sample.

3.2.2. Hydrogeochemistry

The geothermal manifestations are located in Baturraden and Paguyangan areas (Figure 3.7). Chemical composition of hot water samples from these areas are given in Table 3. 2, and as Schoeller diagram in Figure 3. 8. The hot springs from Baturraden (P-3 and P-7) are classified as alkali-chloride-sulfate and alkali-chloride-bicarbonate ($\text{Na}+\text{K}-\text{Cl}-\text{SO}_4$, $\text{Na}+\text{K}-\text{Cl}-\text{HCO}_3$) waters. These waters seem to be products of mixing between bicarbonate and chloride-sulfate waters (Harijoko and Juhri, 2017). High

level of bicarbonate may suggest the mixing with groundwater, while sulfate enrichment of hot waters may be produced due to condensation of volcanic steam (Juhri and Harijoko, 2016). P-3 water composition suggests that it underwent sulfate and bicarbonate enrichment from H₂S and CO₂ rich volcanic vapor mixed with meteoric water near the surface. P-7 has similar composition with P-3 sample but with more enrichment of bicarbonate. Hot water sample from Paguyangan is classified as alkali-chloride (Na+K-Cl) water and is inferred to have similar origin with P-3 and P-7 waters owing to their similar Cl/B ratio (Harijoko and Juhri, 2017). In this respect, Paguyangan water is proposed to represent the outflow zone of the Baturraden geothermal system (Harijoko and Juhri, 2017). Juhri and Harijoko (2016) estimated reservoir temperature of Baturraden (P-7, P-3) and Paguyangan waters sources by applying Na/K cation geothermometry as 294°C and 116°C respectively. The conceptual model of Baturraden geothermal system, based on the study by Harijoko and Juhri (2017), is given in Figure 3. 9.

Table 3.2. *Baturaden water chemistry (in mg/L) (Harijoko and Juhri, 2017).*

ID	T (°C)	pH	K ⁺	Na ⁺	Ca ²⁺	Mg ²⁺	SiO ₂	HCO ₃ ⁻	SO ₄ ²⁻	Cl ⁻	B	TDS
P-7	50	7	76	389	194	185	169	687.3	609	754	4.4	3068
P-3	46	6	77	377	197	185	164	695.4	600	724	3.9	3023
Paguyangan	72	7	2.9	193	63	0.23	58	20.3	8.51	414	3.7	764

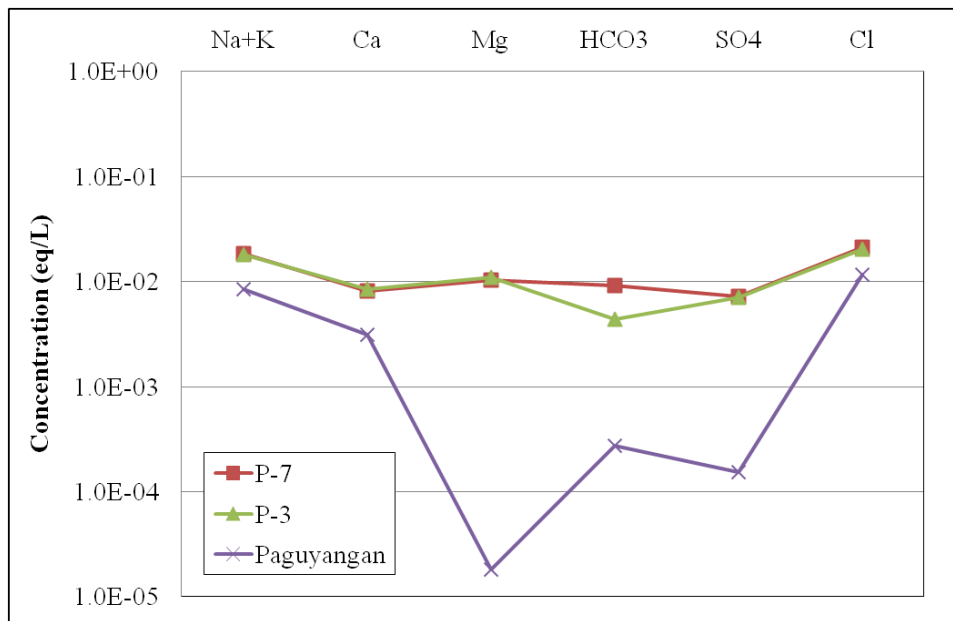


Figure 3.8. Schoeller diagram of Baturaden field waters.

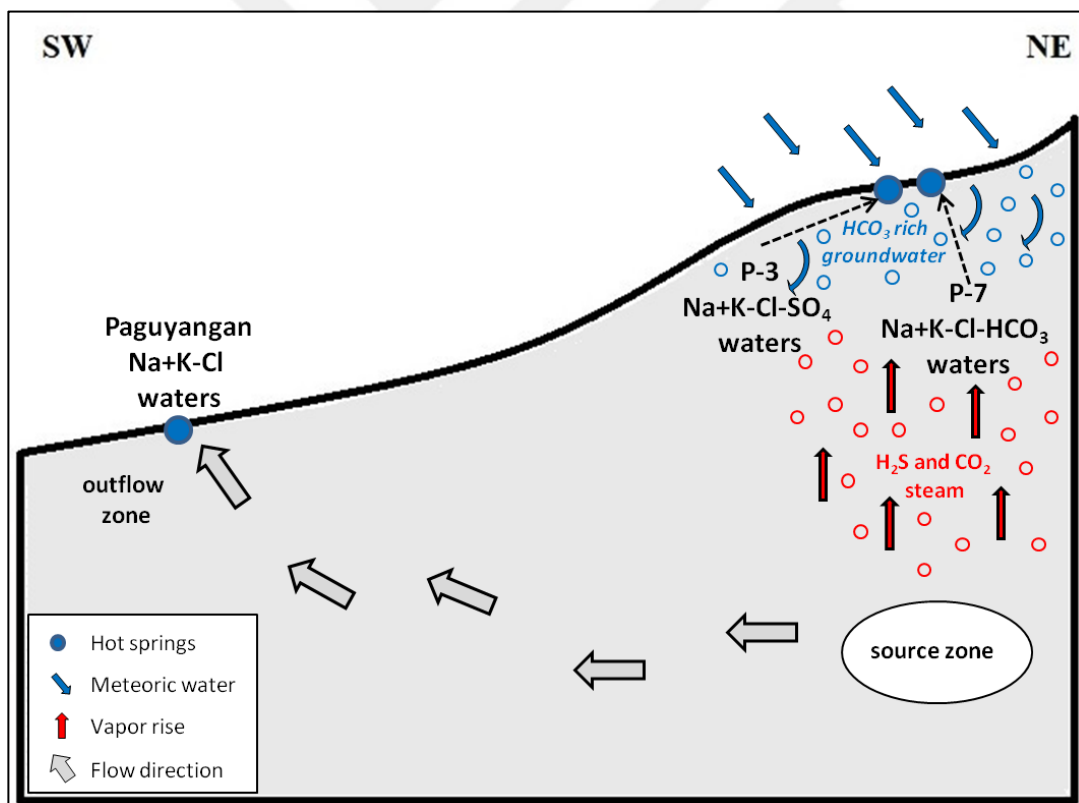


Figure 3.9. Conceptual model of hydrogeochemistry of Baturaden field based on the study of Harijoko and Juhri (2017).

3.2.3. Reservoir Rock Properties

The reservoir of Baturraden field has a thickness in the range of 1000-1250 m, with an elevation of about 0.5-1 km (Utama et al., 2012) corresponding to a depth of about 1600-2000 m from the surface. From geophysical study conducted by Reswara et al. (2014), depth of 1600 to 2000 meters corresponds to Old Slamet volcanics having an estimated rock density of 2.54 g/cm³. Alteration minerals found in Baturraden field are amorphous silica, halloysite and montmorillonite (Indarto et al., 2017).

3.3. Dieng Geothermal Field

3.3.1. Geographic Setting and Geology

Dieng geothermal field is located inside the volcanic highlands of the Dieng Plateau in Central Java at elevations of over 2000 meters. Dieng geothermal field has been generating electricity since 2002 with a capacity of 60 MW. The geology of Dieng field is composed of Tertiary sediments overlain by several volcanic sequences (Figure 3.10). Rambatan Formation containing shale, marl and calcareous sandstone formed during Early-Middle Miocene is the oldest unit in the area (Condon et al., 1996). This unit is unconformably overlain by Tapak Formation consisting of volcanic breccia and tuffaceous sandstone formed during Middle Pliocene and Kalibiuk Formation consisting of marl and claystone respectively. These units are intruded by dioritic rock intrusion which is exposed in the southwestern part of the area (Gaffar, 2017) (Figure 3. 10).

Ligung Formation consisting of andesitic volcanic breccia, hornblende andesitic lava and tuff formed during Early Pleistocene is deposited unconformably above earlier Tertiary units (Condon et al., 1996). Jembangan volcanics which consist of andesitic lava, developed from Early to Late Pleistocene, cover large areas in the northern part of the field (Figure 3. 10). Kaligetas Formation containing of volcanic breccia, lava flows, tuff, tuffaceous sandstone and claystone formed in Middle Pleistocene is

exposed in the northeastern part of the field. Alluvial and lake deposit consisting of sand, silts, muds and clay from Early Holocene overlies these volcanic units.

Dieng volcanic complex composed of andesitic lava and andesite quartz developed during Early to Middle Holocene is deposited above alluvial and lake deposit. Dieng volcanic complex is divided into two growth episodes: 1) Old Dieng (Prahu volcano, Pagerkandang caldera and Pangonan-Merdada caldera) and 2) Young Dieng (Bisma, Pakuwaja, Sikidang, Seroja and Sikunir volcano) (Gaffar, 2017) (Figure 3. 10). This unit is overlain by recent volcanism of Sindoro volcano (Condon et al., 1996). Dieng geothermal system is associated with Pagerkendang and Pangonan-Merdada caldera from Old Dieng volcanic complex (Harijoko et al., 2016). The regional structure of the studied area has a caldera form with local fault trending southeast – southwest (Ramadhan et al., 2013).

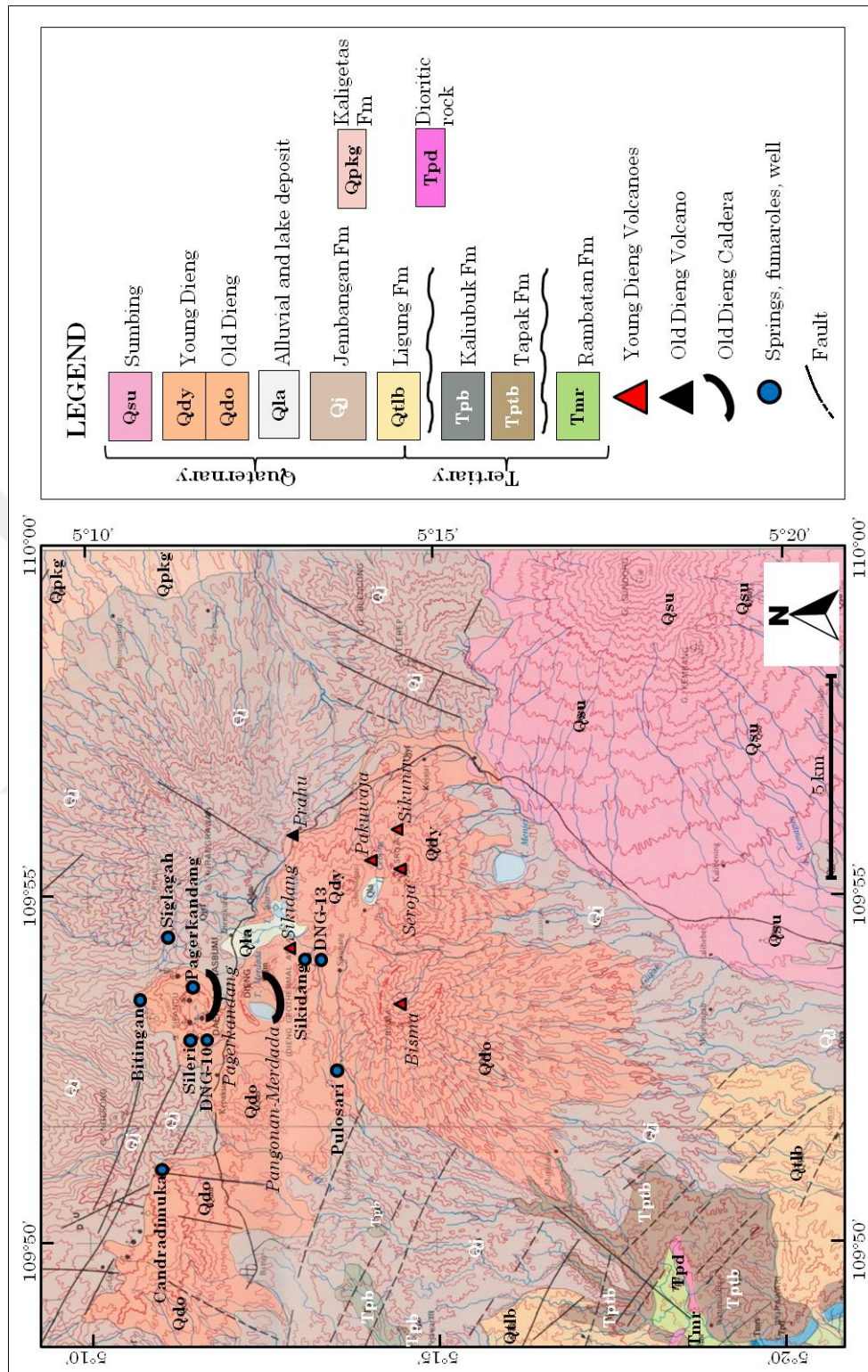


Figure 3.10. Geologic map of Dieng geothermal field (Condon et al., 1996) showing the major volcanoes and the location of geothermal water samples.

3.3.2. Hydrogeochemistry

Geothermal manifestations in Dieng field are found as hot springs in Bitingan, Sileri, Siglagah, Pulosari and Sikidang, fumaroles in Candradimuka and Pagerkandang and mud pools in Sileri and Sikidang craters (Ramadhan et al., 2013). In this study, chemical compositions of spring samples from Bitingan, Sikidang and Sileri, and well samples from Sikidang (DNG-13) and Sileri (DNG-10) are given in Table 3. 3 and plotted as Schoeller diagram in Figure 3. 11. The field consist of two sectors namely; Sileri sector which is dominated by a deep, high-temperature, liquid-dominated reservoir and Sikidang sector which is a moderate depth, high-enthalpy, gas-rich resource (Layman et al., 2002).

Bitingan and Sileri spring waters are of alkali-bicarbonate ($\text{Na}+\text{K}-\text{HCO}_3$) type, with Sileri water having slightly more bicarbonate enrichment. Sikidang spring water is classified as alkali-sulfate ($\text{Na}+\text{K}-\text{SO}_4$). Production well sample of DNG-10 in Sileri sector and DNG-13 in Sikidang sector are classified as alkali-chloride ($\text{Na}+\text{K}-\text{Cl}$) water. Bottom hole temperatures in well DNG-10 (2300m) and DNG-13 (1732m) are measured as 325°C and 255°C (Boedihardi et al., 1991). The hydrogeochemical conceptual model of Dieng field is summarized in Figure 3. 12 (Layman et al., 2002).

Table 3.3. Chemical Compositions of Dieng waters (concentration in mg/L, w: well, s: spring)
(Boedihardi et al., 1991; Ramadhan et al., 2013)

ID	Sector	T (°C)	pH	K ⁺	Na ⁺	Ca ²⁺	Mg ²⁺	SiO ₂	HCO ₃ ⁻	SO ₄ ²⁻	Cl ⁻	TDS
Bitingan (s)	-	59	6.8	28	71.3	11.3	23.4	38.9	243	59.5	18	495.3
Sikidang (s)	Sikidang	88	2.2	52	203	43.5	58.9	58.7	1	862	27.5	1306
Sileri (s)	Sileri	45	6.4	18	53	72	32	175	340	152	15	857
DNG-10 (w)	Sileri	325	5.9	919	3351	405	67	70	366	288	6741	12207
DNG-13 (w)	Sikidang	255	4.1	93	1062	83	1	280	1	450	1508	3478

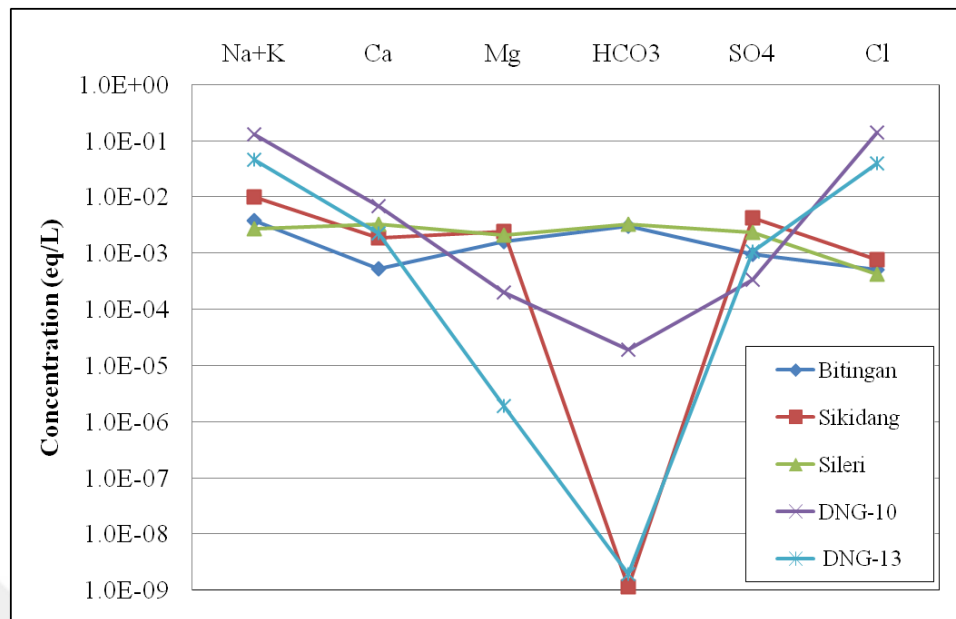


Figure 3.11. Schoeller diagram of Dieng waters

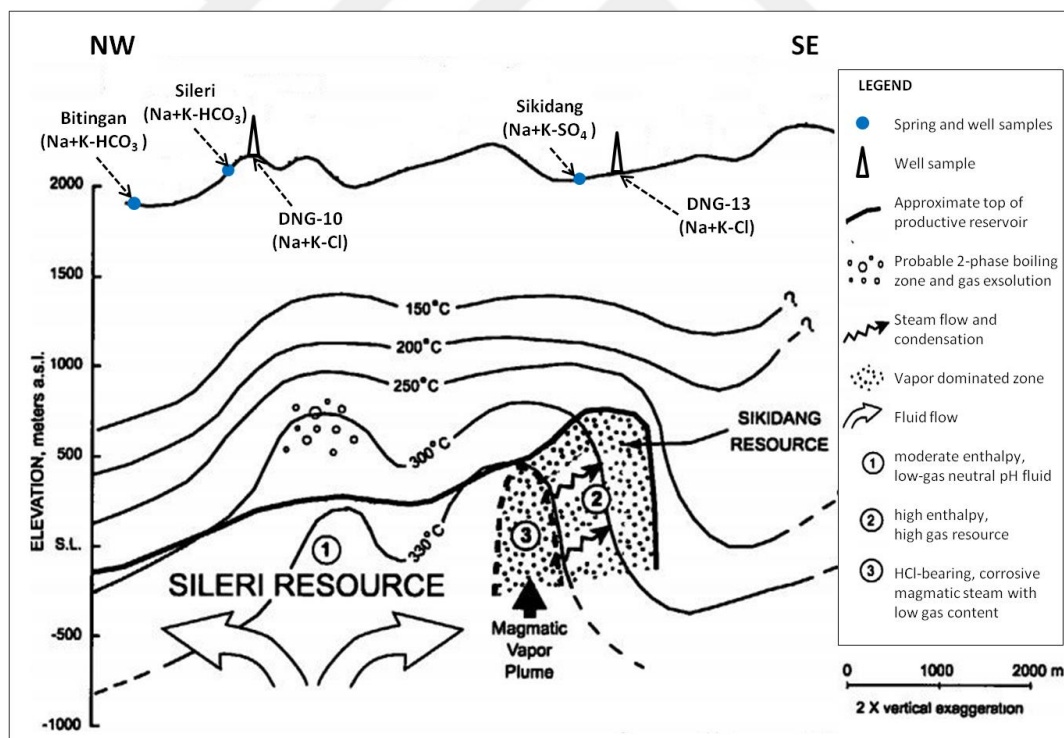


Figure 3.12. Conceptual model of Dieng geothermal system (Layman et al., 2002).

3.3.3. Reservoir Rock Properties

Reservoir rock is located at depth between 2000-2300 meters having a measured well temperature range of 300 to 335°C in Sileri sector, and between 1400- 1500 meters having measured well temperature of 240-300 °C in Sikidang sector (Layman et al., 2002). Dieng geothermal field is associated with the calderas of old Dieng volcanics (Pagerkandang 0.46 Ma, Pangonan—Merdada 0.37 Ma) formed during Upper Pleistocene (Gaffar, 2017). According to Kusdyantono et al. (2016), three alteration zones are present in the field. Argillic alteration occurs at the shallowest depth (1100-1300 m) with temperatures of 150-250°C. Propylitic alteration occurs at intermediate depths (1100-2400 m) with temperatures of 250-300°C. Phyllic alteration occurs in greatest depth (1600-2400 m) at temperature above 300°C. Kusdyantono et al. (2016) identified argillic alteration by presence of clay minerals, propylitic zone by epidote, quartz, calcite, illite and chlorite, and phyllic alteration by the presence of actinolite.

3.4. Awibengkok Geothermal Field

3.4.1. Geography Setting and Geology

The Awibengkok geothermal field is the largest developed geothermal field in Indonesia, currently having installed capacity of 377 MW electrical generation (Acuna et al., 2008). The Awibengkok geothermal system is located in a mountainous area with an elevation ranging from about 950-1500 meter above sea level. The geothermal reservoir is associated with young volcanism and intrusions in a highland area southwest of Salak volcano and east of the Cianten caldera (Aprilina et al., 2015). The oldest rocks are mainly shallow-marine carbonates and epiclastic sediments (mudstones and sandstones containing abundant volcanic ash and lithic debris) (Stimac et al., 2008). Bojongmanik formation (Figure 3.13) from Middle Miocene overlies these rocks and is composed of sandstone, pumiceous tuff, marl, limestone and claystone. This formation is overlain by tuff and breccia formed in Late Miocene (Efendi and Hermanto, 1998). These sedimentary units are overlain unconformably by volcanics units formed during Quaternary.

The Oldest volcanic units are formed during Early Pleistocene and are composed of undifferentiated volcanic rocks, volcanics breccia and volcanic lava (Figure 3.13) (Efendi and Hermanto, 1998). Salak volcanics formed during Middle to Late Pleistocene comprise tuff, lahar, tuffaceous breccia and andesitic basaltic lava. The products of Salak volcanics are Cianten caldera and Salak volcano (Figure 3.13). Andesitic lava of Endut-Perbakti volcanics forms the youngest deposits in the area (Efendi and Hermanto, 1998). Volcanoes namely Perbakti, Gagak, Endut and Awibengkok are included in this unit.

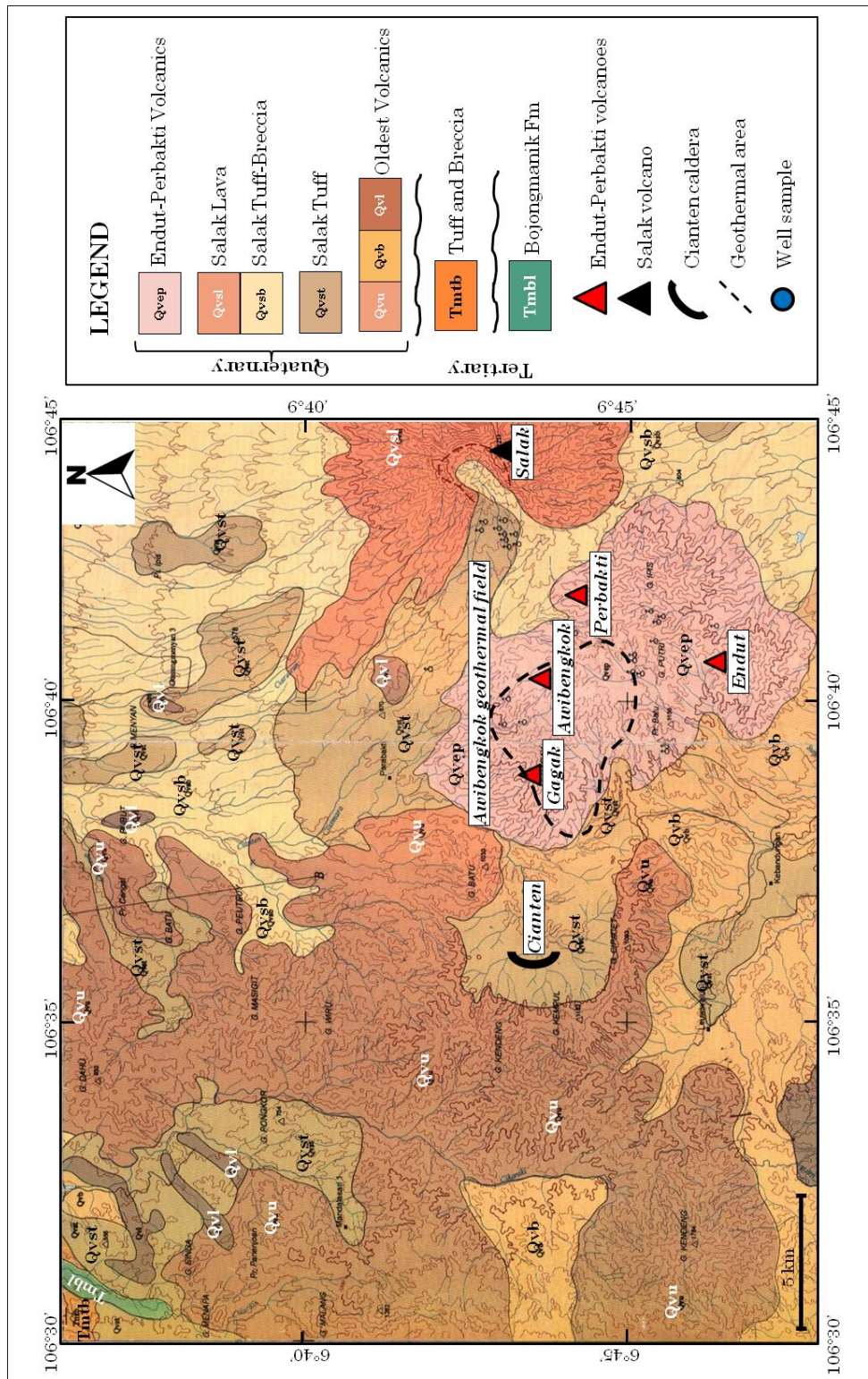


Figure 3.13. Geologic map of Awibengkok geothermal field (Efendi and Hermanto, 1998) showing major volcanoes and well sample location.

3.4.2. Hydrogeochemistry

Geothermal manifestations of Awibengkok field are found in the form of fumarole and hot springs (Figure 3.14). Hot springs comprise of bicarbonate, bicarbonate–chloride and chloride waters with Ratu spring as an exceptional hot water having acid sulfate characteristic (Stimac et al., 2008). Awibengkok field is divided into four sectors based on the fluid chemistry, temperature and flow patterns: Western, Central, Eastern and Far Eastern Cells which are bounded by faults (Stimac et al., 2008) (Figure 3.15). Western Cell hosts 2 wells, Central Cell 5 wells, Eastern and Far Eastern Cells host 4 and 2 wells, respectively. Central Cell has the highest Cl concentration and the lowest gas content compared to the other cells. The highest temperature is measured in the Western Cell, followed by Central, Eastern and Far Eastern Cells.

The chemical compositions of the spring and well waters from Awibengkok field are given in Table 3.4. As can be seen from the table, the full chemical data including both cation and anion concentrations are available for well waters, while for the spring waters, only the anion contents are reported in the previous studies. The bicarbonate and chloride rich compositions of waters are readily apparent from Table 4, except Ratu spring which is of acid sulfate nature. The chemistry of well waters is also presented as Schoeller diagram in Figure 3.16. Well sample Awi-12 in western cell and Awi 1-2 RD in eastern cell are taken from the study of Mahon et al. (2000) and Allis (1999) respectively. Both of the W-12 and Awi 1-2 RD well samples are classified as alkali-chloride (Na+K-Cl) water (Figure 3.16).

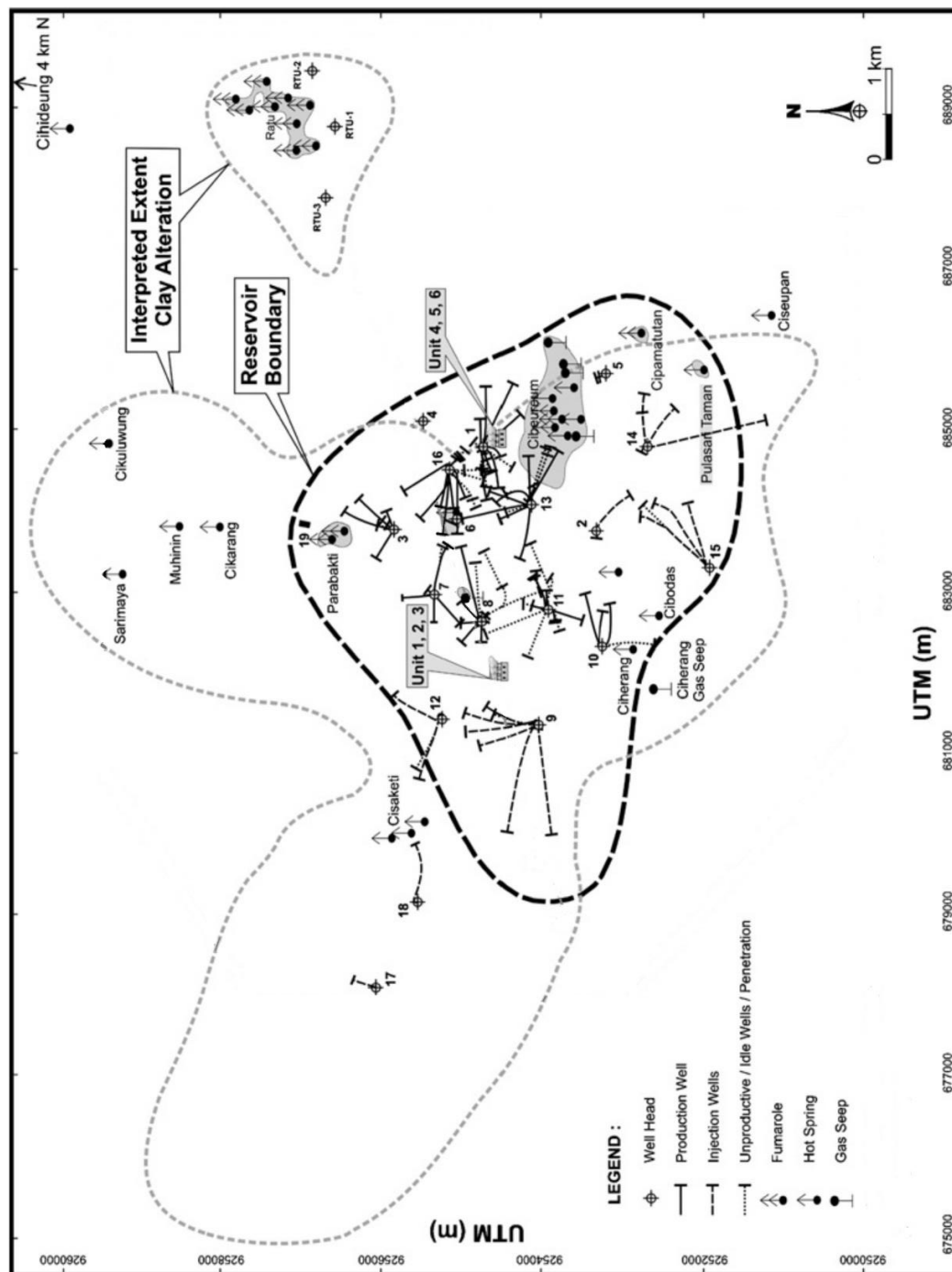


Figure 3.14. Map of Awibengkok geothermal field (powerplant units and wells are numbered based on the sequence of drill sites established) (Stimac et al., 2008).

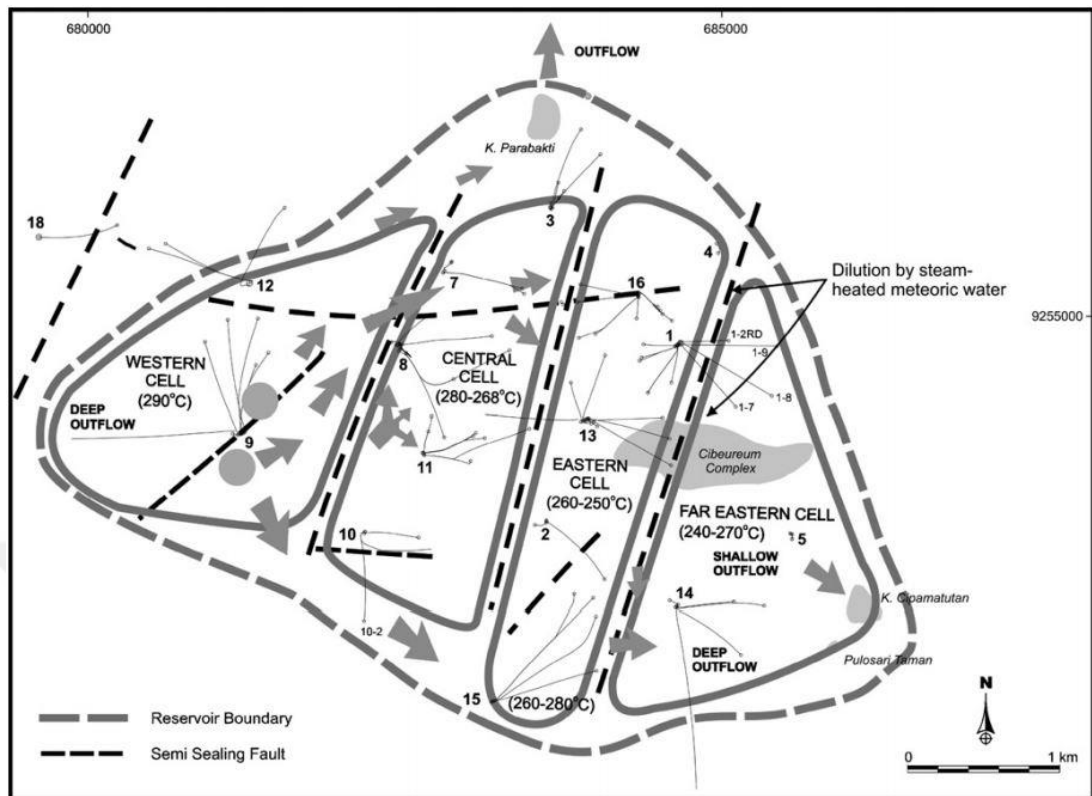


Figure 3.15. Conceptual model for the Awibengkok field showing the sectors, the wells (numbered) and the flow pattern under natural state (pre-exploitation) (Stimac et al., 2008)

Table 3.4. Chemistry of Awibengkok waters (concentration in mg/L, s: spring, w: well) (Allis, 1999; Mahon et al., 2000; Stimac et al., 2008).

ID	T (°C)	pH	K	Na	Ca	Mg	SiO ₂	HCO ₃	SO ₄	Cl	TDS
Sarimaya (s)	57.5	6.4	-	-	-	-	-	513	2.5	3402	-
Ciherang (s)	53	6.5	-	-	-	-	-	713	0.5	1.5	-
Cikarang (s)	75	6.7	-	-	-	-	-	940	41	2.5	-
Muhinin (s)	47.5	6.1	-	-	-	-	-	728	6	5.5	-
Cikuluwung (s)	-	6.7	-	-	-	-	-	1130	3	320	-
Cisketi (s)	41	6.4	-	-	-	-	-	276	3	19.4	-
Cihideung (s)	44.5	6.7	-	-	-	-	-	550	7	580	-
Ciseupan (s)	49	6.5	-	-	-	-	-	544	7.5	0.5	-
Cibodas (s)	60	6.6	-	-	-	-	-	290	1	2	-
Ratu (s)	95	2.5	-	-	-	-	-	0	2340	15	-
Aw1 1-2 RD (w)	250	6.9	630	3680	227	0.7	498	96.2	23.6	6700	12116
W-12 (w)	100	6.7	876	3675	268	1	495	37	20	6810	12452

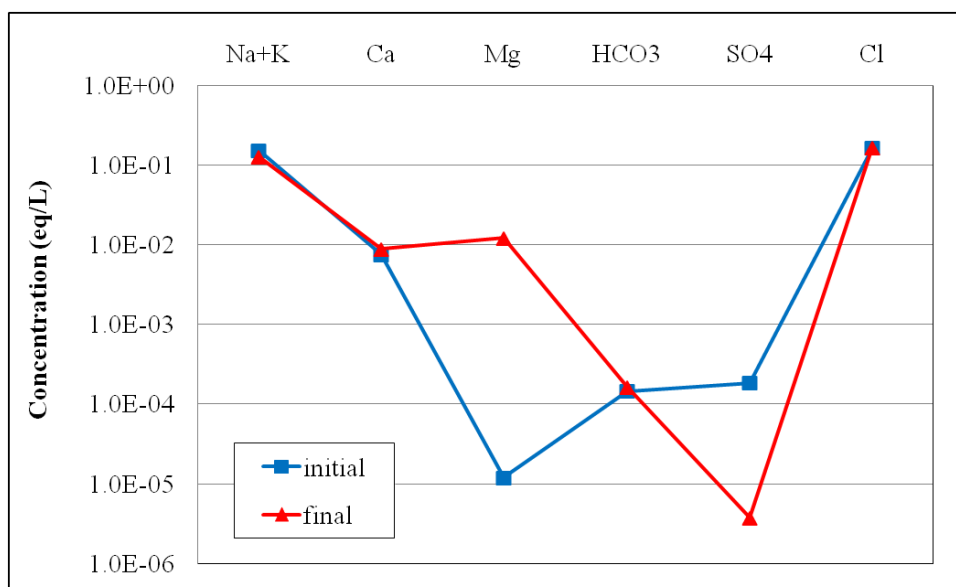


Figure 3.16. Schoeller diagram of Awibengkok well samples.

3.4.3. Reservoir Rock Properties

The four sectors of Awibengkok field are separated by faults whose permeability is partly sealed as a result of intrusion of dikes and sills (Stimac et al., 2008; Aprilina et al., 2015). The Awibengkok reservoir rocks are generally composed of andesitic and lesser basaltic lava, breccia, tuff and lahar (Stimac et al., 2008). The reservoir top is characterized to be deeper and hotter in the western and southern part, while relatively shallower in the eastern part of the field (Acuna et al., 2008). According to Stimac et. al. (2008) reservoir rock is located between Salak volcanics and Perbakti-Endut volcanics and has a mean porosity value of 10.6%. Three alteration zones are found in the field: 1) Argillic alteration zone dominated by smectite and smectite-illite mixed layer clays, with accessory pyrite, silica, hematite, calcite, anhydrite, zeolite and chlorite which act as cap rock, 2) Propylitic alteration zone dominated by epidote, illite, and chlorite but also contains albite, adularia, calcite, wairakite, pyrite and titanite, 3) Phyllic alteration zone dominated by illite, sericite, adularia and quartz, with lesser epidote and chlorite (Stimac and Sugiaman, 2000).

CHAPTER 4

MODELING STUDIES

Geochemical trapping which consists of solubility and mineral trapping is considered to be the safest means of CO₂ fixation. Interaction of the stored CO₂ with both brine and minerals in reservoir rock produces variation in species concentration and pH in the brine leading to precipitation and/or dissolution of minerals and porosity change in rock. The extent and time in which these changes take place can be utilized as means to evaluate the effectiveness of geochemical trapping. One of the means to assess the efficiency of both solubility and mineral trapping is by performing geochemical modeling. Solubility trapping is evaluated by observing the final concentration of carbonic acid, bicarbonate and carbonate dissolved in the brine. Mineral trapping is assessed by calculating the amount of newly formed carbonate precipitates and the length of time needed for the dissolved CO₂ to be transformed into a mineral.

Previous studies concerned with geochemical investigations related to CO₂-water-rock interaction include laboratory experiment for short term observation and numerical simulation for long term prediction. Since geochemical study based on laboratory experiment has a limitation of experiment duration, numerical simulation by the assistance of program such as PHREEQC (Parkhurst and Appelo, 2013) is necessary to predict long term outcome of CO₂-water-rock interaction. Steel et. al. (2018) determined the equilibrium state of CO₂-water-calcite interaction using PHREEQC code. Klajmon et al. (2017) carried out equilibrium and kinetic modeling of CO₂ storage with PHREEQC and predicted the geochemical evolution for a period of 10000 years. Gysi et. al. (2012) conducted geochemical modeling of CO₂ rich water interaction with basaltic glass with the assistance of PHREEQC program.

4.1. Modeling Approach

In this study, modeling is performed using PHREEQC program and assuming a single stage CO₂ injection under a constant temperature and pressure in a static environment where there is no flow in the simulated reservoir. The constant temperature assigned corresponds to the reservoir temperature obtained from either well bottom temperature measurements or geothermometric calculations. The constant pressure corresponds to the hydrostatic pressure present at the reservoir depth. Modeling is performed in two separate batch namely equilibrium and kinetic modeling. From both modeling studies, solubility and mineral trapping mechanisms are evaluated by observing the compositional change in the brine chemistry and the rock mineralogy. The thermodynamic extended llnl.dat database is used during simulation in this study. Klajmon et al. (2017) reported that the phreeqc.dat, pitzer.dat and llnl.dat is unable to predict the solubility of CO₂ in a higher-pressure environment (Figure 4.1). Thus redefinition of CO₂ dissolution reaction and additional Peng-Robinson equation parameters from phreeqc.dat is extended into the llnl.dat database to overcome this limitation. Peng-Robinson equation of state is a modification of original Van der Waals equation that describe the behavior of non-ideal gas and its solubility in water (Peng and Robinson, 1976).

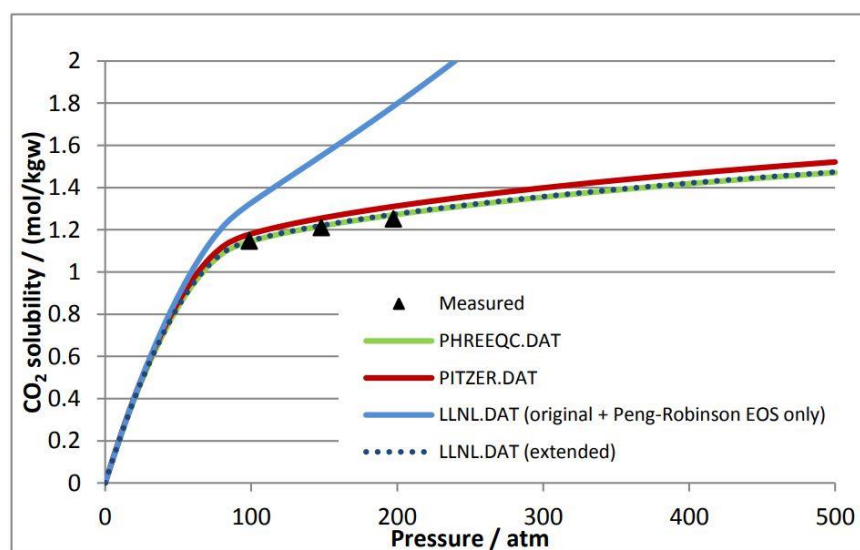


Figure 4.1. CO₂ dissolution in a 0.35 mol kgw⁻¹ NaCl solution at 40°C (Klajmon et al., 2017).

4.1.1. Equilibrium modeling

Equilibrium modeling is performed by reacting brine and reservoir rock composition with CO₂. The purpose of this modeling is to understand the changes in brine chemistry, mineral composition and porosity value of the reservoir rock after equilibrium state is achieved among CO₂-brine-reservoir rocks. The modeling results in the investigation of the variations in a) reservoir rock mineralogy (in terms of mineral mol amount), b) porosity of rock, c) pH and major ion concentrations of the brine. The necessary input required for equilibrium modeling are temperature, pH, volume and concentration of dissolved species in brine and mol amount of minerals in rock (Figure 4.2). For the injected CO₂, the partial pressure and mol amount are used as inputs. Secondary carbonates (calcite, dolomite, ankerite, dawsonite, magnesite, siderite) with an initial mol amount of zero are included in the simulation to evaluate possible mineral trapping mechanism in the reservoir. The parameters are assigned into two different data blocks in PHREEQC program which are: *Solution* data block and *Equilibrium_phase* data block.

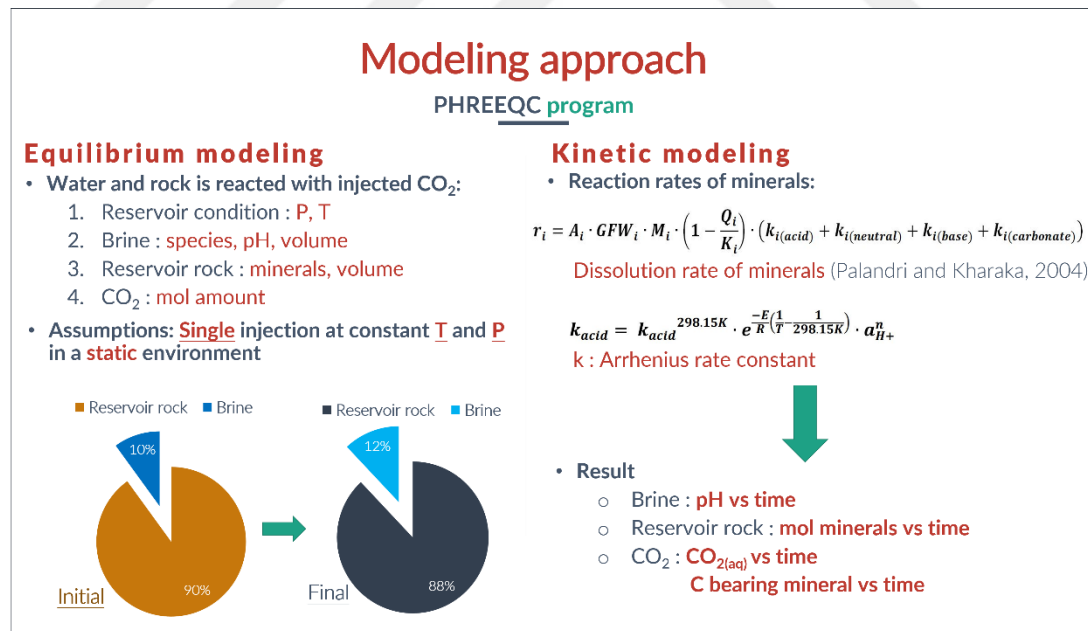


Figure 4.2. Summary of modeling approach.

Solution data block is used to define brine chemistry related parameters and the volume and the density of water. The modeling assumes that 1 liter of brine fills the entire pore space of the reservoir and the volume of reservoir rock is adjusted accordingly. As an example, porosity value of 10% will correspond to 1 liters of brine and 9 liters of reservoir rock. By taking density of water as 1.0 g/cm³, the assumed brine and rock volume correspond to 1000 cm³ and 9000 cm³ respectively (Figure 4.2).

Equilibrium_phase data block is utilized to assign the amount of minerals or gas in units of mol. Mol amount for each mineral can be found using the following equation:

$$M_i = \frac{m_i \cdot V \cdot \rho}{GFW_i}$$

Where M_i is the mol amount (mol) of a mineral, m_i is the volume % of a mineral with respect to total volume of reservoir rock obtained from renormalized CIPW norm (Hollacher, 2018) with the addition of alteration minerals reported in the literature. V is the total rock volume (cm³) adjusted to the porosity value of the reservoir. The symbol ρ is the rock density (g/cm³). GFW_i is the molar weight (g/mol) of each mineral.

The amount of CO₂ gas reacting with brine and rock is determined from the result of CO₂ solubility calculation in the brines of four selected fields. This is because the ratio of CO₂ to H₂O should be kept less than the solubility of CO₂ at reservoir condition (Sigfussona et al., 2015).

For the modeling to resemble reservoir regime, reservoir temperature and hydrostatic pressure at depth are defined. Reservoir temperature is defined in the *Solution* data block, whereas pressure is assigned in the *Equilibrium_phase* data block.

4.1.2. Kinetic modeling

Kinetic modeling is intended to understand how brine and reservoir rock properties transform after CO₂ injection over a period of time until equilibrium state is achieved.

The results of kinetic modeling give insight on how the reactions between CO₂-water-rock proceed by predicting which chemical reaction would be responsible for the dissolution or the precipitation of certain minerals (Figure 4. 2). In addition, the modeling also provides insight on how these reactions affect the brine composition by evaluating the change in pH and dissolved CO₂ through time. The modeling is based on dissolution rate of minerals. The dissolution of minerals is defined by the following reaction rate formula (Palandri and Kharaka, 2004; Klajmon et al., 2017).

$$r_i = A_i \cdot GFW_i \cdot M_i \cdot \left(1 - \frac{Q_i}{K_i}\right) \cdot (k_{i(acid)} + k_{i(neutral)} + k_{i(base)} + k_{i(carbonate)})$$

r_i is the reaction rate (mol/s), A_i is the specific surface area (m²/g), GFW_i is the molecular weight (g/mol) of the mineral and M_i is the molar amount (mol). The symbol Q_i denotes activity product, and K_i is equilibrium constant of the mineral. The character k_i is the Arrhenius rate constant (mol/m² s) of a mineral. Arrhenius rate k_i is quantified for several mechanisms: acid, neutral, base and carbonate reaction mechanisms which are explained in detail inside the work of Palandri and Kharaka (2004). Each mechanism comprises of a single k equation with the following detail:

$$k_{acid} = k_{acid}^{298.15K} \cdot e^{\frac{-E}{R} \left(\frac{1}{T} - \frac{1}{298.15K} \right)} \cdot a_{H^+}^n$$

The example above depicts the acidic reaction mechanism of a mineral. This equation is also applied in other reaction mechanisms. In the above equation, the symbol $k_{acid}^{298.15K}$ denotes the reaction rate (mol/m²s) of a mineral in an acidic condition at 25°C, E is the activation energy of a mineral (kJ/mol) and R is the universal gas constant (8.314 J/mol-K). T is the temperature (Kelvin). The symbol n is the reaction order with respect to H⁺. The list of $\log k_i$ are compiled from various studies in Table 4. 1. Specific surface area of minerals are compiled from various previous work (Klajmon et al., 2017; Carroll-Webb and Walther, 1988; Anovitz et al., 2017; White et al., 1994; Miller et al., 2016) (Table 4. 1). Due to the lack of published studies on precipitation rates of minerals, rates of mineral precipitation are assumed to be the same as rate of mineral dissolution.

Table 4.1. Parameters for the kinetic modeling (activation energy E and specific surface area A are in kJ/mol and m²/g, respectively).

^a . MINERAL	Acid			Neutral		Base			Carbonate			A
	$\log k$	E	n	$\log k$	E	$\log k$	E	n	$\log k$	E	n	
Quartz	-	-	-	-13.4	90	-	-	-	-	-	-	^f . 0.05
Anorthite	-3.5	16.6	1.411	-9.82	31.5	-	-	-	-	-	-	^g . 0.02
Albite	-10.16	65	0.457	-12.56	69.8	-15.6	71	-0.572	-	-	-	^g . 0.02
Orthoclase	-10.06	51.7	0.500	-12.41	38	-21.2	94.1	-0.823	-	-	-	^g . 0.31
^b . Corundum	-8.19	47.6	0.150	-11.36	47.6	-0.29	47.6	-0.550	-	-	-	3.7
Diopside	-6.36	96.1	0.710	-11.11	40.6	-	-	-	-	-	-	^h . 0.03
Enstatite	-9.02	80	0.600	-12.72	80	-	-	-	-	-	-	ⁱ . 9.3
Ilmenite	-8.35	37.9	0.421	-11.16	37.9	-	-	-	-	-	-	^j . 0.21
Magnetite	-8.59	18.6	0.279	-10.78	18.6	-	-	-	-	-	-	^j . 0.1
^c . Titanite	-10.17	53.9	1.268	-17.44	53.9	-	-	-	-	-	-	^k . 0.08
Hematite	-9.39	66.2	1.000	-14.6	66.2	-	-	-	-	-	-	^l . 23
Halloysite	-11.31	65.9	0.777	-13.18	22.2	-17.05	17.9	-0.472	-	-	-	^g . 20
^d . Alunite	-10.65	32.3	0.133	-12.53	39	-12.53	39	-0.194	-	-	-	26
Montmorillonite	-12.71	48	0.220	-14.41	48	-14.41	48	-0.130	-	-	-	^m . 16
^e . Actinolite	-11.15	22	1.000	-12.28	22	-11.78	22	-1.000	-	-	-	0.46
Epidote	-10.6	71.1	0.338	-11.99	70.7	-17.33	79.1	-0.556	-	-	-	ⁿ . 0.25
Chlorite	-11.11	88	0.500	-12.52	88	-	-	-	-	-	-	^g . 1.6
Calcite	-0.3	14.4	1.000	-5.81	23.5	-	-	-	-3.48	35.4	1.000	^g . 0.15
Dolomite	-3.76	56.7	0.500	-8.6	95.3	-	-	-	-5.37	45.7	0.500	^o . 0.09
Magnesite	-6.38	14.4	1.000	-9.34	23.5	-	-	-	-5.22	62.8	1.000	^p . 0.07
Anhydrite	-	-	-	-2.79	0	-	-	-	-	-	-	^g . 0.12

- Reaction rate parameters compiled from Palandri and Kharaka (2004) excluding corundum, titanite, alunite and actinolite
- Rate parameters (Declercq and Oelkers, 2014) and A (Carroll-Webb and Walther, 1988)
- Titanite parameters taken similar to kyanite as both arenesosilicate.
- Alunite's reaction rate parameters and A are taken from Miller et al. (2016).
- Reaction rate parameters and A are taken from Critelli et al. (2014)
- Casey et al. (1990)
- Klajmon et al. (2017)
- Daval et al. (2010)
- Anovitz et al. (2017)
- White et al. (1994)
- Oelkers and Schott. (1994)
- Bruno et al. (1992)
- Diamond and Kinter. (1956)
- Rose. (1991)
- Gautelier et al. (2007)
- Porovsky et al. (2009)

Similar to the equilibrium modeling, constant temperature and constant pressure is kept in kinetic modeling to resemble reservoir condition. The inputs for kinetic modeling are assigned using the following data blocks: 1) *Solution* data block, 2) *Equilibrium_phase* data block, 3) *Rates* data block and 4) *Kinetics* data block. The *Solution* and *Equilibrium_phase* data block functions used in this modeling is similar to functions described in equilibrium modeling.

Rates data block is utilized to assign a set of general mathematical rate expressions of specific minerals. In this study, the rate expression of each mineral is based on the reaction rate defined in the work of Palandri and Kharaka (2004). The rate expression in PHREEQC is modified for practical reason and the following abbreviation is noted:

A command to let mineral precipitate is added into this *Rates* data block and an initial SA value of 0.00001 is assigned (Koenen et al., 2014). This command states that if the mol of a mineral is zero and its SI > 0, then the mineral will start to precipitate with a (SA) surface area value of 0.00001 m². This value is an estimate reflecting the surface of the very first pre-crystalline precipitate of the given secondary mineral. The reaction rate for dissolution and precipitation of a mineral is calculated per second of time. The rate reaction is then multiplied by the time steps assigned to the simulation in order to calculate the final mol of minerals that is either dissolved or precipitated. The number of steps is assigned in the *Kinetics* data block. *Rates* data block of a single mineral is shown, as an example, in Figure 4. 3.

```

RATES
Anorthite
-start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_anort = SI("Anorthite")
30 if (M <= 0 and si_anort < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_anort > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-3.5)*EXP(-16.60e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.411)
70 k_neut = 10^(-9.82)*EXP(-31.50e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_anort))
190 moles = r * TIME
200 SAVE moles
-end

```

Figure 4.3. Example of a Rates data block. The expression PARM (1) is the molar surface area MSA which is the product of Specific Surface Area *A_i* and molar weight of a mineral *GFW_i*. The term SA is denoted as the product of PARM(1) multiplied by the mol assemblage of a mineral *M_i*.

Kinetics data block is used to assign kinetic modeling input and to define time step in which kinetic modeling is done. The inputs include the initial mol amount of a mineral *M_i* and the product of *Specific Surface Area (A_i)* and *molar weight of a mineral (GFW_i)* which is denoted by **PARM(1)** (Figure 4. 3). Mol tolerance required by the PHREEQC and denoted as (**tol**) is also specified as 10⁻⁹. A set of time step is defined in this data block. For this specific study, the time of simulation is assigned a range of 100 to 10000 years. The time step which is assigned to the program is in seconds. *Kinetics* data block of minerals is shown, as an example, in Figure 4. 4.

```

KINETICS 1
Quartz
  -formula SiO2 1
  -m 69.09
  -m0 69.09
  -parms 2.956
  -tol 1e-09
Anorthite
  -formula CaAl2(SiO4)2 1
  -m 19.07
  -m0 19.07
  -parms 5.548
  -tol 1e-09
-steps 3 30 300 3000 30000 300000 3000000 30000000 300000000
-cvode true

```

Figure 4.4. Example of a Kinetics data block.

4.2. Modeling of Individual Fields

The modeling of individual fields is implemented by using, as inputs, i) water chemistry and temperature of the sample most representative of the field, ii) depth, porosity and normative mineralogy of reservoir rock and iii) the amount of injected CO₂ based on solubility test.

4.2.1. Ungaran Geothermal Field

Given that the highest concentration levels are recorded in sample UW-8B (see Table 3. 1), this sample is taken to represent the water composition of Ungaran geothermal field. Phuong et al. (2012) reported that the Ungaran reservoir temperature is estimated between 72-143 C° by applying silica geothermometer. Given, however, the presence of water mixing in the field (Phuong et al., 2012), temperature estimates from silica geothermometers are likely to be underestimates, therefore a further attempt is made here for reservoir temperature estimate by using silica-enthalpy mixing model. This calculation yielded a range of 699-1000 J/kg enthalpy corresponding to temperature of 166-233°C (Figure 4. 5). Based on this temperature range, reservoir temperature is assigned a value of 200°C in modeling. The main reservoir unit is assigned as the Old Ungaran volcanics which is reported to be within the depth of 1000 and 3500 meters below surface at the geothermal prospect area (Setyawan et al., 2009). From the reported depth range of Ungaran volcanics, depth of injection is taken as 2500 m which corresponds to a hydrostatic pressure of 249 atm. Taking into account that the Old Ungaran volcanics are located in the same volcanic belt as Salak volcanics in Awibengkok field, the porosity is taken to be 0.10 similar to that of Awibengkok reservoir (Stimac et al., 2008).

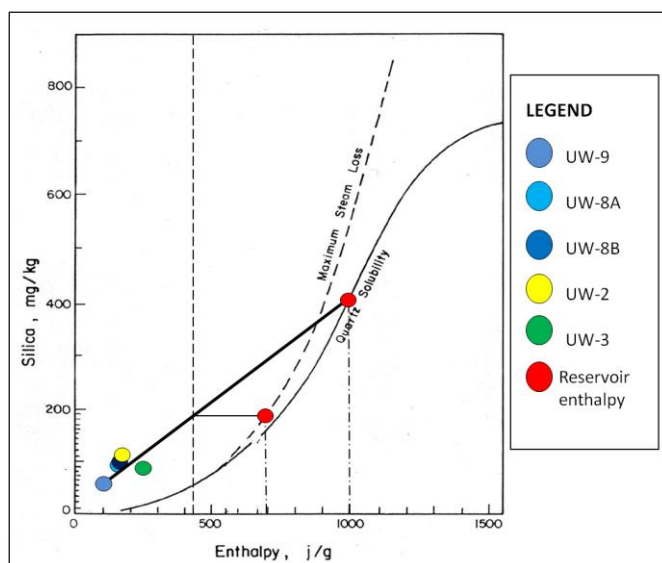


Figure 4.5. Silica-enthalpy mixing diagram of Ungaran waters.

Major element chemistry of Old Ungaran volcanics from the study of Claproth (1989) are plotted into CIPW Norm. This calculation yields a normative mineralogy comprising of the following volumetric fractions: 15.7% quartz, 24.47% anorthite, 21.04% albite, 20.61% orthoclase, 3.13% corundum, 13.35% enstatite, 0.77% ilmenite, 0.64 apatite and 0.02% zircon (Table 4. 2). Taking into account the observation of the previous researchers (Phuong et al., 2012) that there are secondary minerals (quartz, halloysite and alunite) in the reservoir lithology, additional alteration minerals are included in the modeling. In this manner, 10% volume fraction which resemble 0.9 L (900 cm³) of total simulated reservoir rock is assigned to be composed of alteration minerals. This amount of volume fraction is distributed equally between quartz, halloysite and alunite. The CIPW norms are then renormalized to 100% to represent the reservoir rock mineralogy shown in Table 4. 2. Renormalized volume fractions are converted to mol amounts to be inputs in PHREEQC. This conversion is based on the total rock volume, molar weight of individual minerals and Old Ungaran average rock density of 2.64 g/cm³ (Setyawan et al., 2009).

Solubility of CO₂ in brine (UW-8B) is simulated using PHREEQC at various pressure values and the assigned temperature of 200°C (473.15 K). This simulation yielded the approximate solubility of CO₂ as 1.5 mol/kgw at 2500 m depth (249 atm). In this

respect, the amount of injected CO₂ is assigned as 1.4 mol, below the measured solubility value (Figure 4. 6).

Table 4.2. *Parameters of reservoir rock minerals in Ungaran (volume fraction in %).*

MINERAL	Weight Norm	Density (g/cm ³)	^a . Volume fraction	^b . Renormalized volume fraction	GFW (g/mol)	^c . mol amount
Quartz	14.49	2.65	15.70	17.47	60.08	69.09
Anorthite	23.79	2.76	24.47	22.27	277.41	19.07
Albite	19.21	2.62	21.04	18.94	263.02	17.11
Orthoclase	18.78	2.56	20.61	18.55	278.327	15.83
Corundum	4.34	3.98	3.13	2.82	101.96	6.56
Enstatite	17.25	3.71	13.35	12.02	100.39	28.44
Ilmenite	1.27	4.75	0.77	0.69	151.71	1.09
Apatite	0.72	3.20	0.64	0.58	504.30	0.27
Zircon	0.03	4.56	0.02	0.02	603.61	0.01
Halloysite			-	3.33	258.16	3.06
Alunite			-	3.33	414.21	1.91
Calcite			-	-	100.10	-
Anhydrite			-	-	138.15	-

a. Mineral volume fraction obtained from CIPW Norm calculation.

b. Renormalized mineral volume fraction after 10% alteration mineral addition.

c. mol amount of minerals converted from volume fraction in b.

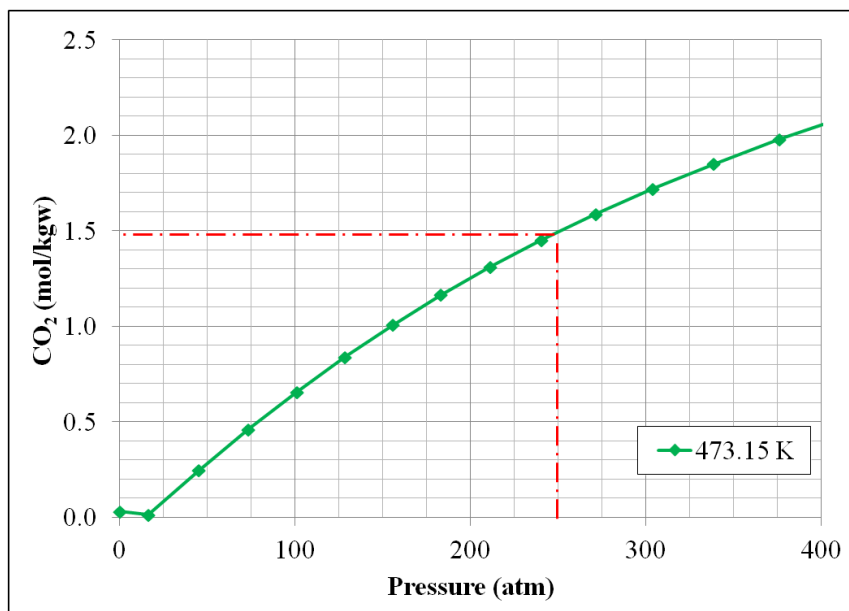


Figure 4.6. CO₂ solubility vs pressure graph of Ungaran field.

4.2.2. Baturaden Geothermal Field

Previous study of Harijoko and Juhri (2017) reported that three hot water samples represent Baturraden geothermal field, namely P-3, P-7 and Paguyangan water. The same study refers to P-3 and P-7 as the main geothermal water and Paguyangan as the outflow zone. Since sample P-3 has less meteoric contribution (see chapter 3.2), this sample is selected to represent the brine composition of Baturraden geothermal field. Given the temperature range of 200 to 210 °C reported by Utama et al. (2012) as geothermometry estimates, reservoir temperature of the modeling study is taken to be 200°C. Considering the reported reservoir elevation range of 500-1000 m (Utama et al., 2012) and the elevation of Slamet volcano of around 3000 m (Djuri et al., 1996), the injection depth is assumed to be 2000 meters. This depth corresponds to hydrostatic pressure of 194 atm. Old Slamet volcanics, the major reservoir lithology, are located in the same volcanic belt as Salak volcanics in Awibengkok field and, hence, the porosity is taken to be 0.10 similar to that of Awibengkok reservoir

Major element chemistry of Old Slamet volcanics taken from Vukadinovic and Sutawidjaja (1995) is plotted into CIPW Norm. This procedure corresponds to normative mineralogy with volume fractions of 1.59% quartz, 31.52% anorthite, 32.16% albite, 10.93% orthoclase, 8.5% diopside, 14.32 enstatite, 0.98% and 0.01% zircon. Indarto et. al. (2017) reported that amorphous silica, halloysite and montmorillonite are the main alteration minerals. From the total simulated rock volume of 9 L (9000 cm³), these additional alteration minerals with a volume of 0.9 L (900 cm³) is added to the mineralogy. The calculated data are renormalized to 100% to represent the reservoir rock mineralogy shown in Table 4. 3. Renormalized volume fraction is converted into mol amount based on the total rock volume, molar weight of individual minerals and Old Slamet volcanics average density of 2.54 g/cm³ (Reswara and Seha, 2014). Solubility simulation yielded the solubility of CO₂ in P-3 water at pressure regime of 194 atm as 1.2 mol/kg water. The amount of injected CO₂ is assigned as 1.1 mol, below the measured solubility value (Figure 4. 7).

Table 4.3 Parameters of reservoir rock minerals in Baturraden (volume fraction in %).

MINERAL	Weight Norm	Density (g/cm ³)	^a . Volume fraction	^b . Renormalized volume fraction	GFW (g/mol)	^c . mol amount
Quartz	1.46	2.65	1.59	4.761	60.08	18.12
Anorthite	30.15	2.76	31.52	28.368	277.41	23.38
Albite	29.19	2.62	32.16	28.944	263.02	25.16
Orthoclase	9.69	2.56	10.93	9.837	278.327	8.08
Diopside	10.01	3.40	8.5	7.65	216.55	8.08
Enstatite	17.88	3.61	14.32	12.888	100.39	29.35
Ilmenite	1.61	4.75	0.98	0.882	151.71	1.33
Zircon	0.01	4.56	0.01	0.009	603.61	0.00
Halloysite			-	3.33	258.16	2.95
Montmorillonite			-	3.33	366.67	2.08
Dolomite			-	-	184.4	-

a. Mineral volume fraction obtained from CIPW Norm calculation.

b. Renormalized mineral volume fraction after 10% alteration mineral addition.

c. mol amount of minerals converted from volume fraction in b.

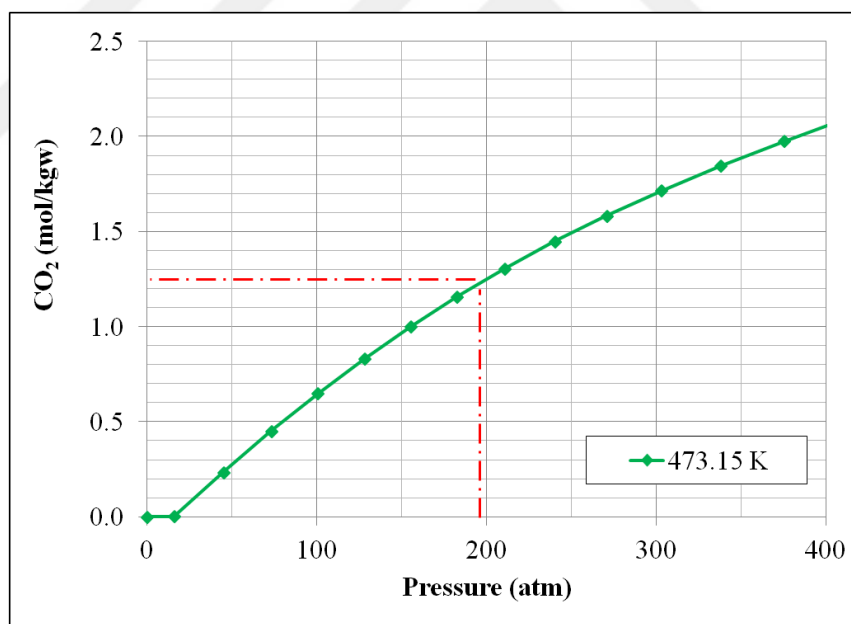


Figure 4.7. CO₂ solubility vs pressure graph of Baturraden field.

4.2.3. Dieng Geothermal Field

Sileri sector of Dieng field is selected to be modeled in this study. DNG-10 well in Sileri is taken to be the injection site with its measured well bottom temperature of 325°C and depth of 2300 m (Boedihardi et al., 1991). However, due to PHREEQC limitation, temperature of 300°C is assigned in the simulation. As for the reservoir pressure, a value of 223 atm corresponding hydrostatic pressure at depth of 2300 meters is assigned. According to Harijoko et al. (2016), the Sileri sector of the field is spatially associated with Pagerkandang volcano of Old Dieng volcanic complex. Thus, the representative reservoir lithology of the Dieng field is defined by using the composition of the samples from Pagerkandang volcano (Harijoko et al., 2016). Taking into account that the volcanics are located in the same volcanic belt as Salak volcanics in Awibengkok field, the porosity is taken to be 0.10 similar to that of Awibengkok reservoir (Stimac et al., 2008).

Major element chemistry of Pagerkandang volcanics is compiled from Harijoko et al. (2016) and plotted into CIPW Norm calculation. From the calculation, the normative mineralogy of the reservoir is summarized in terms of volume fractions: 10.63% quartz, 29.68% anorthite, 24.88% albite, 15.31% orthoclase, 3.74% diopside, 14.22% enstatite, 1.11% ilmenite, 0.44% apatite and 0.01% zircon. Given that i) there are three alteration zones (argillic, propylitic and phyllic) in the field (Kusdyantono et al., 2016) and ii) the depth of DNG 10 well and its temperature correspond to the phyllic alteration zone, 5% volume fraction of actinolite – characteristic of phyllic alteration - is added to the mineralogy calculated by CIPW Norm. This amount of actinolite corresponds to 0.45 L of the total simulated rock unit. The added calculation data are re-normalized to 100% to represent the reservoir rock mineralogy shown in Table 4. 4. Dieng volcanic complex is located in the same Quaternary volcanic belt as Ungaran volcano (Harijoko et al., 2016). Hence it can be assumed both volcanics have similar rock densities of 2.64 g/cm³ (Setyawan et. al., 2009). The solubility simulation of CO₂ in DNG-10 water at a pressure regime of 223 atm yielded a value of 1.3 mol/kg water. Consequently, the amount of injected CO₂ is taken as 1.2 mol (Figure 4. 8).

Table 4.4 Parameters of reservoir rock minerals in Dieng (volume fraction in %).

MINERAL	Weight Norm	Density (g/cm ³)	^a . Volume fraction	^b . Renormalized volume fraction	GFW (g/mol)	^c . mol amount
Quartz	9.73	2.65	10.63	10.10	60.08	42.16
Anorthite	28.26	2.76	29.68	28.20	277.41	25.49
Albite	22.51	2.62	24.88	23.64	263.02	22.54
Orthoclase	13.53	2.56	15.31	14.54	278.327	13.11
Diopside	4.39	3.40	3.74	3.55	216.55	4.11
Enstatite	17.73	3.61	14.22	13.51	100.39	33.75
Ilmenite	1.82	4.75	1.11	1.05	151.71	1.74
Apatite	0.49	3.20	0.44	0.42	504.3	0.21
Zircon	0.03	4.56	0.01	0.01	231.53	0.03
Actinolite			-	5.00	853.16	1.47
Dolomite			-	-	184.4	-

a. Mineral volume fraction obtained from CIPW Norm calculation.

b. Renormalized mineral volume fraction after 10% alteration mineral addition.

c. mol amount of minerals converted from volume fraction in b.

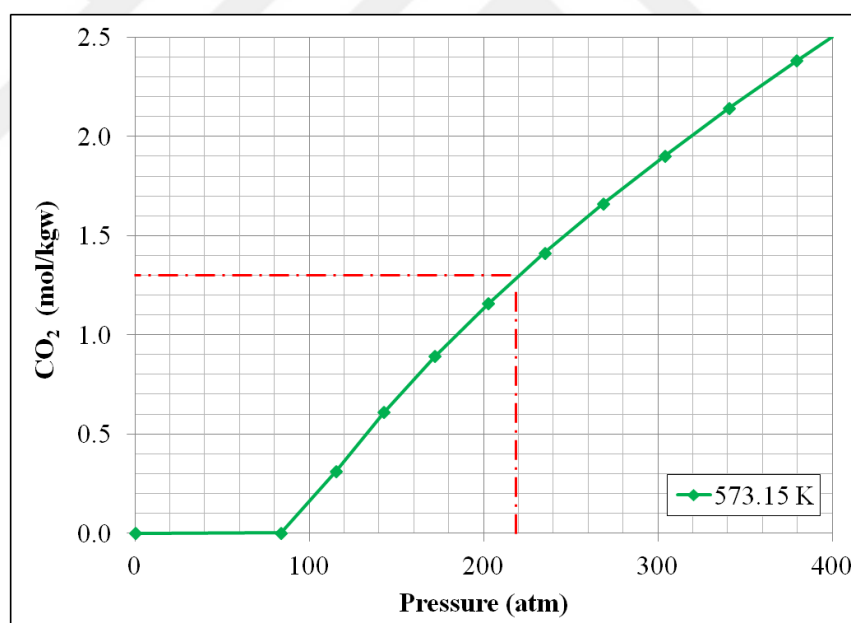


Figure 4.8. CO₂ solubility vs pressure graph of Dieng field.

4.2.4. Awibengkok Geothermal Field

Eastern cell of Awibengkok field is assigned to be the modeling site. AWI 1-2 well in this cell is taken to be the injection site. This well has a measured well bottom temperature of 250°C with a depth of 1600 m (Allis, 1999). The hydrostatic pressure that is present in the depth of 1600 in AWI 1-2 well bottom corresponds to a value of 160 atm. Taking into account the study of Stimac et al. (2008) that the reservoir rock is located between Salak volcanics and Perbakti-Endut volcanics, the chemistry of Salak volcanics is selected to be represent the reservoir rock mineralogy. Stimac et al. (2008) also noted that the reservoir has a mean porosity value of 0.11. In this respect, porosity value for this modeling study is taken to be 0.10.

Major element chemistry of Salak volcanics compiled from Handley et. al. (2008) is plotted into CIPW Norm. This calculation yielded to a normative mineralogy with volumetric fraction of 13.51% quartz, 25.23% anorthite, 38.11% albite, 10.24% orthoclase, 0.44% diopside, 4.78% enstatite, 0.27% ilmenite, 1.82% titanite, 4.76% hematite, 0.82% apatite and 0.02% zircon. By considering the reservoir temperature and presence of alteration minerals, 10% volume fraction of epidote, chlorite and calcite is added into the reservoir mineralogy to accommodate the presence of propylitic alteration (Stimac and Sugiaman, 2000), and the normative mineralogy is renormalized to 100% (Table 4.5). Given that Awibengkok volcanic complex is located in the same Quaternary volcanic belt as the other geothermal fields (Purnomo et al., 2016), it is assigned a rock density of 2.64 g/cm³. CO₂ solubility is simulated with respect to AWI 1-2 water at pressure condition of 160 atm and is found to be 1.0 mol/kg water. Consequently, the amount of injected CO₂ is assigned as 0.9 mol, below the measured solubility value (Figure 4. 9).

Table 4.5 Parameters of reservoir rock minerals in Awibengkok (volume fraction in %).

MINERAL	Weight Norm	Density (g/cm ³)	^a . Volume fraction	^b . Renormalized volume fraction	GFW (g/mol)	^c . mol amount
Quartz	12.59	2.65	13.51	12.16	60.08	48.09
Anorthite	24.48	2.76	25.23	22.71	277.41	19.45
Albite	35.12	2.62	38.11	34.30	263.02	30.98
Orthoclase	9.22	2.56	10.24	9.22	278.33	7.87
Diopside	0.50	3.22	0.44	0.40	142.48	0.66
Enstatite	5.40	3.21	4.78	4.30	100.39	10.18
Ilmenite	0.44	4.75	0.27	0.24	151.71	0.38
Titanite	2.24	3.50	1.82	1.64	196.04	1.99
Hematite	8.78	5.25	4.76	4.28	159.69	6.37
Fluorapatite	0.93	3.20	0.82	0.74	504.30	0.35
Zircon	0.04	4.56	0.02	0.02	603.61	0.01
Epidote			-	3.34	519.30	1.53
Chlorite			-	3.33	67.45	11.73
Calcite			-	3.33	100.10	7.90
Dolomite			-	-	184.4	-

a. Mineral volume fraction obtained from CIPW Norm calculation.

b. Renormalized mineral volume fraction after 10% alteration mineral addition.

c. mol amount of minerals converted from volume fraction in b.

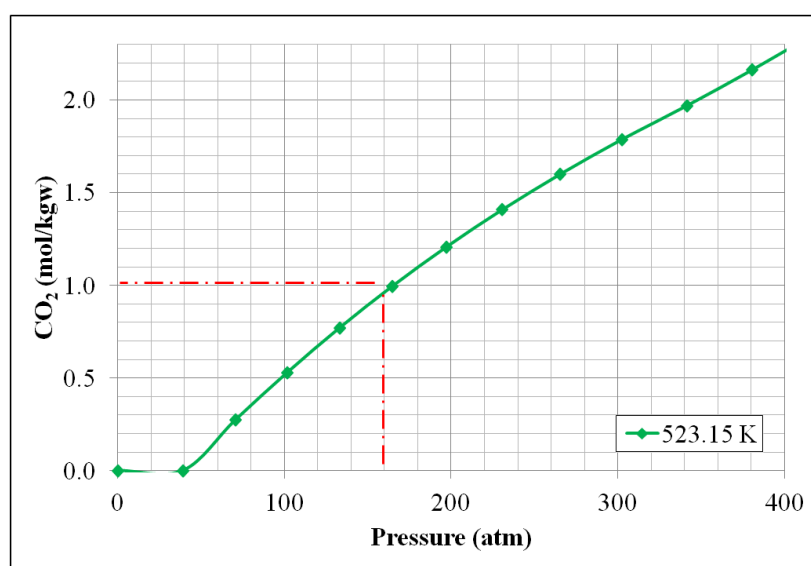


Figure 4.9. CO₂ solubility vs pressure graph of Awibengkok field.

A summary of the reservoir parameters used as inputs in modelling study is given in Table 4.6.

Table 4.6 *Reservoir parameters used as inputs in modelling studies.*

Field	Ungaran	Baturraden	Dieng	Awibengkok
Depth (P in atm)	2500 m 249 atm	2000 m 194 atm	2300 m 223 atm	1600 m 160 atm
Temp (T°C)	200 °C	200 °C	300 °C	250 °C
Water type	Na+K-Cl	Na+K-Cl	Na+K-Cl	Na+K-Cl
pH	6.80	6.00	5.90	6.92
Minerals	Quartz Anorthite Albite Orthoclase Corundum Enstatite Ilmenite Apatite Zircon Hyalosite Alunite	Quartz Anorthite Albite Orthoclase Diopside Enstatite Ilmenite Zircon Hyalosite Montmorillonite	Quartz Anorthite Albite Orthoclase Diopside Enstatite Ilmenite Apatite Zircon Actinolite	Quartz Anorthite Albite Orthoclase Diopside Enstatite Ilmenite Titanite Hematite Fluorapatite Zircon Epidote Chlorite Calcite
Porosity	0.10	0.10	0.10	0.10
CO ₂	1.4 mol/kgw	1.1 mol/kgw	1.2 mol/kgw	0.9 mol/kgw

CHAPTER 5

RESULT AND DISCUSSION

The results of modeling study in four selected fields is divided into two parts: Equilibrium modeling and kinetic modeling results.

Result of equilibrium modeling is assessed based on the changes in brine chemistry, mineral composition and porosity value of the reservoir rock. The calculation of porosity change is performed based on the assumption of no mass transfer in the reservoir. Thus, the initial brine plus rock volume before and after modeling is conserved. Porosity change is calculated by subtracting the final porosity from the initial porosity assigned as 0.10. Final porosity of reservoir rock is calculated by subtracting the final volume of rock from the conserved total brine plus rock volume (10000 cm³). Final volume of rock can be obtained using the following formula:

$$V_f = \sum \frac{M_f \cdot GFW_i}{\rho}$$

Where V_f is the sum of final mineral volume (cm³), M_f is the final mol amount of a mineral. GFW_i is the molar weight (g/mol) of each mineral and ρ is the rock density (g/cm³).

Result from kinetic modeling is evaluated based on the changes occurring in mineral composition and brine chemistry over a period of time. As for mineral composition, the modeling examines the dissolution and precipitation of minerals over that period of time. For brine chemistry, result of kinetic modeling is presented in terms of temporal evolution of pH value and dissolved CO₂ concentration. The observation obtained from both brine chemistry and mineral composition are combined and used to predict the occurrence of possible geochemical (solubility and mineral) trapping mechanisms as long-term effect of carbon storage.

5.1. Ungaran field

5.1.1. Equilibrium modeling

Equilibrium modeling shows the addition of CO₂ result in an increase in sulfate (SO₄) and a decrease in calcium, magnesium and bicarbonate (Ca, Mg, HCO₃) concentrations (Figure 5. 1). In terms of mineral composition, the modeling shows that CO₂ addition give way to the complete dissolution of halloysite and alunite, and partial dissolution of anorthite and albite (Table 5. 1). This interaction also induces the precipitation of quartz, orthoclase, corundum as well as the precipitation of anhydrite. Mol amounts of enstatite, ilmenite, apatite and zircon remain unchanged. The introduction of CO₂ leads to the precipitation of calcite which can be suggested as the mineral trapping mechanism in the field. Interaction among CO₂-brine-rock result in an increase in pH and minor increase in porosity value (Table 5. 2). Result of the PHREEQC simulation is given in Appendix A.

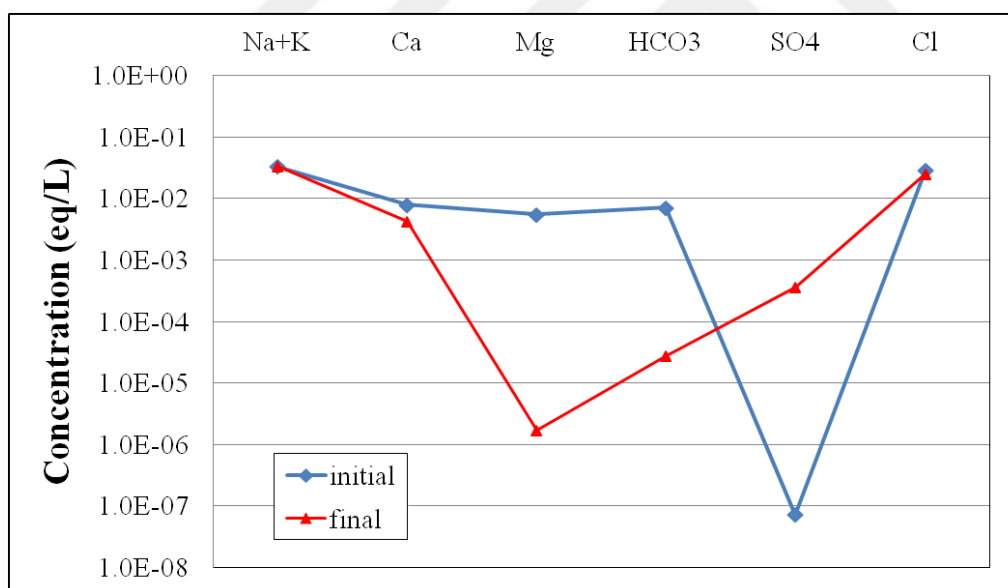


Figure 5.1. Ungaran water (UW-8B) chemistry plotted in Schoeller diagram.

Table 5.1. Ungaran reservoir mineralogy change.

MINERAL	(chemical formula)	Mineral mol amount		
		Initial	Final	Difference
Quartz	SiO ₂	69.09	79.98	10.89
Anorthite	CaAl ₂ Si ₂ O ₈	19.07	13.82	-5.25
Albite	NaAlSi ₃ O ₈	17.11	17.10	-0.01
Orthoclase	KAlSi ₃ O ₈	15.83	17.74	1.91
Corundum	Al ₂ O ₃	6.56	16.78	10.22
Enstatite	MgSiO ₃	28.44	28.45	0.01
Ilmenite	FeTiO ₃	1.09	1.09	0.00
Apatite	Ca ₅ (PO ₄) ₃ F	0.27	0.27	0.00
Zircon	ZrSiO ₄	0.01	0.01	0.00
Halloysite	Al ₂ Si ₂ O ₅ (OH) ₄	3.06	0.00	-3.06
Alunite	KAl ₃ O ₈ (SO ₄) ₂ (OH) ₆	1.91	0.00	-1.91
Calcite	CaCO ₃	0.00	1.43	1.43
Anhydrite	CaSO ₄	0.00	3.82	3.82

Table 5.2. Porosity and pH change in Ungaran reservoir.

Properties	Initial	Final	Delta
Porosity (%)	10.0	10.6	0.6
pH	6.80	7.17	0.37

5.1.2. Kinetic modeling

The result shows the complete dissolution of 1.4 mol of injected CO₂ at the first 1 hour of simulation leading to the maximum dissolved CO₂ amount in the brine (Figure 5. 2). This value decreases gradually to its minimum value in 1 year (Figure 5. 2). Dissolved CO₂ in brine lowers the pH during the first 10 hours, followed by a progressive increase until the end of the first year.

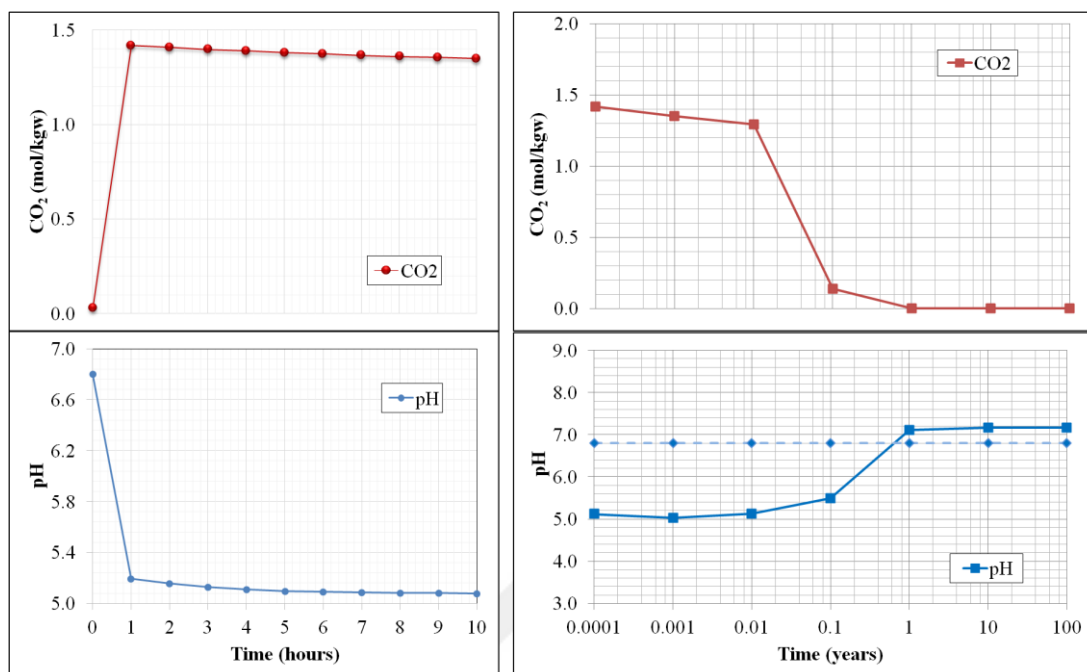


Figure 5.2. CO₂ solubility and pH evolution in Ungaran brine in the first ten hours (left) and 100 years period (right). Dashed line represents the initial pH value.

In terms of mineral evolution, kinetic modeling is performed by considering the reactive minerals that either dissolve or precipitate (quartz, anorthite, albite, orthoclase, corundum, halloysite, alunite, calcite, and anhydrite). The results of modeling are depicted in Figure 5. 3 where mol amounts of minerals are plotted against time after injection.

The modeling result show that dissolution of anorthite, albite and alunite accompanied by precipitation of quartz, orthoclase and corundum, occur immediately after simulation started. Between the time interval 4-36 days after injection (time interval II of Figure 5. 3), the progress of quartz and corundum precipitation and anorthite dissolution continue while alunite dissolved completely, and orthoclase reached equilibrium. Between 4-365 days (time interval II-III of Figure 5. 3) dissolution of anorthite parallels the precipitation of corundum, anhydrite and calcite. During the same period, quartz precipitation continues to take place. Halloysite starts dissolution in about 36 days (time interval III-IV of Figure 5. 3) and becomes totally dissolved in about 10 years. Result of the kinetic modeling in PHREEQC is given in Appendix B.

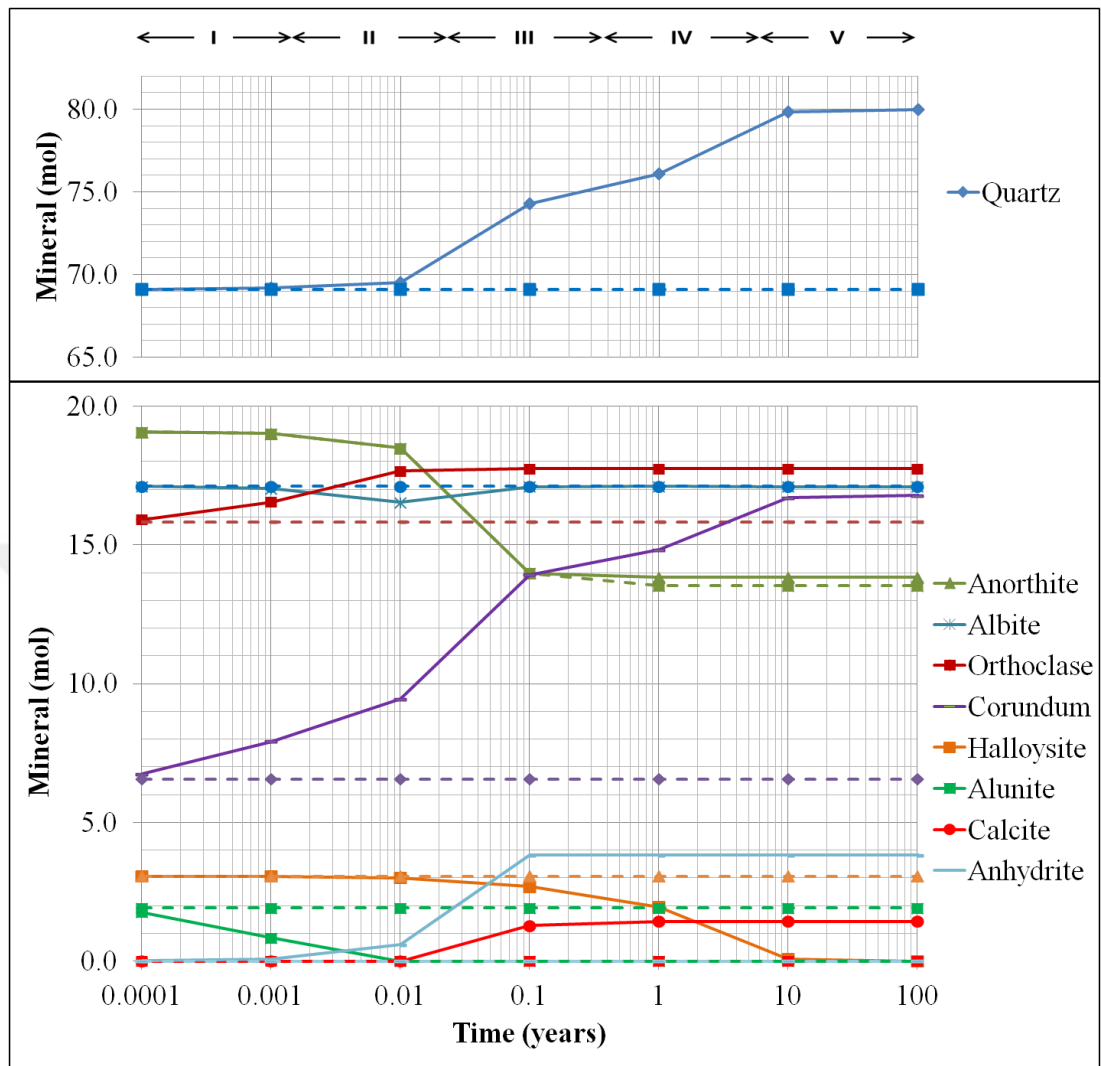
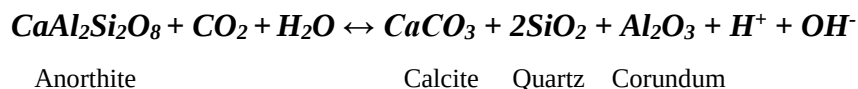


Figure 5.3. Mineral evolution in Ungaran based on mol amount against time, the dashed line shows the initial mol amount of each mineral. The graph is divided into 5 time intervals.

Kinetic modeling detects the occurrence of solubility trapping at the first hour of simulation shown by the complete dissolution of injected CO_2 . The contribution of solubility trapping gradually decreases and is replaced by mineral trapping starting from the first hour, but especially significant after 4 days of simulation (Figure 5. 2). Complete transition from solubility to mineral trapping occur in the period between 4 days to 1 year after injection. This process is indicated by the decrease of dissolved CO_2 paralleled by the precipitation of calcite (Figure 5. 3). Equilibrium among CO_2 -brine-reservoir rock is achieved 10 years after injection (Figure 5. 3). Anorthite

dissolution into calcite is inferred to be the main CO₂ mineral trapping mechanism described by the following formula:



5.2. Baturraden field

5.2.1. Equilibrium modeling

Equilibrium modeling suggest that CO₂ addition leads to increase in alkali, bicarbonate, sulfate and chloride (Na+K, HCO₃, SO₄ and Cl) and the decrease in calcium and magnesium (Ca and Mg) concentration (Figure 5. 4). In terms of mineralogy, CO₂-brine-rock interaction leads to the complete dissolution of quartz and montmorillonite, and partial dissolution of anorthite and enstatite (Table 5. 3). This interaction also promotes the precipitation of albite, diopside and halloysite. Orthoclase, ilmenite and zircon are identified as the non-reactive minerals. The introduction of CO₂ to brine-rock leads to the precipitation of dolomite which may indicate a probable mineral trapping mechanism. Interaction among CO₂-brine-rock results in increase of pH and decrease in porosity value (Table 5. 4). Result of equilibrium modeling in PHREEQC is given in Appendix C.

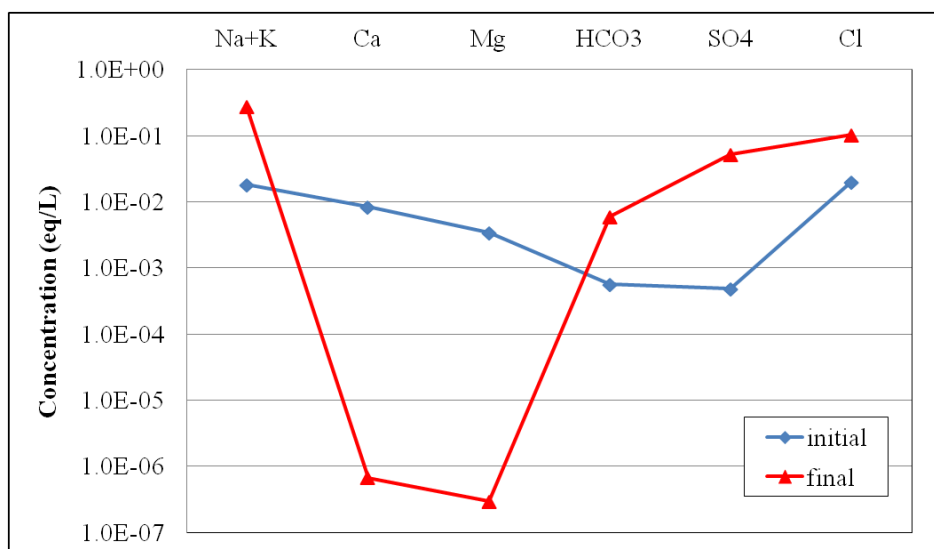


Figure 5.4. Baturraden brine chemistry plotted in Schoeller diagram.

Table 5.3. Baturaden reservoir mineralogy change.

MINERAL	(chemical formula)	Mineral mol amount		
		Initial	Final	Delta
Quartz	SiO ₂	18.12	0.00	-18.12
Anorthite	CaAl ₂ Si ₂ O ₈	23.38	1.13	-22.24
Albite	NaAlSi ₃ O ₈	25.16	25.79	0.63
Orthoclase	KAlSi ₃ O ₈	8.08	8.08	0.00
Diopside	MgCaSi ₂ O ₆	8.08	29.73	21.65
Enstatite	MgSiO ₃	29.35	7.79	-21.56
Ilmenite	FeTiO ₃	1.33	1.33	0.00
Zircon	ZrSiO ₄	0.00	0.00	0.00
Halloysite	Al ₂ Si ₂ O ₅ (OH) ₄	2.95	26.60	23.65
Montmorillonite	(Na,Ca) _{0.33} (Al,Mg) ₂ (Si ₄ O ₁₀)	2.08	0.00	-2.08
Dolomite	CaMg(CO ₃) ₂	0.00	0.61	0.61

Table 5.4. Porosity and pH change in Baturraden reservoir.

Properties	Initial	Final	Delta
Porosity (%)	10.00	6.51	-3.49
pH	6.00	8.54	2.54

5.2.2. Kinetic modeling

Kinetic modeling result suggests that the injected CO₂ (1.1 mol) dissolves completely at the initial stage (< 1 hour) of CO₂-brine-rock interaction. This amount of dissolved CO₂ decreases to 0.9 mol/kg water in the first 1 hour (Figure 5. 5). This value gradually decreases to its minimum value from the first hour until the first 4 days of simulation (Figure 5. 5). Dissolution of CO₂ in brine induce a drop in pH value during the initial stage (< 1 hour) of simulation. The pH value increases as dissolved CO₂ concentration decreases.

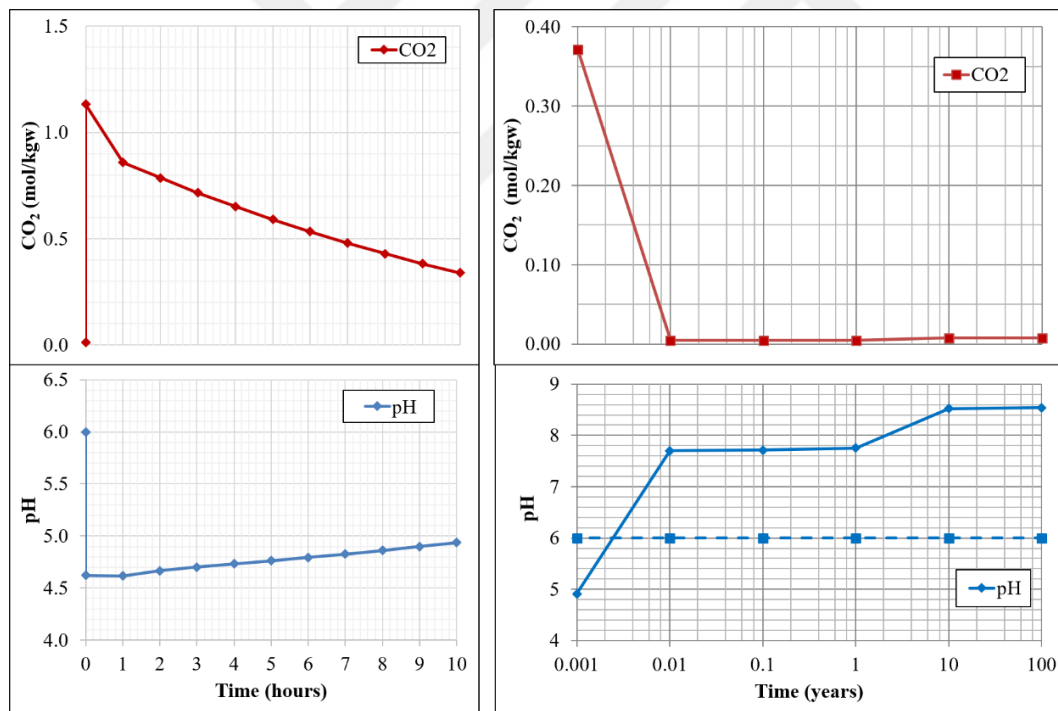


Figure 5.5. CO₂ solubility and pH evolution in Baturraden brine in the first ten hours (left) and 100 years period (right). Dashed line represents the initial pH value.

In terms of mineral evolution, kinetic modeling excludes the presence of non-reactive minerals namely orthoclase, ilmenite and zircon. The modeling identifies two episodes

of mineral evolution in the field. The first takes place in the first 10 hours (Figure 5. 6) and the second episode occurs between 10 hours and 10 years time interval (Figure 5. 7).

The first mineral evolution episode is marked by minor dissolution of enstatite and diopside accompanied by minor precipitation of quartz and montmorillonite. During the similar time period, formation of dolomite is also observed (Figure 5. 6). In the second episode, mineral evolution is seen intense between 0.1 and 10 years (time interval III-IV of Figure 5. 7), in which complete dissolution of quartz and montmorillonite, partial dissolution of enstatite and anorthite and precipitation of albite, diopside and halloysite occur. Equilibrium of the system is achieved approximately 10 years after the start of simulation. Result of the kinetic modeling in PHREEQC is given in Appendix D.

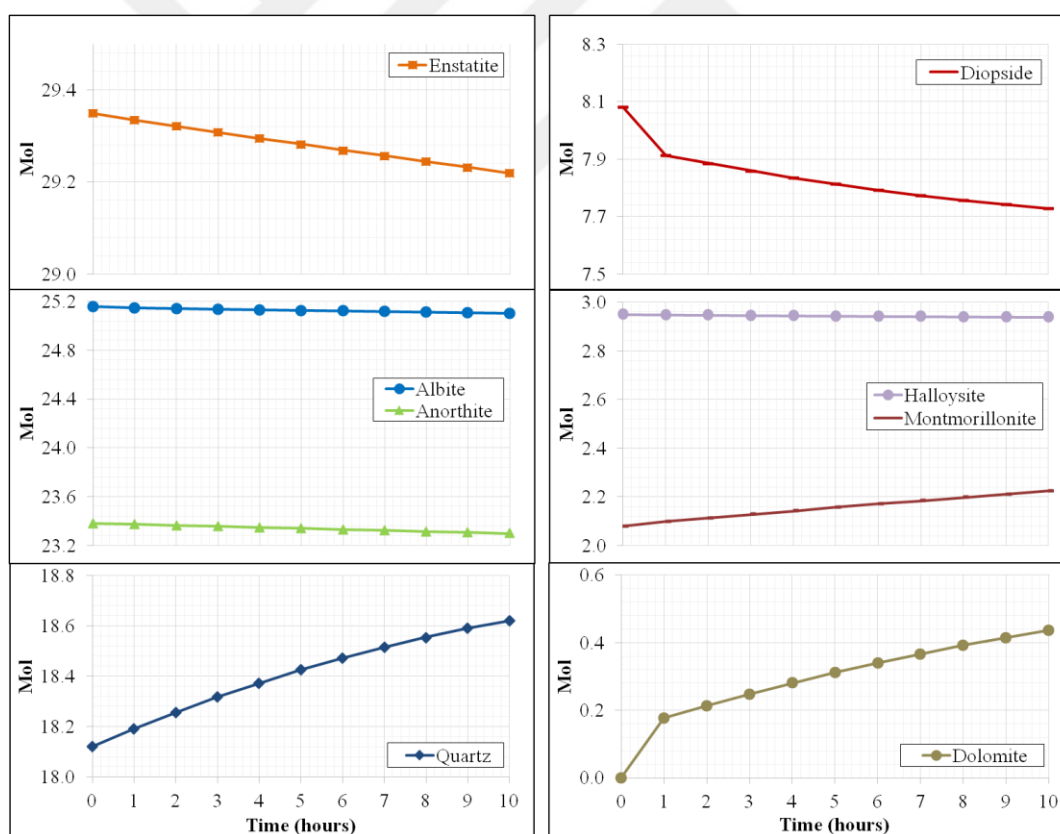


Figure 5.6. Mineral evolution in Baturraden in the first 10 hours based on mol amount against time.

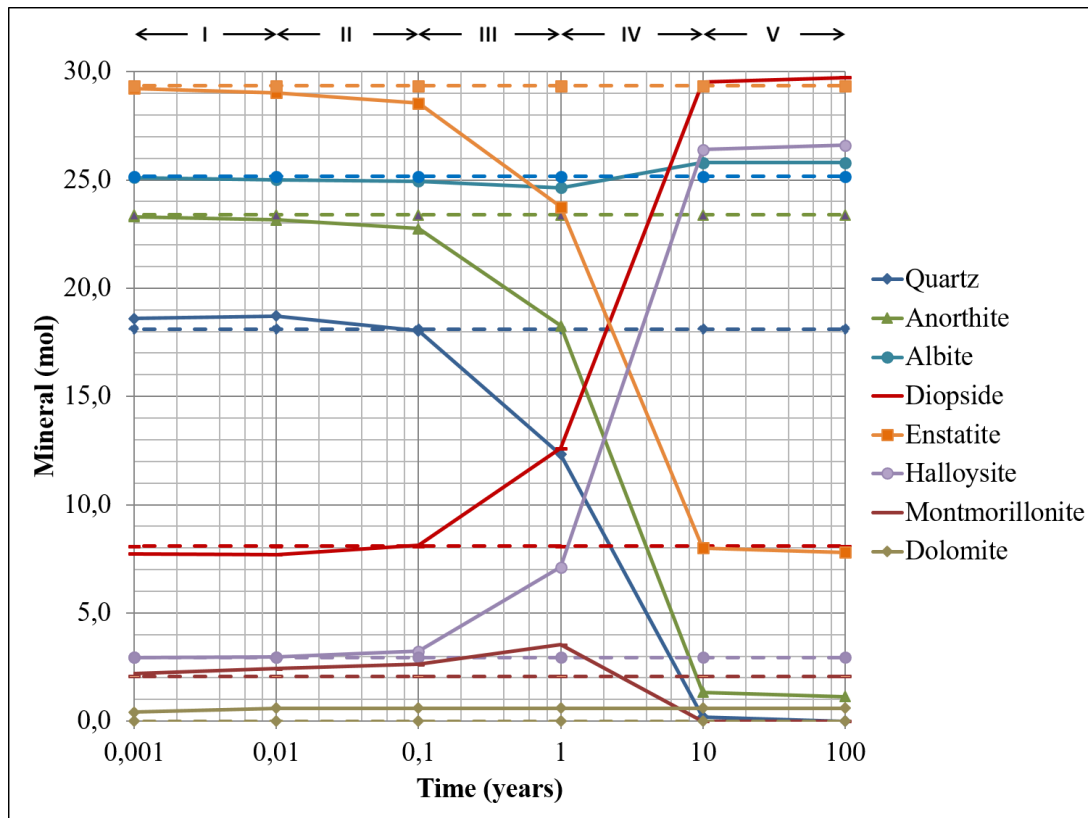
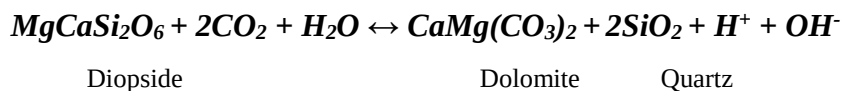


Figure 5.7. Mineral evolution in Baturraden based on mol amount against time, the dashed line show initial mol amount of minerals. The graph is divided into 5 time intervals.

Kinetic modeling result suggests that solubility trapping occur at the initial stage of injection (< 1 hour) and its contribution decreases until the 4th day when the dissolved CO₂ reaches its lowest concentration (Figure 5. 5). Solubility trapping is then replaced by mineral trapping marked by the formation of dolomite (Figure 5.6 and Figure 5. 7). Equilibrium among CO₂-brine-reservoir rock is achieved approximately after 10 years of simulation. Diopside dissolution into dolomite in the first 10 hours (Figure 5.6) is inferred to be the main mineral trapping mechanism at the first episode of mineral evolution described by the following formula:



After this time (until the equilibrium is reached at the end of 10 year) there seems to be no reaction involving carbonate minerals.

5.3. Dieng field

5.3.1. Equilibrium modeling

Equilibrium modeling show that the introduction of CO₂ induces the decrease in calcium and sulfate (Ca and SO₄) and increase in bicarbonate (HCO₃) concentration (Figure 5.8). The introduction of CO₂ result in the partial dissolution of albite and diopside (Table 5. 5). This is accompanied by the precipitation of quartz, minor precipitation of anorthite and orthoclase and the formation of dolomite. Enstatite, ilmenite, apatite, zircon and actinolite are seen to be non-reactive during simulation. CO₂ injection seems to contribute to minor decrease in pH value and minor decrease in rock porosity (Table 5. 6). Result of PHREEQC simulation is given in Appendix E.

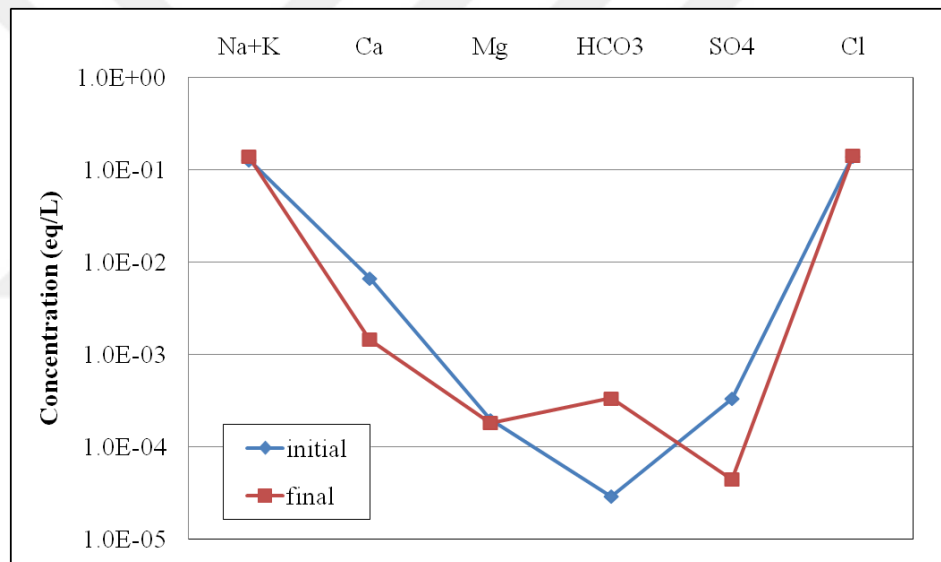


Figure 5.8. Dieng brine chemistry plotted in Schoeller diagram.

Table 5.5. *Dieng reservoir mineralogy change.*

MINERAL	(chemical formula)	Mineral mol amount		
		Initial	Final	Delta
Quartz	SiO ₂	42.16	43.04	0.88
Anorthite	CaAl ₂ Si ₂ O ₈	25.49	25.50	0.01
Albite	NaAlSi ₃ O ₈	22.54	22.52	-0.02
Orthoclase	KAlSi ₃ O ₈	13.11	13.12	0.01
Diopside	MgCaSi ₂ O ₆	4.11	3.68	-0.44
Enstatite	MgSiO ₃	33.75	33.75	0.00
Ilmenite	FeTiO ₃	1.74	1.74	0.00
Apatite	Ca ₅ (PO ₄) ₃ F	0.21	0.21	0.00
Magnetite	Fe ₃ O ₄	0.03	0.03	0.00
Actinolite	Ca ₂ (MgFe ²⁺) ₅ Si ₈ O ₂₂ (OH) ₂	1.47	1.47	0.00
Dolomite	CaMg(CO ₃) ₂	0.00	0.43	0.43

Table 5.6. *Porosity and pH change in Dieng reservoir.*

Properties	Initial	Final	Delta
Porosity (%)	10.00	4.83	-0.17
pH	5.90	5.25	-0.65

5.3.2. Kinetic modeling

Kinetic modeling result indicates that the injected CO₂ dissolved completely at the initial stage (< 1 hour) of simulation. The result shows that the initial amount of dissolved CO₂ (1.2 mol/kg water) starts to decrease before the first 1 hour of simulation (Figure 5. 9). This value continues to decrease to 0.35 mol/kg water during the first 10 hours. This trend is associated with the pH evolution where the pH value initially decreases from its original value and started to rise as dissolved CO₂ decreases. The value of dissolved CO₂ and pH do not change after the first 10 hours of simulation.

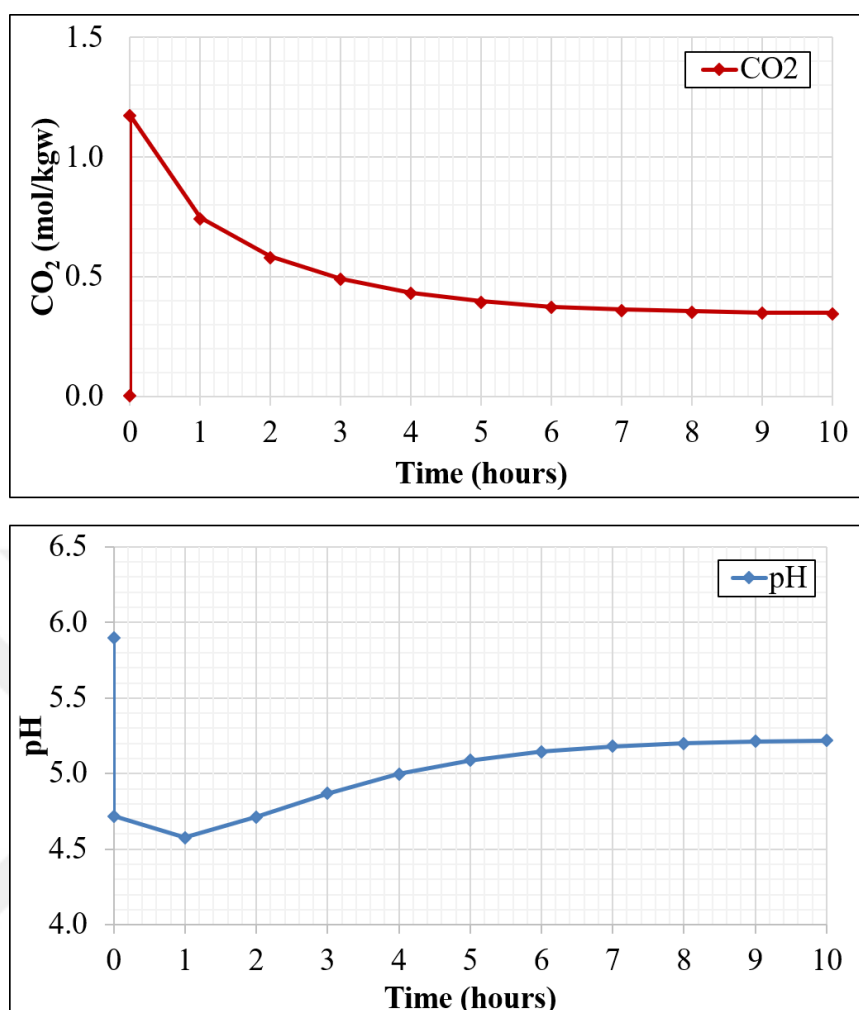


Figure 5.9. CO₂ solubility and pH evolution in Dieng brine in the first 10 hours of simulation.

Mineral evolution in Dieng field seem to occur only in the first 10 hours (Figure 5. 10). After this period, the mol amount of simulated minerals do not change until 100 years of simulation. Minerals such as quartz, anorthite, albite, orthoclase, diopside, enstatite, actinolite and dolomite are included in the simulation to evaluate mineral evolution. Kinetic modeling result suggests that CO₂ injection only has significant effect on the dissolution of diopside and precipitation of dolomite. The other simulated minerals seem to undergo minor change. Equilibrium state is achieved among CO₂-brine-rock after 10 hours of simulation. Result of kinetic modeling in PHREEQC simulation is given in Appendix F

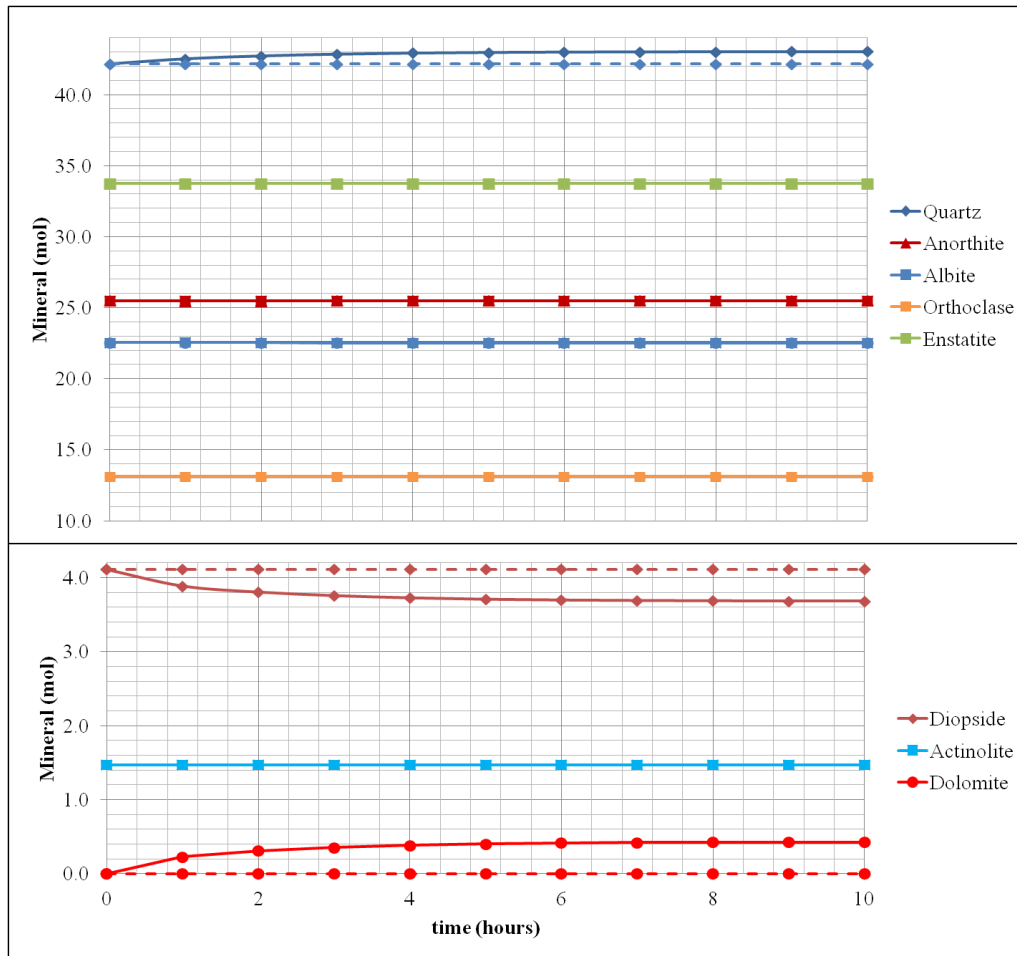
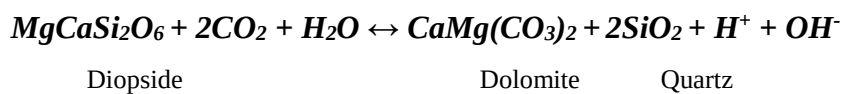


Figure 5.10. Mineral evolution in Dieng based on mol amount against time, the dashed line shows the brine-rock model, solid line show CO₂-brine-rock model.

Modeling results show the occurrence of both solubility and mineral trapping in Dieng. At the initial stage of simulation, solubility trapping is shown by almost complete dissolution of injected CO₂ (1.2 mol/kg water) (Figure 5. 9). Mineral trapping starts to appear as dissolved CO₂ concentration decreases and is partially converted into dolomite. Precipitation of dolomite accounts for the conversion of approximately 72% of injected CO₂ into mineral phase. The remaining injected CO₂ is suggested to be trapped as dissolved aqueous state. Precipitation of quartz and dolomite at the expense of diopside dissolution is identified as reaction controlling mineral trapping mechanism described by the following reaction:



5.4. Awibengkok field

5.4.1. Equilibrium modeling

Result from equilibrium modeling shows that CO₂ injection increases magnesium (Mg) and decreases sulfate (SO₄) concentrations (Figure 5. 11). CO₂-brine-rock interaction leads to the complete dissolution of diopside, titanite and calcite, and partial dissolution of anorthite, enstatite, hematite, chlorite (Table 5. 7). The modeling also shows the precipitation quartz, albite, ilmenite and epidote, and minor precipitation of orthoclase. Introduction of CO₂ induced the formation of magnesite which implies mineral trapping mechanism occurring in the field. Apatite and zircon are identified as non-reactive minerals (Table 5. 7). Interaction between CO₂-brine-rock result in decrease in pH value and decrease in porosity value (Table 5. 8). Result of equilibrium modeling in PHREEQC is given in Appendix G.

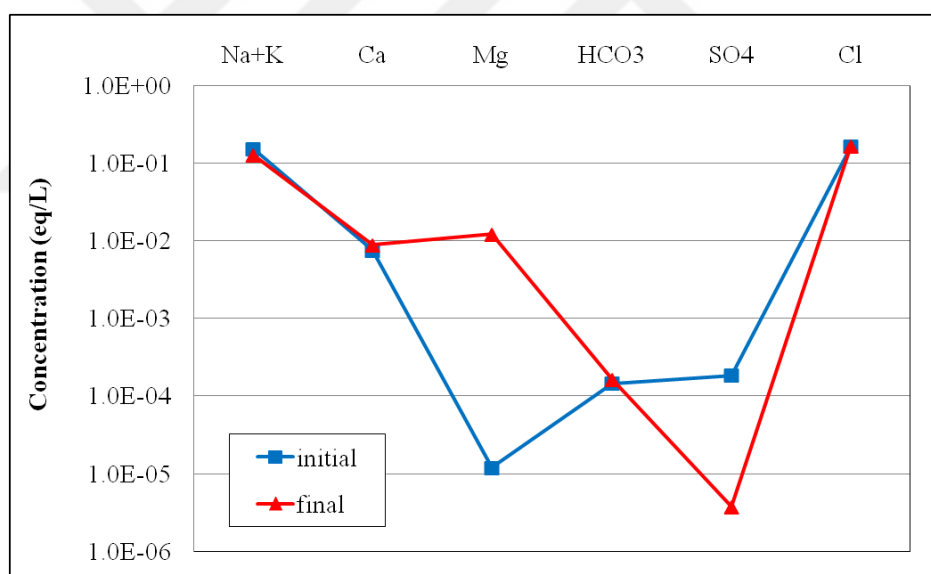


Figure 5.11. Awibengkok brine chemistry plotted in Schoeller diagram.

Table 5.7. Awibengkok reservoir mineralogy change.

MINERAL	(chemical formula)	Mineral mol amount		
		Initial	Final	Delta
Quartz	SiO ₂	48.09	48.76	0.67
Anorthite	CaAl ₂ Si ₂ O ₈	19.45	10.85	-8.60
Albite	NaAlSi ₃ O ₈	30.98	31.01	0.03
Orthoclase	KAlSi ₃ O ₈	7.87	7.88	0.01
Diopside	MgCaSi ₂ O ₆	0.66	0.00	-0.66
Enstatite	MgSiO ₃	10.18	2.18	-8.00
Ilmenite	FeTiO ₃	0.38	2.37	1.99
Titanite	CaTiSiO ₅	1.99	0.00	-1.99
Hematite	Fe ₂ O ₃	6.37	1.58	-4.79
Apatite	Ca ₅ (PO ₄) ₃ F	0.35	0.35	0.00
Zircon	ZrSiO ₄	0.01	0.01	0.00
Epidote	Ca ₂ FeAl ₂ Si ₃ O ₁₂ (OH)	1.53	11.11	9.58
Chlorite	Fe ₂ Al ₂ SiO ₅ (OH) ₄	11.73	10.74	-0.99
Calcite	CaCO ₃	7.90	0.00	-7.90
Dolomite	CaMg(CO ₃) ₂	0.00	0.00	0.00
Magnesite	MgCO ₃	0.00	8.64	8.64

Table 5.8. Porosity and pH change in Awibengkok reservoir.

Properties	Initial	Final	Delta
Porosity (%)	10.00	7.11	-2.89
pH	6.92	4.79	-2.13

5.4.2. Kinetic modeling

Kinetic modeling show that injected CO₂ (0.9 mol) dissolves completely at the initial stage (< 1 hour) of modeling which is marked by abrupt decrease in pH value (Figure 5. 12). After its complete dissolution, CO₂ concentration decreases in the first 1 hour to 0.1 mol/kg water accompanied by slight increase in pH value. This is followed by gradual increase of dissolved CO₂ and decrease in pH until the first 36 days of

simulation (Figure 5. 12). After approximately 36 days, the amount of dissolved CO₂ remain approximately constant (0.21 mol/kg water) throughout the simulation.

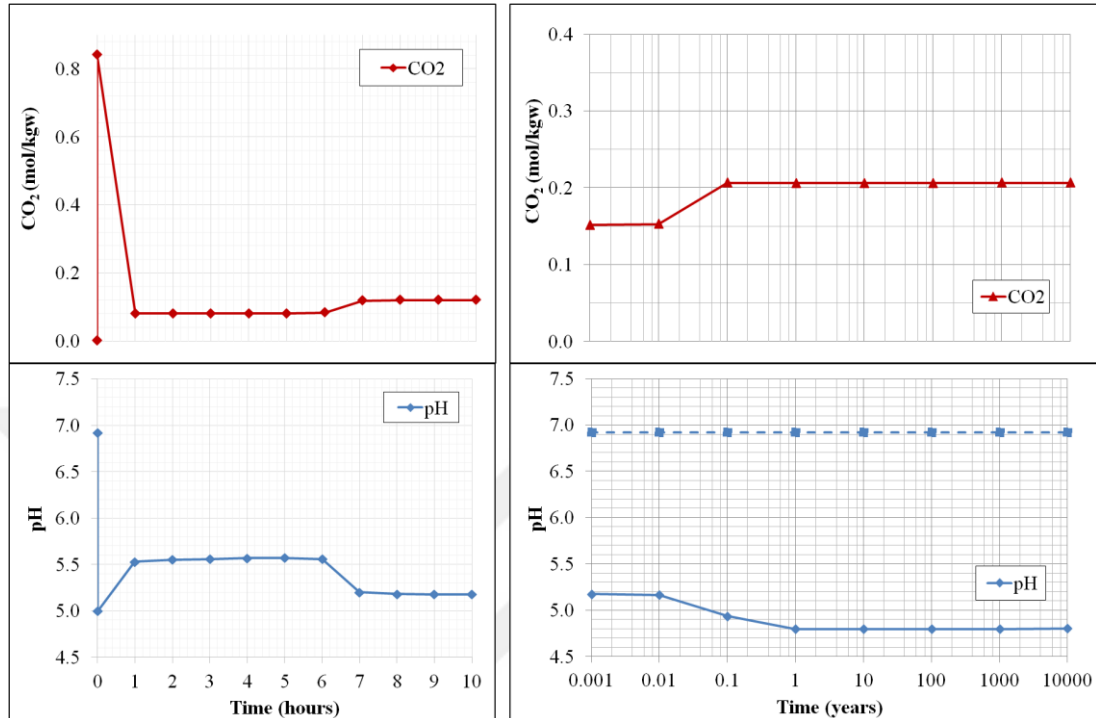


Figure 5.12. CO₂ solubility and pH evolution in Awibengkok brine first ten hours (left) and 10000 years period (right). Dashed line represents the initial pH value.

In evaluating mineral evolution, kinetic modeling excludes the non-reactive minerals (orthoclase, apatite, zircon) that was included in equilibrium modeling. Mineral evolution after CO₂ injection can be divided into three stages. The first takes place in the first 10 hours, the second occurs between 10 hours and 1 year and the third between 100 and 10000 years. The result of modeling is plotted as mol amounts of minerals against time after injection (Figure 5.13 to 5.15).

During the first stage, the modeling result identifies complete dissolution of calcite and partial dissolution of chlorite (Figure 5. 13). This process is observed together with minor precipitation of quartz, hematite and epidote and the formation of dolomite. Rapid dissolution of enstatite is observed parallel to precipitation of

diopside in the first hour, followed by enstatite precipitation concurrent with complete diopside dissolution after six hours of simulation (Figure 5. 13).

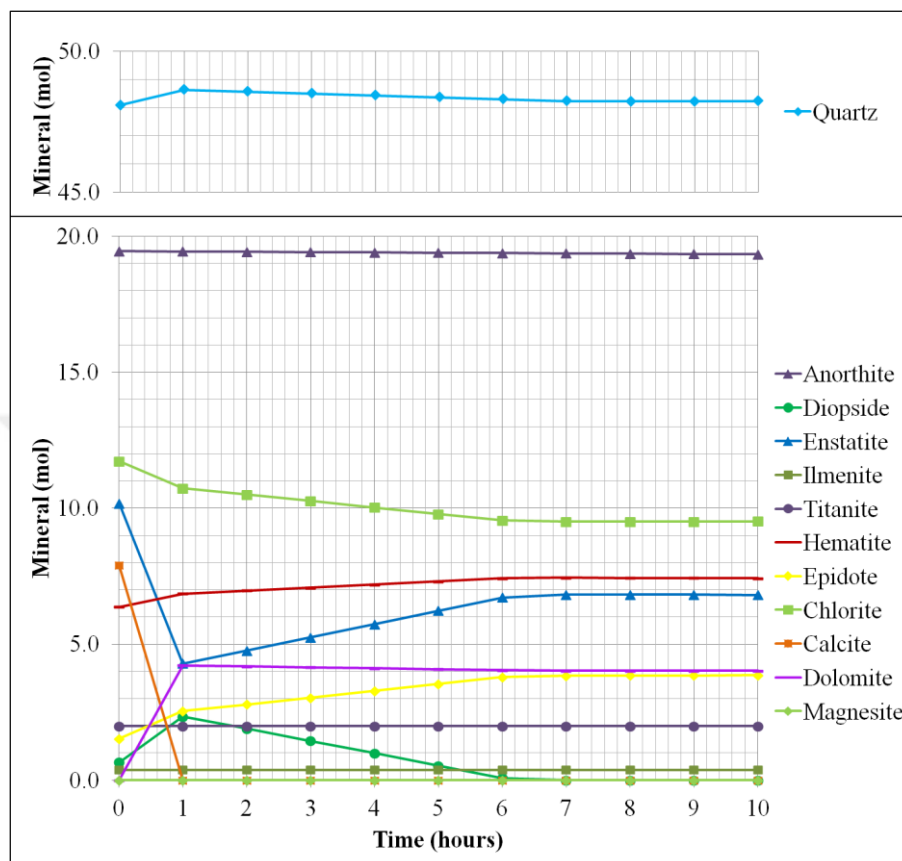


Figure 5.13. Mineral evolution in Awibengkok in the first 10 hours of simulation.

The beginning of the second stage (10 hours to 4 days) is marked by the precipitation of quartz and chlorite (time interval I-II of Figure 5. 14). In time interval 10 hours and 1 year, dissolution of anorthite, hematite, enstatite and dolomite occur together with the precipitation of epidote and magnesite (time interval I-III of Figure 5. 14). The system reaches apparent equilibrium between the 1 year and 100 years period (time interval IV-V of Figure 5. 14). Between 100 and 10000 years of simulation (Figure 5. 15), dissolution of chlorite, hematite and titanite and precipitation of epidote and ilmenite is observed. The final equilibrium state in the system is achieved after 10000 years. Result of the PHREEQC simulation is given in Appendix H.

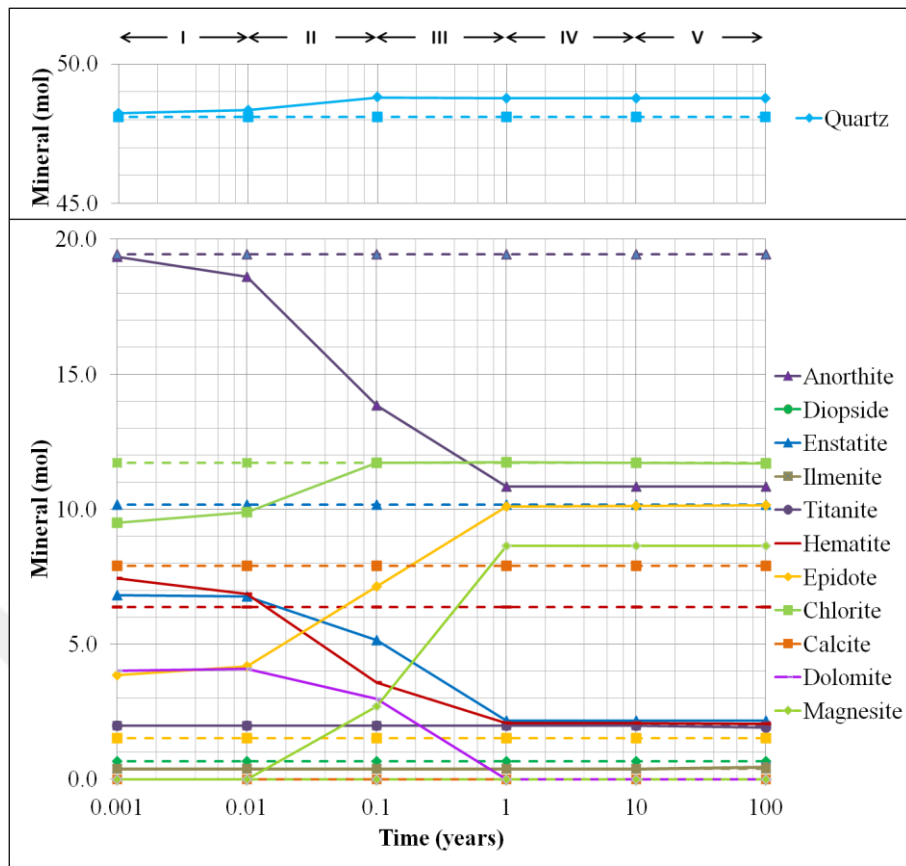


Figure 5.14. Mineral evolution in Awibengkok between 0.001 years (~10 hours) and 100 years of simulation. The graph is divided into 5 time intervals.

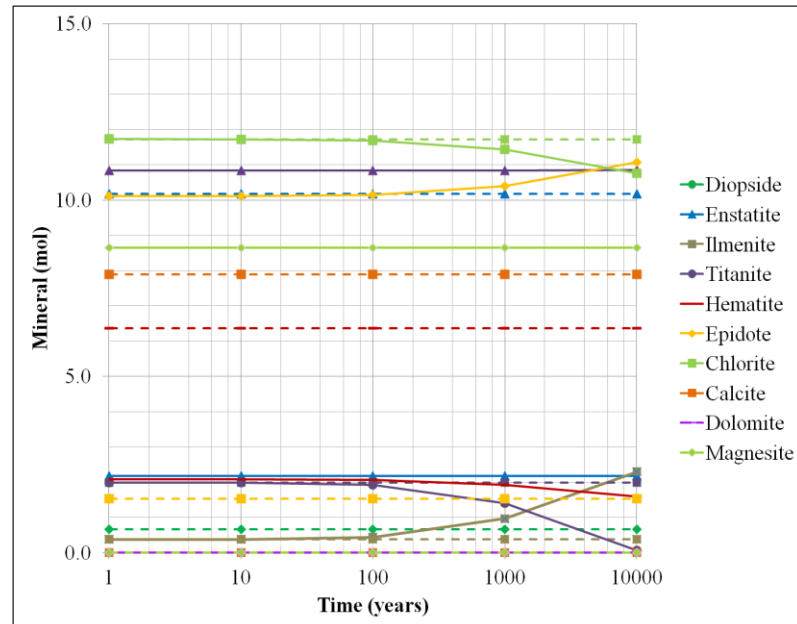
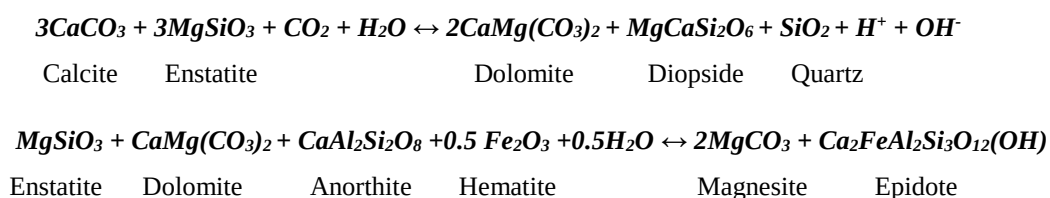


Figure 5.15. Mineral evolution in Awibengkok between 1 year and 10000 years of simulation.

Modeling result suggest that both solubility and mineral trapping take place in the field. Solubility trapping start to occur at initial stage of simulation shown by the complete dissolution of injected CO₂ (0.9 mol) into brine (Figure 5. 12) and its contribution decreases as dissolved CO₂ concentration drops to 0.1 mol/kg water within the first 1 hour (Figure 5. 12). After this period, dissolved CO₂ concentration increases gradually until the brine reaches its maximum concentration of 0.21 mol/kg water. Mineral trapping starts to occur in the first hour indicated by dolomite precipitation (Figure 5. 13). Dolomite is then replaced by magnesite during the 1 year of simulation (Figure 5. 14).

Solubility trapping accounts for approximately 23% of the total injected CO₂ while the remaining injected CO₂ is converted into mineral phase. The identified mineral trapping occurs via a complex chemical reaction involving calcite, dolomite and magnesite. Initially, precipitation of dolomite, diopside and quartz at the expense of calcite and enstatite occurs in the first hour (Figure 5. 12). This process is followed by the precipitation of magnesite and epidote as a product from the dissolution of enstatite, dolomite, anorthite and hematite between 4 days and 1 year (Figure 5. 14). Both predicted reactions is explained by the following formula:



5.5. Discussion

5.5.1. Equilibrium modeling

Equilibrium modeling reveals the potential for the possible mineral trapping mechanism by identifying which mineral dissolution or precipitation is influenced by the introduction of CO₂. The modeling results suggest changes in fluid chemistry is indicated by HCO₃ increase in Baturraden and Dieng, and decrease in Ungaran fields

without a pronounced change in Awibengkok field (Figure 5.16). Ca and Mg contents seem to have decreased in Ungaran, Baturaden and Dieng fields, pointing to the possibility of calcite and/or dolomite precipitation, and increased in Awibengkok field. This increase in Awibengkok field, however, does not necessarily rule out the possibility of carbonate mineral precipitation which is further assessed by kinetic modeling. Equilibrium modeling also predicts the change in pH and the porosity of the rock. The pH value seems to be increasing in Ungaran and Baturaden and decreasing in Dieng and Awibengkok fields. Regarding the porosity, a decrease is observed in all fields except Ungaran field.

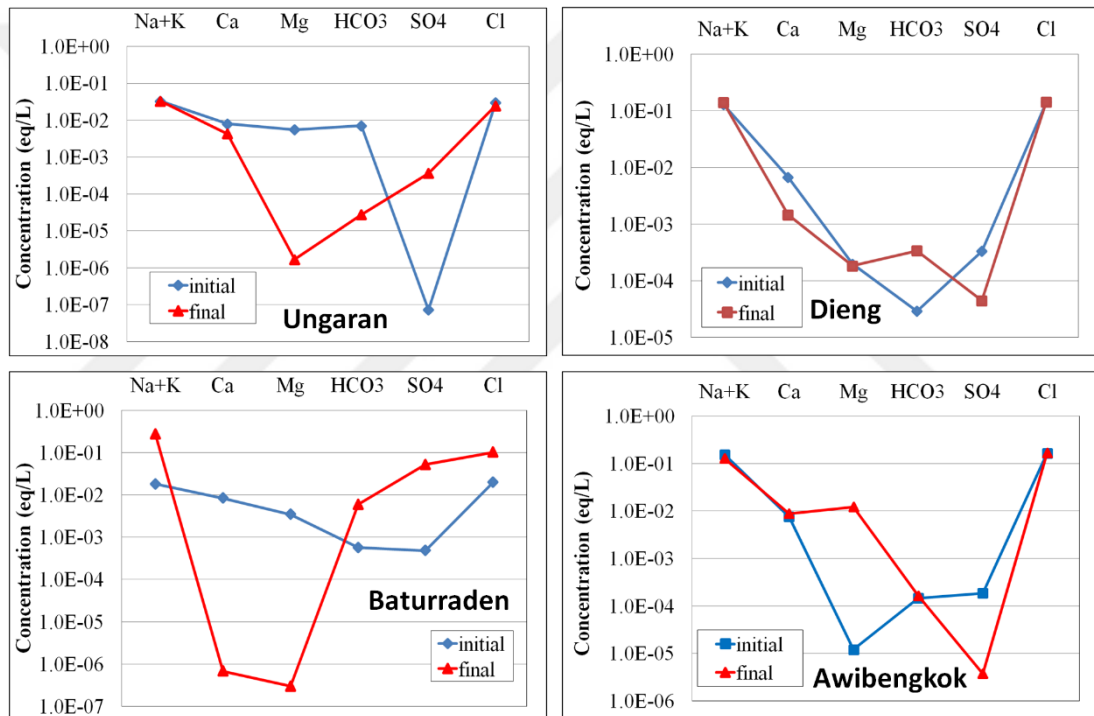


Figure 5.16. Change of brine chemistry in all four fields.

5.5.2. Kinetic modeling

Kinetic modeling provides a better understanding of CO₂-brine-rock interaction by considering the dissolution and precipitation rates of minerals. This enables the modeling to observe the changes in both brine chemistry and rock mineralogy at any time scale.

Result of kinetic modeling indicate that solubility trapping occurs at the beginning of simulation. Solubility trapping initially makes the greatest contribution to CO₂ fixation shown by the complete dissolution of injected CO₂. This value then drops to its minimum value followed by the formation of new carbonate minerals indicating the occurrence mineral trapping. In Ungaran and Baturraden fields, solubility trapping is replaced completely by mineral trapping marked by the formation of calcite and dolomite, respectively (Figure 5.17). The result from Dieng (Figure 5.18) and Awibengkok (Figure 5.19) fields suggested that solubility trapping is replaced partially by mineral trapping indicated by the formation of dolomite and magnesite, respectively. The final (increased) pH value in Ungaran and Baturraden fields may be due to the absence of dissolved CO₂ since all the injected CO₂ is converted into mineral phases. The presence of dissolved CO₂ at equilibrium state in brines of Dieng and Awibengkok seems to be compatible with the decreased pH values in these fields. This observation seems to be related with the water properties of the studied area. In Ungaran and Baturraden fields, the water has relatively lower TDS of 4224 and 3023 mg/L respectively. Dieng and Awibengkok field has a TDS value of 12207 and 12116 mg/L.

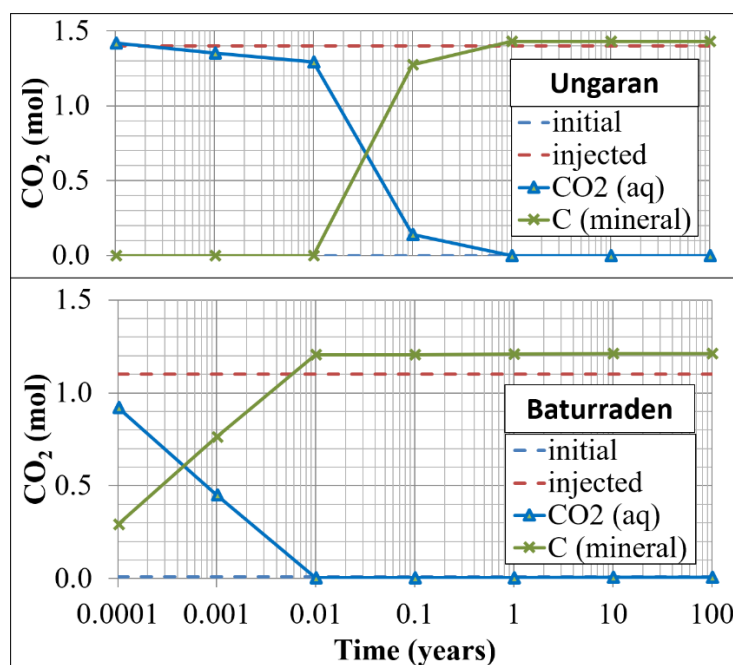


Figure 5.17. Evolution of CO₂ in Ungaran and Baturraden field.

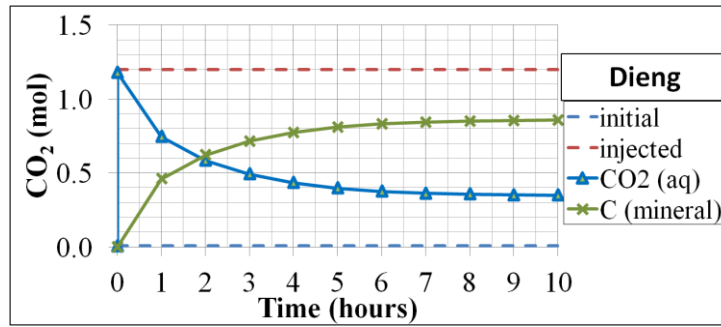


Figure 5.18. Evolution of CO₂ in Dieng field.

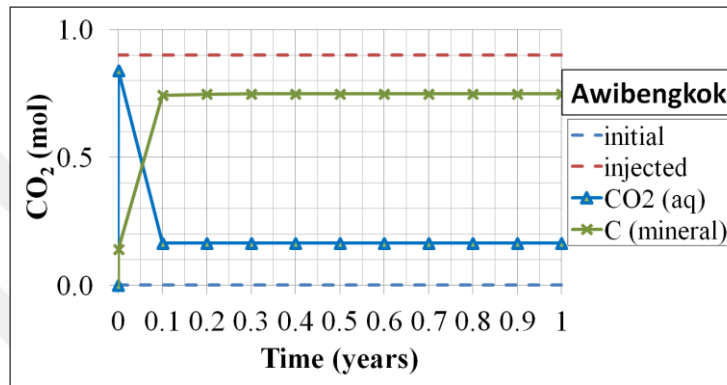


Figure 5.19. Evolution of CO₂ in Awibengkok field.

As for mineral trapping, kinetic modeling results from all four fields identified several reactions involved in the formation of these carbonates: i) anorthite dissolution to calcite in Ungaran field, ii) diopside dissolution to dolomite in Baturraden field and Dieng field and iii) calcite dissolution followed by dolomite dissolution to magnesite in Awibengkok field. These reactions are predicted to occur within the periods of 4 days to 1 year in Ungaran field, 1 hour to 4 days in Baturraden, 1 hour to 10 hours in Dieng field, and 1 hour to 36 days in Awibengkok field. The CO₂-brine-rock interaction reaches equilibrium state in 10 years in Ungaran and Baturraden, 10 hours in Dieng and 10000 years in Awibengkok.

Results from both equilibrium and kinetic modeling reveal the occurrence of solubility and mineral trapping. Solubility trapping is evaluated based on the change in dissolved CO₂ concentration and pH value. As for mineral trapping, the mechanism is evaluated by observing the change in mineral composition, as well as in the fluid chemistry. Modeling results show that solubility trapping in four selected fields occurs

immediately after injection within 1 hour of simulation. Solubility trapping is later replaced completely or partially by mineral trapping indicated by the decrease in dissolved CO₂ concentration and the formation of new carbonate minerals.

Based on these observations, the studied fields for possible future carbon capture and storage can be divided into two groups: 1) Ungaran and Baturraden fields with mineral trapping, 2) Dieng and Awibengkok fields with combined (solubility and mineral) trapping. In the first group, the injected CO₂ which initially dissolved as aqueous phase is converted completely to new carbonate minerals. As for the second group, result of Dieng field show that approximately 30% of injected CO₂ is converted to permanent dissolved CO₂ (0.35 mol/kgw) and 70% into carbon bearing mineral dolomite (0.43 mol), and in Awibengkok field, 28% of the injected CO₂ is transformed completely into dissolved CO₂ (0.2 mol/kgw) and the remaining is turned in to magnesite (0.7 mol). The time required for the system to reach equilibrium is site specific.

5.5.3. Sensitivity analysis

The results of modelling performed in the thesis study are subject to uncertainties associated with the assumptions regarding the i) alteration mineral proportion in the mineral assemblage, ii) rock porosity. The sensitivity analyses related to these uncertainties are given below.

5.5.3.1. Alteration Mineral Proportions

Given the lack of access to the rock samples (drill cores or cuttings) that will be representative of reservoir rock mineralogy of the fields, the normative (not the modal) mineralogy specified by applying CIPW Norm calculation is used during modelling throughout the thesis. Because the definition of normative mineralogy is based on primary rock forming minerals, the alteration minerals reported by the previous researchers for the respective fields are added to the mineral assemblage obtained by CIPW norm calculations. However, although the mineral names are reported, the proportions of alteration minerals are not specified in the previous studies. Therefore,

it is assumed in the thesis that the proportion of alteration minerals is 10% of the total mineral assemblage, and the mineral proportions in the assemblage are renormalized to 100%. The assumption of this 10% proportion is subject to uncertainty. In order to understand the uncertainty associated with the modeling output induced by the variation of alteration mineral abundance, sensitivity analysis is performed in this section for both Ungaran and Awibengkong fields. This analysis is done by changing the amount of alteration mineral percentage. Five batches of equilibrium model are simulated, using 5%, 7.5%, 10%, 12.5% and 15% alteration mineral proportions. Each batch is simulated under constant pressure and temperature conditions applied, and the same amount of CO₂ specified in the modelling (Chapter 4) for the relevant fields. The result of each batch is further analyzed in terms of brine chemistry and rock mineralogy.

Ungaran Field:

In terms of brine chemistry, the variation of alteration mineral abundance has effect on the final Ca and SO₄ concentrations (Figure 5.20). The decrease in the final Ca and the increase in the final SO₄ concentrations seems to be enhanced as the proportion of the alteration minerals in the assemblage increases. However, this enhancement does not exceed 0.39 mmol/L for Ca, and 0.018 mmol/L for SO₄ for 5% increase in the proportion of the alteration minerals. The decrease in Mg and HCO₃ concentrations seem not to have been affected by change in the alteration mineral proportions. In terms of pH, the difference in pH show very minor increase as the alteration mineral abundance increases (Figure 5.21).

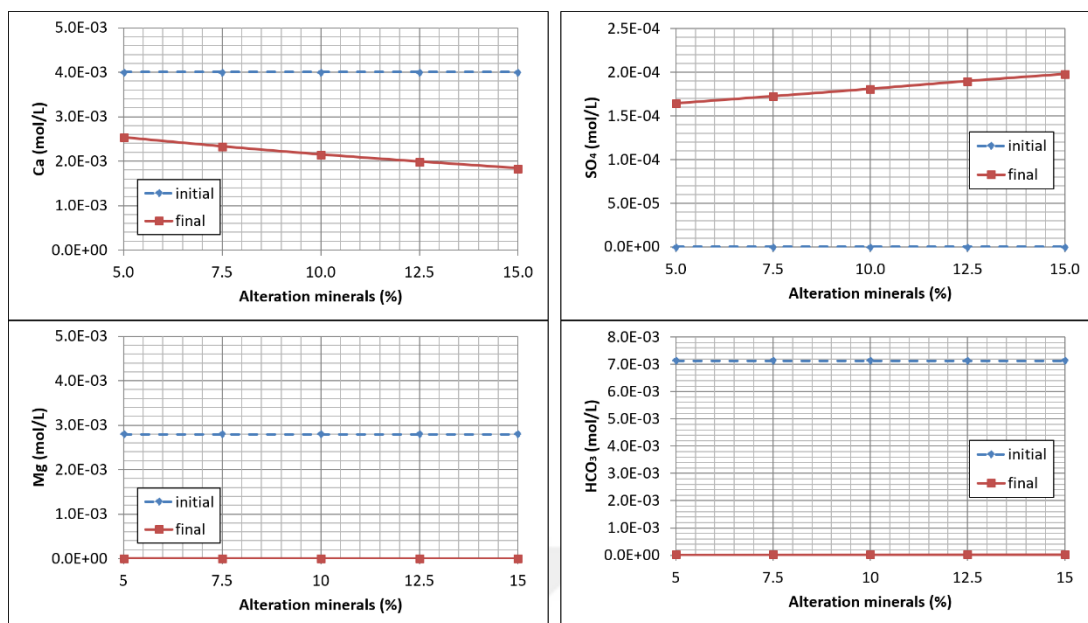


Figure 5.20. Change of species in Ungaran water plotted against the change in proportion of alteration minerals in the mineral assemblage.

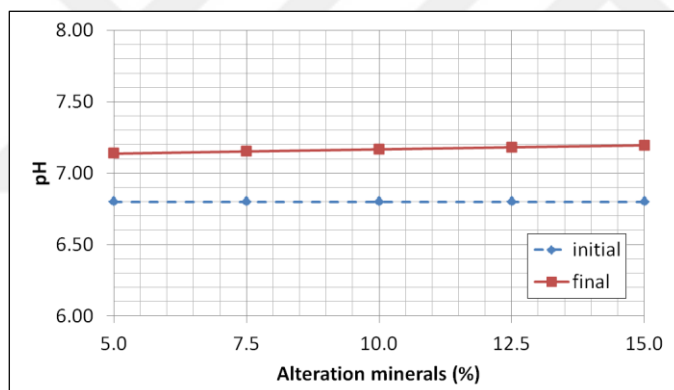


Figure 5.21. Change of pH in Ungaran water plotted against the change in proportion of alteration minerals in the mineral assemblage.

In terms of rock mineralogy, the amount of calcite precipitated is similar (1.4 mol) for all batches (5%, 7.5%, 10%, 12.5% and 15%). Quartz, orthoclase, anhydrite and albite precipitate more as the amount of alteration minerals increases (Figure 5.22). Enstatite, alunite, corundum, halloysite and anorthite seem to be dissolving more with increasing alteration mineral proportion (Figure 5.22). The increase of anhydrite precipitation may point to the increase of anorthite dissolution. Given that anhydrite precipitation occurs more than anorthite dissolution, this process may be correlated with the enhancement of Ca decrease in brine chemistry (Figure 5.20). Dissolution of

alunite with the increase of alteration minerals is in line with enhancement of SO_4 increase in brine (Figure 5.20). In terms of porosity, increase in alteration mineral proportion leads to greater porosity increase (Figure 5.23).

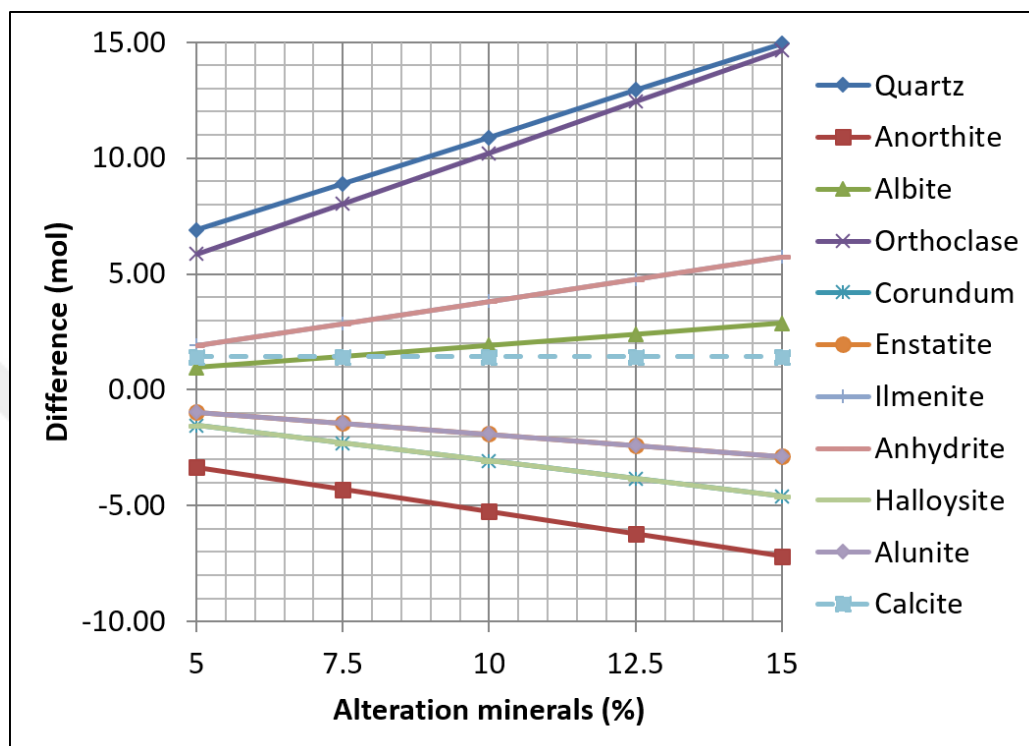


Figure 5.22. Change of mineral mol amount in Ungaran field plotted against the change in proportion of alteration minerals in the mineral assemblage (note that the trends for enstatite and alunite, and corundum and halloysite overlap with each other).

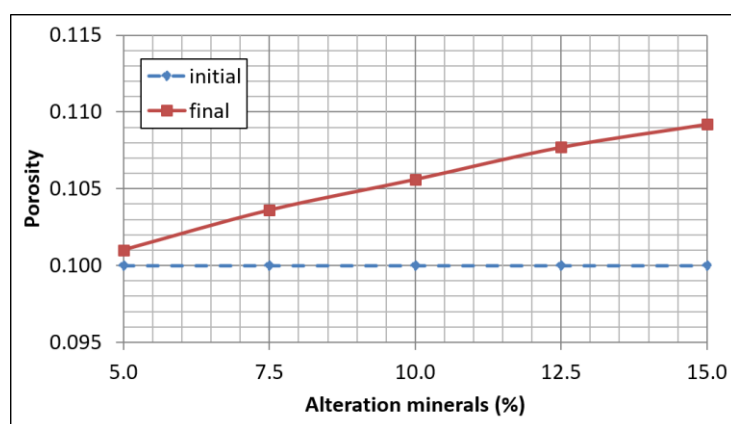


Figure 5.23. Porosity change against change in alteration mineral abundance in Ungaran field.

Awibengkok field:

In terms of brine chemistry, the variation of alteration mineral abundance has effect on the final Ca, SO₄, Mg and HCO₃ concentrations (Figure 5.24). The increase in the final Ca and SO₄ concentrations seems to be enhanced as the proportion of the alteration minerals in the assemblage increases. The increase in the final concentration of Mg seems to rise from 5% to 10 % alteration mineral proportion, while it starts to decrease between 10% and 15%. The final concentration of HCO₃ seems to be unaffected up to 10% alteration mineral proportion, but then starts to increase. In terms of pH, similar amount of change is observed for various values of alteration mineral proportions (Figure 5.25)

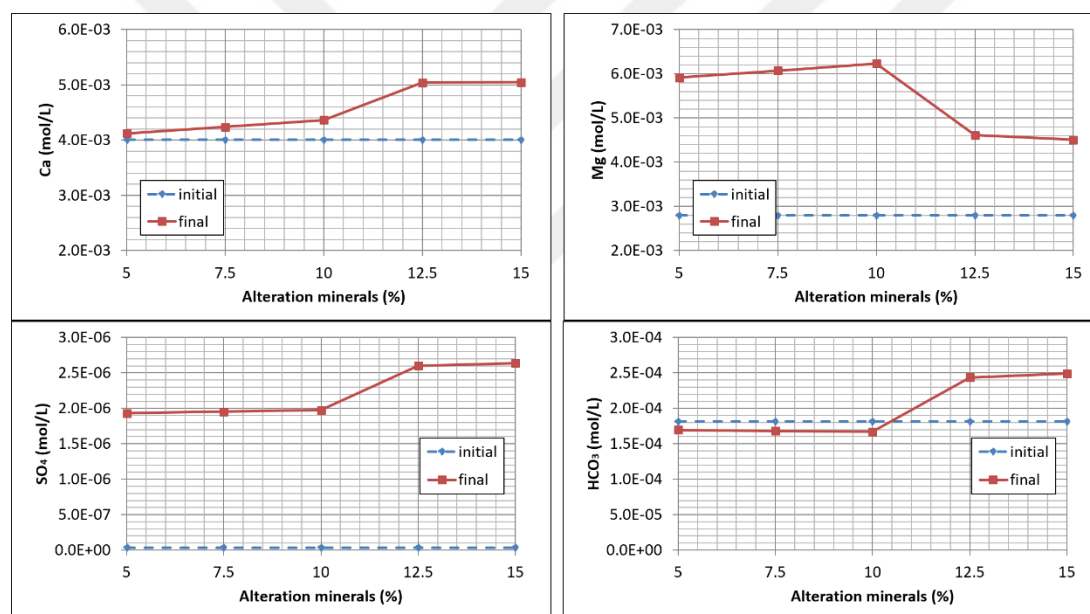


Figure 5.24. Change of species in Awibengkok water plotted against the change in proportion of alteration minerals in the mineral assemblage.

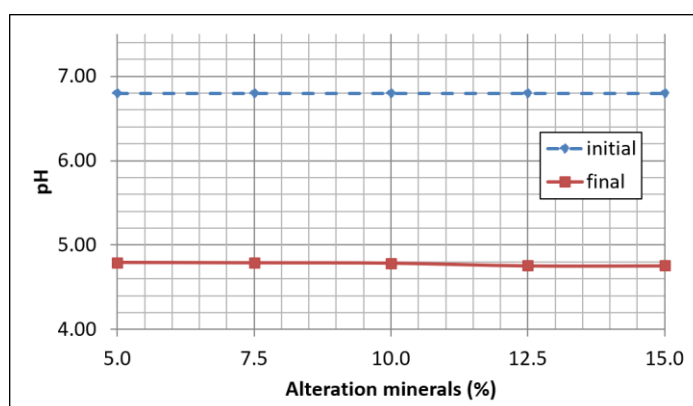


Figure 5.25. Change of pH in Awibengkok water plotted against the change in proportion of alteration minerals in the mineral assemblage.

In terms of rock mineralogy, the amount of magnesite precipitation increases as alteration mineral proportion increases from 5% to 12.5%. When the proportion increases up to 15%, the amount of magnesite precipitation decreases accompanied by the start of dolomite precipitation (Figure 5.26). The increase in magnesite precipitation as well as the occurrence of dolomite at higher alteration mineral proportion seems to be accompanied by an increase in the dissolution of calcite. Epidote precipitates more as the amount of alteration minerals increases. Hematite, calcite, enstatite and anorthite seem to be dissolving more with increasing alteration mineral proportion (Figure 5.26). The change in albite, orthoclase, diopside, ilmenite, titanite and chlorite seem to be unaffected by the increase in alteration mineral proportion. In terms of porosity, increase in alteration mineral proportion leads to more pronounced decrease in porosity (Figure 5.27).

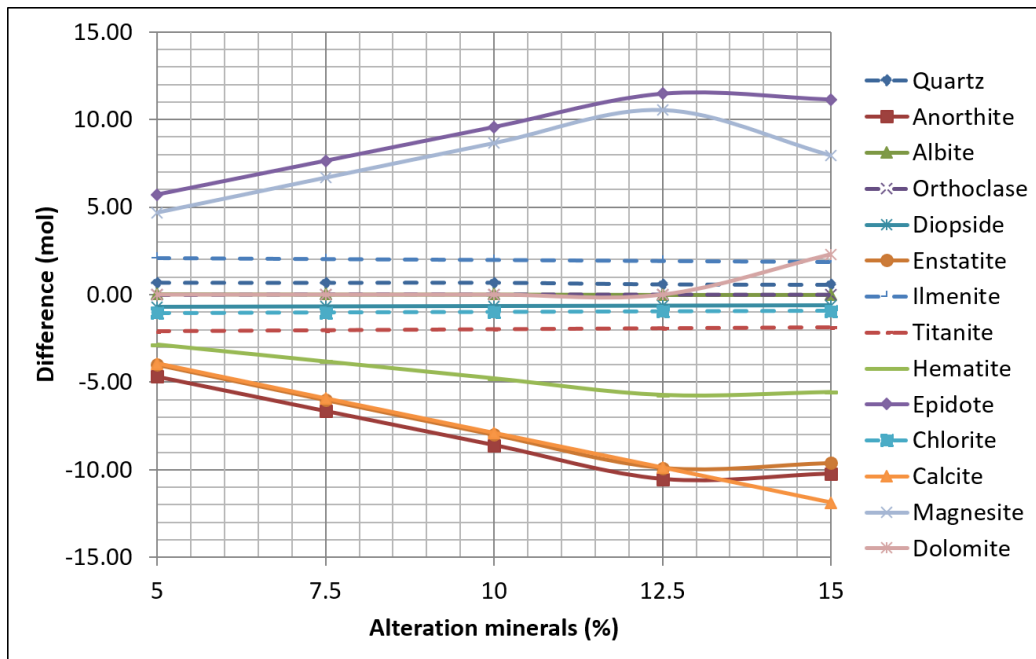


Figure 5.26. Change of mineral mol amount in Awibengkok field plotted against the change in proportion of alteration minerals in the mineral assemblage (note that the trends for enstatite and alunite, and corundum and halloysite overlap with each other).

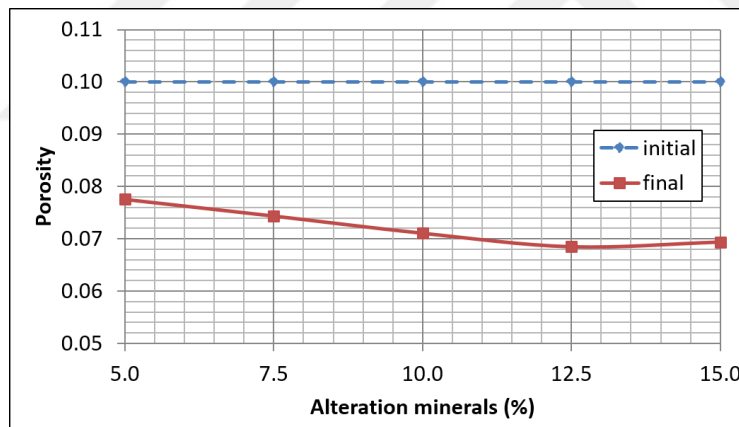


Figure 5.27. Porosity change against change in alteration mineral abundance in Awibengkok field.

5.5.3.2. Porosity value

Givent that i) all the fields studied in this thesis have volcanic rocks as reservoir lithology and ii) the measured porosity of the Awibengkok field is reported as 10% (Stimac et al., 2008), the reservoir porosity used in modelling is taken as 10% in the thesis. In order to understand the uncertainty associated with the modelling output induced by the variation of porosity value, sensitivity analysis is performed here for

both Ungaran and Awibengkok fields. This analysis is performed by changing the porosity value between 0.05 and 0.15. Five batches of equilibrium model are simulated, using 5%, 7.5%, 10%, 12.5% and 15% porosity. Each batch is simulated under constant pressure and temperature conditions set up, and the same amount of CO₂ specified in the modelling (Chapter 4) for the relevant fields. The result of each batch is further analyzed in terms of brine chemistry and rock mineralogy.

Ungaran field:

In terms of brine chemistry, the variation of porosity has effect on the final Ca and SO₄ concentrations (Figure 5.28). The decrease in the final Ca and the increase in the final SO₄ concentrations seems to get smaller as the porosity increases. However, this reduction is just about 0.28 mmol/L for Ca, and 0.012 mmol/L for SO₄ for 5% increase in porosity. The decrease in Mg and HCO₃ concentrations seem not to have been affected by change porosity. In terms of pH, the difference in pH show very minor decrease as the porosity increases (Figure 5.29).

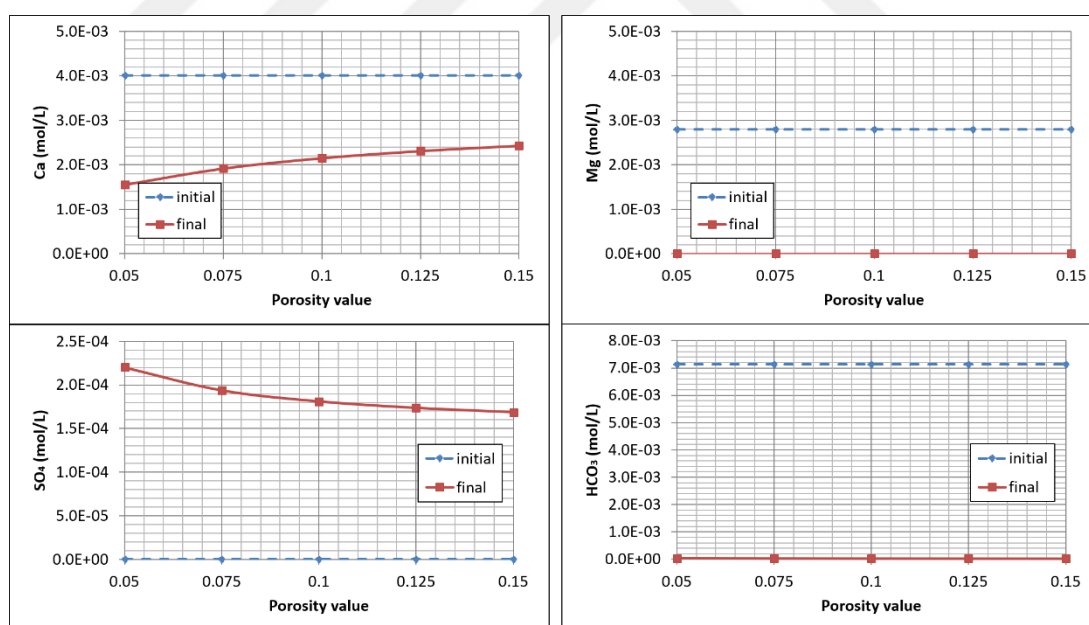


Figure 5.28. Change of species in Ungaran water plotted against the change in porosity value.

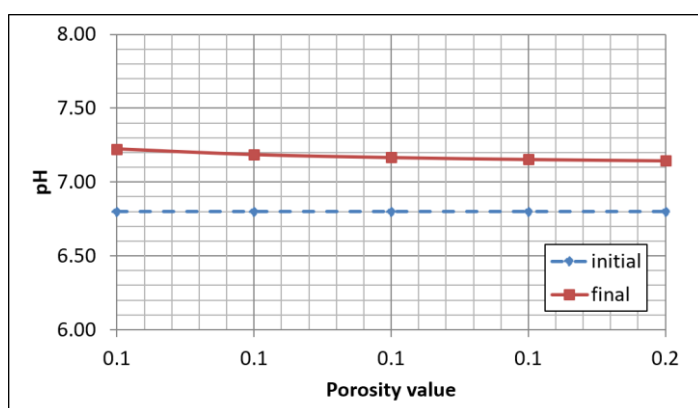


Figure 5.29. Change of pH in Ungaran water plotted against porosity value.

In terms of rock mineralogy, the amount of calcite precipitated is similar (1.4 mol) for all batches (5%, 7.5%, 10%, 12.5% and 15%). Quartz, orthoclase, ilmenite and albite precipitate more as the amount of porosity increases (Figure 5.30). Enstatite, corundum and anorthite seem to be dissolving more with increasing porosity (Figure 5.30). Anhydrite, halloysite and alunite do not display any change with the change in porosity.

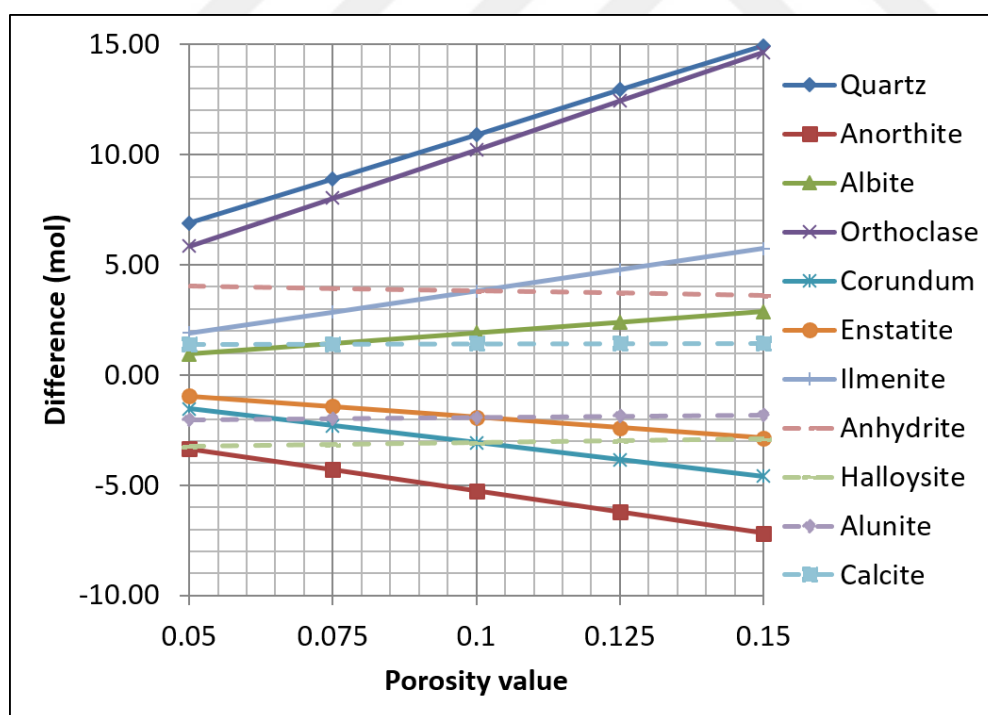


Figure 5.30. Change of mineral mol amount in Ungaran field plotted against porosity change.

Awibengkok field:

In terms of brine chemistry, the variation of porosity has effect on the final Ca, Mg and HCO_3 concentrations (Figure 5.31). The increase in the final Ca and Mg concentrations seems to get smaller as the porosity increases. The decrease in the final HCO_3 concentration seems to get smaller with increasing porosity. The increase in SO_4 concentration seem not to have been affected by the change in porosity. In terms of pH, the difference in pH show no significant change as the porosity increases (Figure 5.32).

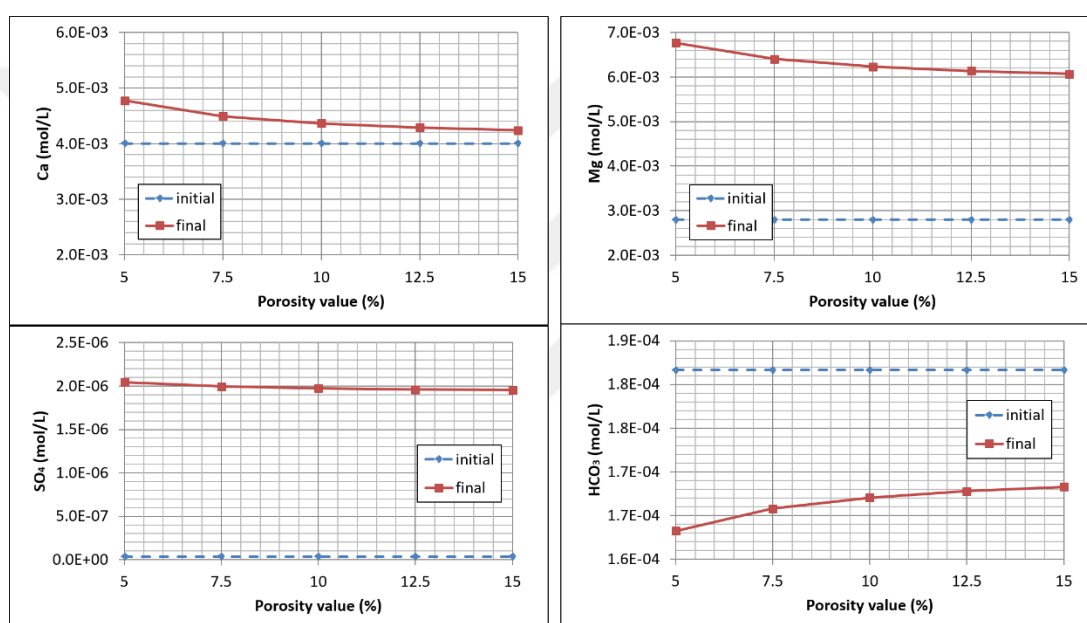


Figure 5.31. Change of species in Awibengkok water plotted against the change in porosity value.

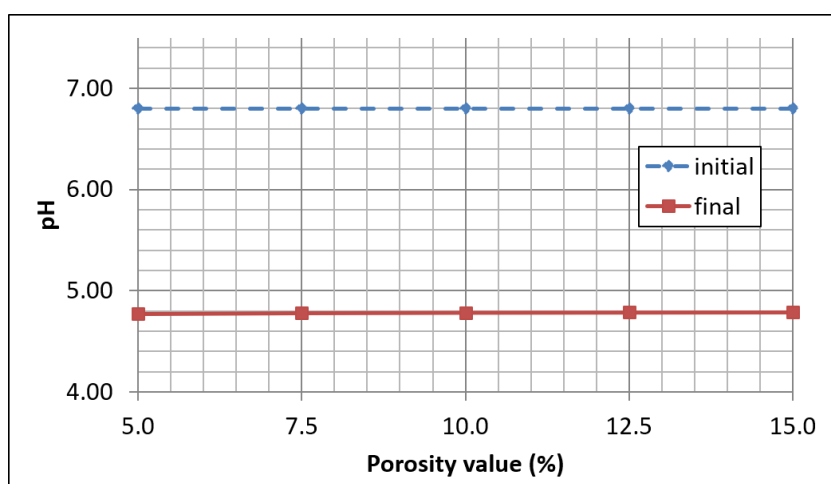


Figure 5.32. Change of pH in Awibengkok water plotted against porosity value.

In terms of rock mineralogy, the amount of magnesite and epidote precipitated slightly decreases as porosity is increased (Figure 5.33). Dissolution of hematite, calcite, enstatite and anorthite seems to get smaller with increasing porosity. Albite, orthoclase, diopside, ilmenite, titanite, chlorite and dolomite do not display any change with the change in porosity.

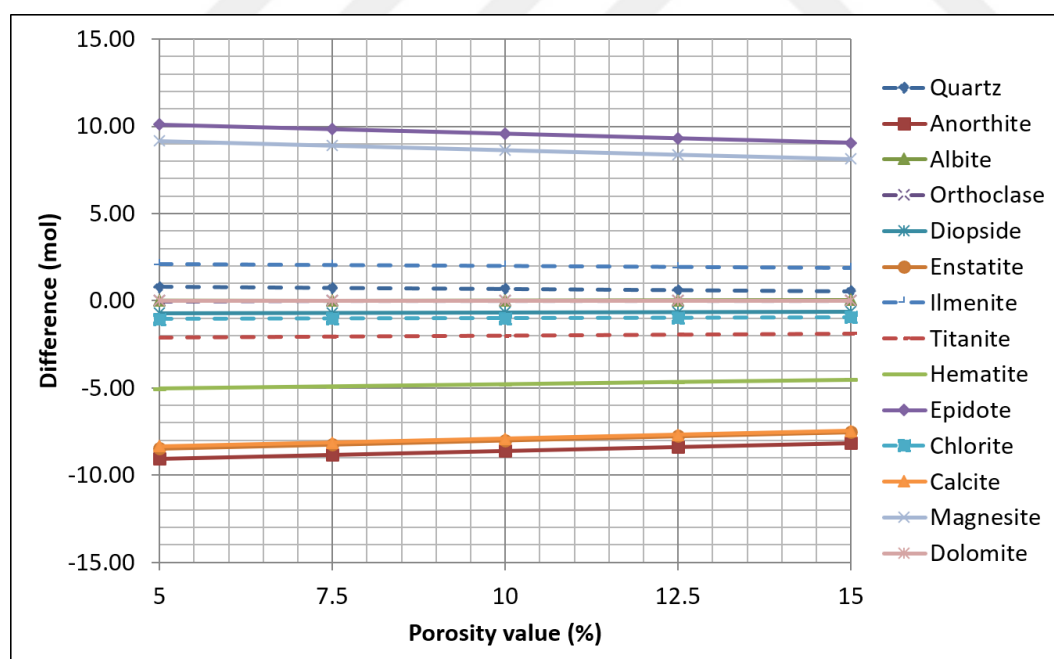


Figure 5.33. Change of mineral mol amount in Awibengkok field plotted against porosity change (note that trends for calcite-enstatite and albite-dolomite-orthoclase are overlapping).

Regarding the sensitivity analyses in both fields (Ungaran and Awibengkok), effect of alteration mineral proportion is seen to be more dominant compared to porosity variation. However, in terms of carbonate minerals controlling the ability of the geothermal reservoir to trap injected CO₂, in Ungaran field there is almost no change in the amount of precipitation of calcite which is the sole carbonate mineral in the system. In Awibengkok field, the mol difference between the amount of new carbonate minerals formed (magnesite and dolomite) and the amount of pre-existing calcite dissolution seem to match the amount of CO₂ injected suggesting that the variation in the proportion of alteration minerals does not change the ability of the field to convert CO₂ to mineral phase.

CHAPTER 6

CONCLUSION AND RECOMENDATION

Geochemical modeling to study the behavior of CO₂ inside a geothermal reservoir is done in four selected geothermal fields of Indonesia for a possible future Carbon Capture and Storage operation.

Equilibrium modeling results forecast the potential for mineral trapping by observing the formation of new carbonate minerals. Kinetic modeling results in identifying the occurrence of solubility and mineral trapping mechanisms in terms of time scale in which these processes take place. Kinetic modeling reveals that solubility trapping existed immediately after CO₂ injection and is followed by complete or partial replacement of mineral trapping mechanism suggested by the drop of dissolved CO₂ concentration accompanied by precipitation of new carbonate minerals. The results from four selected field can be summarized by the following:

- In terms of brine chemistry, Ungaran field experiences a rise in pH value accompanied by decrease in bicarbonate, calcium and magnesium concentration. Porosity value increases from 0.100 to 0.105. Mineral trapping mechanism is identified to be the main CO₂ fixation described by the dissolution of anorthite into calcite. Equilibrium among CO₂-brine-rock is achieved in 10 years.
- The brine chemistry in Baturraden field witnesses a rise in pH value accompanied by an increase in bicarbonate and decrease in calcium and magnesium contents. Porosity value decreases from 0.10 to 0.065. Mineral precipitation is the main CO₂ trapping mechanism described by the formation of dolomite from diopside dissolution. Equilibrium among CO₂-brine-rock is achieved in 10 years.

- For Dieng field, the drop in pH is accompanied by an increase in bicarbonate and a decrease in calcium and magnesium concentrations. Porosity change is minor, from 0.050 to 0.043. Solubility and mineral trapping mechanisms are both active in Dieng field. Almost 30% of injected CO₂ is transformed into dissolved aqueous phase while 70% is converted into mineral phase in the form of dolomite. Dolomite formation is caused by diopside dissolution. Equilibrium among CO₂-brine-rock is achieved approximately 10 hours after injection
- In Awibengkok field the brine chemistry experience a drop in pH, increase in bicarbonate, calcium and magnesium. The porosity value changes from 0.10 to 0.071. Similar to Dieng field, solubility and mineral trapping mechanism are both responsible for the CO₂ fixation. Approximately 23% of injected CO₂ is dissolved permanently as aqueous phase, while the remaining 77% is transformed into magnesite. Equilibrium among CO₂-brine-rock is achieved 10000 years after injection.

The result of this modeling study classifies the studied fields into two groups: 1) Ungaran and Baturraden fields with mineral trapping, 2) Dieng and Awibengkok fields with combined (solubility and mineral) trapping. This grouping seems to be related to the proportion of the dissolved CO₂ which can be correlated with the TDS content and pH value of the brine.

Given i) the lack of published studies on the precipitation rates of minerals, and ii) the assumption, in the kinetic modeling, of the similarity between dissolution and precipitation rates of minerals, the results of the present study suffer from limitation in predicting accurate time for mineral trapping. Nonetheless, result of this study provide relevant information on how CO₂-water-rock interaction can be assessed for a possible future CCS project to be carried out in these areas. However, because the simulations done are restricted to static environment in which flow regime is neglected, dynamic mass transport study is strongly recommended for future work in order to refine the conclusions obtained from the present study.



REFERENCES

- Acuna, J.A., Stimac, J., Sirad-Azwar, L., Pasikki, R.G., 2008. Reservoir management at Awibengkok geothermal field, West Java, Indonesia. *Geothermics*, 37, pp.332-346.
- Alam, M.A., Sanchez, P., Parada, M.A., 2010. Interplay of volcanism and structural control in defining the geothermal system(s) along the Liquine-Ofqui fault zone, in the south-central Chile. *GRC Transactions*, 34, p.747–750.
- Allis, R.G., 1999. Present day hydrothermal conditions in the vicinity of AWI 1-2, Awibengkok Geothermal Field, Indonesia. *Geothermal Resources Council Transactions*, 23, pp.3-8.
- Anovitz, L.M., Rondinone, A.J., Sochalski-Kolbus, L., Rosenqvist, J., Chesire, M.C., 2017. Nano-scale synthesis of the complex silicate minerals forsterite and. *Journal of Colloid and Interface Science*, 495, pp.94-101.
- Aprilina, N.V., Satya D.Y., Rejeki S., Golla G., Waite M., 2015. Geologic Modeling Workflow for Volcanic Hosted Geothermal Reservoirs: Case Study from Salak Geothermal Field. In *Proceedings World Geothermal Congress 2015*. Melbourne, 2015.
- Bachu, S., Bonijoly, D., Bradshaw, J., Burruss, R., Holloway, S., Christensen, N.P., Mathiassen OM., 2007. CO₂ storage capacity estimation: Methodology and gaps. *Int. J. Greenhouse Gas Control*, 1, pp.430-443.
- Bemmelen, V., 1949. *The Geology of Indonesia. vol. 1A: General geology of Indonesia and adjacent archipelagoes*. the Hague: Martinus Nijhoff.
- Best, M.G., 2003. The CIPW Normative Composition. In Best, M.G. *Igneous and Metamorphic Petrology*. Melbourne: Blackwell. pp.56-60.

- Boedihardi, M., Suratno., Sudarman, S., 1991. Evaluation of the Dieng geothermal field: Review of development strategy. In *Proceeding Indonesia Petroleum Association Twentieth Annual Convention.*, 1991.
- Bruno, J., Stumm, W., Wersin, P., Brandberg, F., 1992. On the influence of carbonate in mineral dissolution: I. The thermodynamics and kinetics of hematite dissolution in bicarbonate solutions at $T = 25^{\circ}\text{C}$. *Geochimica et Cosmochimica Acta*, 56, pp.1139-1147.
- Buscheck, T.A., Bielicki, J.M., Chen, M., Sun, Y., Hao, Y., Edmunds, T.A., Saar, M.O., Randolph, J.B., 2014. Integrating CO₂ storage with geothermal resources for dispatchable renewable electricity. *Energy Procedia*, 63, pp.7619-7630.
- Captuready, 2018. *CCS History*. [Online] Available at: <http://www.captureready.com/EN/Channels/OverViews/showDetail.asp?objID=2,ClassID=1> [Accessed 15 September 2018].
- CarbFix, 2018. *The CarbFix Project*. [Online] Available at: <https://www.carbfix.com/carbfix-project> [Accessed 19 January 2019].
- Carroll-Webb, S.A. , Walther, J.V., 1988. A surface complex reaction model for the pH-dependence of corundum. *Geochimica et Cosmochimica Acta*, 52, pp.2609-2623.
- Casey, W.I., Lasaga, A.C., Gibbs, G.V., 1990. Mechanisms of silica dissolution as inferred from the kinetic isotope effect. *Geochimica et Cosmochimica Acta*, 54, pp.3369-3378.
- CCP, 2015. *CO₂ Trapping Mechanisms*. [Online] Available at: https://www.co2captureproject.org/co2_trapping.html [Accessed 27 March 2019].
- CCSA, 2018. *Carbon Capture and Storage Association*. [Online] Available at: <http://www.ccsassociation.org/what-is-ccs/> [Accessed 27 March 2019].

- Claproth, R., 1989. *Petrography and geochemistry of volcanic rocks from Ungaran, Central Java, Indonesia*. Doctor of Philosophy thesis, Department of Geology, University of Wollongong.
- CO2-Earth, 2018. *Global Warming Update*. [Online] Available at: <https://www.co2.earth/global-warming-update> [Accessed 14 September 2018].
- Condon, W.H. Pardyanto, L., Ketner, K.B., Amin, T.C., Gafoer, S., Samodra, H., 1996. *Peta geologi lembar Banjarnegara dan Pekalongan, Jawa Skala 1:100.000*. Geologic map. Pusat Penelitian dan Pengembangan Geologi, Departemen Pertambangan dan Energi.
- Critelli, T. Marini, L., Schott, J., Mavromatis, V., Apollaro, C., Rinder, T., De Rosa, R., Oelkers, E.H., 2014. Dissolution rates of actinolite and chlorite from a whole-rock experimental study of metabasalt dissolution from $2 \leq \text{pH} \leq 12$ at 25 °C. *Chemical Geology*, 390, pp.100-108.
- Cui, G., Zhang, L., Tan, C., Ren, S., Zhuang, Y., Enechukwu, C., 2017. Injection of supercritical CO₂ for geothermal exploitation from sandstone and carbonate reservoirs: CO₂-water-rock interaction and their effect. *J. CO₂ Utilization*, 20, pp.113-128.
- Daval, D. Hellmann, R., Corvisier, J., Tisserand, D., Martinez, I., Guyot, F., 2010. Dissolution kinetics of diopside as a function of solution saturation state: Macroscopic measurements and implications for modeling of geological storage of CO₂. *Geochimica et Cosmochimica Acta*, 74, pp.2615-2633.
- Declercq, J., Oelkers, E.H., 2014. *CarbFix Report PHREEQC mineral dissolution kinetics database*. Kinetics database compilation. Toulouse: Geoscience Environment.
- Diamond, S., Kinter, E.B., 1956. Surface areas of clay minerals as derived from measurements of glycerol retention. *Clay and Clay Minerals*, 5, pp.334-347.

- Djuri, M., Samodra, H., Amin, T.C., Gafoer, S., 1996. *Geological Map of the Purwokerto and Tegal Quadrangle, Java, scale 1:100.000*. Geologic Map. Bandung: Geological Research and Development Centre.
- Duan, Z., Sun, R., 2003. An improved model calculating CO₂ solubility in pure water and aqueous NaCl solutions from 273 to 533 K and from 0 to 2000 bar. *Chemical Geology*, 193, pp.257-271.
- Duan, Z., Sun, R., Zhu, C., Chou, I.M., 2006. An improved model for the calculation of CO₂ solubility in aqueous solutions containing Na⁺, K⁺, Ca²⁺, Mg²⁺, Cl⁻, SO₄²⁻. *Marine Chemistry*, 98, pp.131-139.
- Efendi, K., Hermanto, B., 1998. *Geological Map of the Bogor Quadrangle, Jawa*. Geologic map. Bandung: Geological Research and Development Centre.
- ESDM, 2016. *Geothermal Investment Opportunities in Indonesia*. Jakarta: Ministry of Energy and Mineral Resources Indonesia Directorate General of New, Renewable Energy and Energy Conservation.
- Ezekiel, J., Saar, M.O., 2016. *Geothermal energy and geofluids: Assessment and optimization of carbon storage and combined EGR-CPG development from high-temperature natural gas reservoir*. [Online] Available at: <https://geg.ethz.ch/project-cpg-egr/> [Accessed 22 December 2018].
- Gaffar, E.Z., 2017. The subsurface structure investigation of Dieng Plateau, Central Java, Indonesia by using the magnetotelluric data. *Teknologi Indonesia*, 40 (1), pp.44-54.
- Gautelier, M., Schott, J., Oelkers, E.H., 2007. An experimental study of dolomite dissolution rates at 80 °C as a function of chemical affinity and solution composition. *Chemical Geology*, 242, pp.509-517.
- Gilfillan, S.M.V., Sherk, G.W., Poreda, R.J., Haszeldine, R.S., 2017. Using noble gas fingerprints at the Kerr Farm to assess CO₂ leakage allegations linked to the

- Weyburn-Midale CO₂ monitoring and storage project. *International Journal of Greenhouse Gas Control*, 63, pp.215-225.
- Gislason, S.R., Oelkers, E.H., 2014. Carbon Storage in Basalt. *Science*, 344 (6182), pp.373-374.
- Global CCS Institute, 2014. *The Global Status of CCS: 2014*. Melbourne: Global Carbon Capture and Storage Institute. Available at: <https://hub.globalccsinstitute.com/sites/default/files/publications/180923/global-status-ccs-2014.pdf> [Accessed 12 February 2019].
- GlobalCCSI, 2018. *Global CCS Institute*. [Online] Available at: <https://www.globalccsinstitute.com/understanding-ccs/what-is-ccs> [Accessed 28 September 2018].
- GRREBS, 2018. *CCS monitoring*. [Online] Available at: http://grrebs.ete.inrs.ca/en/csc/csc_surveillance/ [Accessed 12 February 2019].
- Gysi, A.P., Stefansson, A., 2012. Experiments and geochemical modeling of CO₂ sequestration during hydrothermal basalt alteration. *Chemical Geology*, 306-307, pp.10-28.
- Hall, R., 2002. Cenozoic geological and plate tectonic evolution of SE Asia and the SW Pacific: computer-based reconstructions, model and animations. *Journal of Asian Earth Sciences*, 20 (4), pp.353-431.
- Hamilton, W.B., 1979. *Tectonics of the Indonesian region*. Report of USGS. U.S. Geological Survey.
- Handley, H.K., Davidson, J.P., Macpherson, C.G., Stimac, J.A., 2008. Untangling differentiation in arc lavas: Constraints from unusual minor and trace element variations at Salak Volcano, Indonesia. *Chemical Geology*, 255, pp.360-376.

- Harijoko, A., Juhri, S., 2017. Cl/B ratio of geothermal fluid around Slamet Volcano, Jawa Tengah, Indonesia. *IOP Conf. Series: Earth and Environmental Science* 012015, 103.
- Harijoko, A., Uruma, R., Wibowo, H.E., Setijadji, L.D., Imai, A., Yonezu, K., Watanabe, K., 2016. Geochronology and magmatic evolution of the Dieng Volcanic Complex Central Java, Indonesia and their relationships to geothermal resources. *Journal of Volcanology and Geothermal Research*, 310, pp.209-224.
- Hochstein, M.P., Sudarman, S., 2015. Indonesian Volcanic Geothermal Systems. In *Proceedings World Geothermal Congress 2015*. Melbourne, 2015.
- Hoffmann-Rothe, A., Ritter, O., Haak, V., 2001. Magnetotelluric and geomagnetic modeling reveals zones of very high electrical conductivity in the upper crust of Central Java. *Physics of the Earth and Planetary Interiors*, 124, pp.131-151.
- Hollacher, 2018. *Petrology, GEO-320*. [Online] Available at: <https://www.whitman.edu/geology/winter/Petrology/CIPW%20Norm%20Hollacher.xls> [Accessed 18 December 2018].
- Indarto, S. Permana, H., Gaffar, E.Z., Bakti, H., Kautsar, A.A., Nurohman, H., Sudarsono., Sudradjat, Y., Setiawan, I., Ismayanto, A.F., 2017. Geological structure and lithology as the control of Guci and Baturaden hot spring appearances, Central Java. *Riset Geologi dan Pertambangan*, 27 (1), pp.97-109.
- IPCC, 2005. *IPCC Special Report on Carbon Dioxide Capture and Storage*. Working Group III of the Intergovernmental Panel on Climate Change. Cambridge University Press.
- IPCC, 2014. *Climate Change 2014: Mitigation of Climate Change*. Contribution of Working Group III to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change. Cambridge University Press.
- Juhri, S., Harijoko, A., 2016. Karakteristik geokimia air panas bumi di sekitar gunung Slamet. In *PROCEEDING, SEMINAR NASIONAL KEBUMIHAN KE-9.*, 2016.

- Klajmon, M. Havlova, V., Cervinka, R., Mendoza, A., Francu, J., Berenblyum, R., Arild, O., 2017. REPP-CO₂: Equilibrium Modelling of CO₂-Rock-Brine Systems. *Energy Procedia*, 114, pp.3364-3373.
- Koenen, M., Heege, J.T., Peeters, R., 2014. *Transport properties of intact caprocks and effects of CO₂-water-rock interaction: CO₂-induced mineral reactions in sandstone reservoirs (CATO2-WP3.03-D12)*. CATO-2 project public report. CATO-2 project public report.
- Kusdyantono, W., Pamungkas, T.S., Pradana, Y.S., Suyanto, I., 2016. Investigation of hydrothermal fluid continuity and geological structure using magnetic method in Dieng geothermal area, central Java. In *41 Pekan Ilmiah Tahunan Himpunan Ahli Geofisika Indonesia*. Lampung, 2016.
- Kvamme, B., Aromada, S.A., 2018. Alternative Routes to Hydrate Formation during Processing and Transport of Natural Gas with a Significant Amount of CO₂: Sleipner Gas as a Case Study. *J. Chem. Eng. Data*, 63 (3), pp.832-844.
- Layman, E.B., Agus, I., Warsa, S., 2002. The Dieng Geothermal Resource, Central Java, Indonesia. *Geothermal Resources Council Transactions*, 26, pp.573-579.
- Liu, B., Zhao, F., Xu, J., Qi, Y., 2019. Experimental Investigation and Numerical Simulation of CO₂-Brine-Rock Interactions during CO₂ Sequestration in a Deep Saline Aquifer. *Sustainability*, 11(317).
- Mahon, T., Harvey, C., Crosby, D., 2000. The chemistry of geothermal fluids in Indonesia and their relationship to water and vapour dominated systems. In *Proceedings World Geothermal Congress 2000*. Kyushu-Tohoku, 2000.
- Miller, J.L. Madden, A.S.E., Phillip-Lander, C.M., Pritchett, B.N., Madden, M.E., 2016. Alunite dissolution rates: Dissolution mechanisms. *Geochimica et Cosmochimica Acta*, 172, pp.93-106.

- MIT, 2016. *Carbon capture and sequestration technologies MIT: In Salah Fact Sheet*. [Online] Available at: https://sequestration.mit.edu/tools/projects/in_salah.html [Accessed 24 March 2019].
- NOAA, 2017. *Global Climate report*. [Online] Available at: <https://www.ncdc.noaa.gov/sotc/global/201713> [Accessed 14 September 2018].
- Oelkers, E.H., Schott, J., 1994. Experimental study of kyanite dissolution rates as a function of Al and Si concentration. In *Goldschmidt Conference 1994*. Edinburgh, 1994.
- Palandri, J.L., Kharaka, Y.K., 2004. *A compilation of rate parameters of water-mineral interaction kinetics for application to geochemical modeling*. Open-File Report 2004-1068. Menlo Park, California: U.S. Geological Survey open file report 2006-1068 U.S. Geological Survey.
- Parkhurst, D.L., Appelo, C.A.J., 2013. *Description of input and examples for PHREEQC version 3-A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations*. Denver: U.S. Geological Survey Techniques and Methods.
- Peng, D.Y., Robinson, D.B., 1976. A new two-constant equation of state. *Ind. Eng. Chem. Fundam.*, 15, pp.59-64.
- Phuong, N.K., Harijoko, A., Itoi, R., Unoki, Y., 2012. Water geochemistry and soil gas survey at Ungaran geothermal field, central Java, Indonesia. *Journal of Volcanology and Geothermal Research*, 229-230, pp.23-33.
- Phuong, N.K., Hendrayana, H., Harijoko, A., Itoi, R., Unoki, R., 2005. Geochemistry of the Ungaran Geothermal System, Central Java, Indonesia. *Proceedings joint Convention Surabaya - HAGI-IAGI-PERHAPI*, pp.64-77.
- Porovsky, O.S., Golubev, S.V., Jordan, G., 2009. Effect of organic and inorganic ligands on calcite and magnesite dissolution rates at 60 °C and 30 atm pCO₂. *Chemical Geology*, 265, pp.33-43.

- Purnomo, B.J., Pichler, T., 2014. Geothermal systems on the island of Java, Indonesia. *Journal of Volcanology and Geothermal Research*, 285, pp.47-59.
- Purnomo, B.J., Pichler, T., You, C., 2016. Boron isotope variations in geothermal systems on Java, Indonesia. *Journal of Volcanology and Geothermal Research*, 311, pp.1-8.
- Putranto, T.T., Rde, T.R., 2016. Hydrogeological Model of an Urban City in a Coastal Area, Case study: Semarang, Indonesia. *Indonesian Journal on Geoscience*, 3(1), pp.17-27.
- Ramadhan, Y., Channel, K., Herdianita, N.R., 2013. Hotwater geochemistry for interpreting the condition of geothermal reservoir, Dieng plateau case, Banjarnegara-Wonosobo regency, central Java. *Indonesian Journal of Geology*, 8 (2), pp.95-102.
- Reswara, A., Seha., 2014. Pendugaan lapisan reservoir panas bumi di kawasan gunungapi Slamet dengan memanfaatkan data anomali medan gravitasi citra satelit. *Berkala Fisika*, 17 (2), pp.45-54.
- Ringrose, P.S., Mathieson, A.S., Wright, I.W., Selama, F., Hansen, O., Bissell, R., Saoula, N., Midgley, J., 2013. The In Salah CO₂ storage project: lessons learned and knowledge transfer. *Energy Procedia*, 37, pp.6226-6236.
- Rose, N.M., 1991. Dissolution rates of prehnite, epidote, and albite. *Geochimica et Cosmochimica Acta*, 55, pp.3273-3286.
- Rosenbauer, R.J., Koksalan, T., Palandri, J.L., 2005. Experimental investigation of CO₂-brine-rock interactions at elevated temperature and pressure: Implications for CO₂ sequestration in deep-saline aquifers. *Fuel Processing Technology*, 86, pp.1581-1597.
- Setiadji, L.D., 2010. Segmented volcanic arc and its association with geothermal fields in Java island, Indonesia. In *Proceedings World Geothermal Congress 2010.*, 2010.

- Setyawan, A. Ehara, S., Fujimitsu, Y., Nishijima, J., Saibi, H., Aboud, E., 2009. The Gravity Anomaly of Ungaran Volcano, Indonesia: Analysis and Interpretation. *J Geotherm. Res. Soc. Japan*, 31(2), pp.107-116.
- Sigfussona, B. Gislasonb, S.R., Matter, J.M., Stute, M., Gunnlaugssona, E., Gunnarssona, I., Aradottir, E.S., Sigurdardottir, H., Mesfin, K., Alfredsson, H.A., 2015. Solving the carbon-dioxide buoyancy challenge: The design and field. *International Journal of Greenhouse Gas Control*, 37, pp.213-219.
- Simandjuntak, T.O., Barber, A.J., 1996. Contrasting tectonic styles in the Neogene orogenic belts of Indonesia. *Geological Society, Special Publications*, 106 (1), pp.185-201.
- Snaebjornsdottir, S.O., Tomasdottir, S., Sigfusson, B., Aradottir, E.S., Gunnarsson, G., Niemi, A., Basirat, F., Dessirier, B., Gislason, S.R., Oelkers, E.H., 2018. The geology and hydrology of the CarbFix2 site, SW-Iceland. *Energy Procedia*, 146, pp.146-157.
- Steel, L., Mackay, M., Maroto-Valer, M., 2018. Experimental investigation of CO₂-brine-calcite interactions under reservoir conditions. *Fuel Processing Technology*, 169, pp.122-131.
- Stimac, J., Nordquist, G., Suminar, A., Sirad-Azwar, L., 2008. An overview of the Awibengkok geothermal system, Indonesia. *Geothermics*, 37, pp.300-331.
- Stimac, J., Sugiaman, F., 2000. The AWI 1-2 core research program: part I, geologic overview of the Awibengkok geothermal field, Indonesia. In *Proceedings World Geothermal Congress 2000*. Kyushu-Tohoku, 2000.
- Sutawidjaja, I.S., Sukhyar, R., 2009. Cinder cones of Mount Slamet, Central Java, Indonesia. *Jurnal Geologi Indonesia*, 4 (1), pp.57-75.
- Thanden, E.R., Sumadirdja, H., Richards, P.W., 1975. *Geologic map of the Magelang and Semarang Quadrangles, Java*. Geologic Map. Geological Survey of Indonesia, Scale 1:100,000.

- Torp, T.A., 2011. *CO2 Capture and Storage: Sleipner Project*. [Online] Available at: http://www.co2captureandstorage.info/project_specific.php?project_id=26 [Accessed 24 March 2019].
- Utama, A.P. Dwinanto, A., Situmorang, J., Hikmi, M., Irsamukhti, R., 2012. Green field geothermal systems in Java, Indonesia. In *PROCEEDINGS, 1st ITB Geothermal Workshop 2012*. Bandung, 2012.
- Vukadinovic, D., Sutawidjaja, I., 1995. Geology, mineralogy and magma evolution of Gunung Slamet Volcano, Java, Indonesia. *Journal of Southeast Asian Earth Science*, 11 (2), pp.135-164.
- Wang, K., Xu, T., Wang, F., Tian, H., 2016. Experimental study of CO2-brine-rock interaction during CO2 sequestration in deep coal seams. *Int. J. Coal. Geol.*, 154, pp.265-274.
- White, A.F., Peterson, M.L., Hochella, M.F., 1994. Electrochemistry and dissolution kinetics of magnetite and ilmenite. *Geochimica et Cosmochimica Acta*, 58 (8), pp.1859-1875.
- Whittaker, S., Rostron, B., Hawkes, C., Gardner, C., White, D., Johnson, J., Chalaturnyk, R., Seeburger, D., 2011. A decade of CO2 injection into depleting oil fields: monitoring and research activities of the IEA GHG Weyburn-Midale CO2 Monitoring and Storage Project. *Energy Procedia*, 4, pp.6069-6076.
- Xu, T.F., Apps, T.A. , Pruess, K., 2005. Mineral sequestration of carbon dioxide in a sandstone-shale system. *Chemical Geology*, 217, pp.295-318.
- Yang, L., Xu, T., Yang, B., Tian, H., Lei, H., 2014. Effect of mineral composition and heterogeneity on the reservoir quality evolution with CO2 intrusion. *Geochemistry Geophysic Geosystems*, 15, pp.605-618.

APPENDIX A

EQUILIBRIUM MODELING RESULT IN UNGARAN FIELD

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\l1n1.dat

Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
NAMED_EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\l1n1.dat
SOLUTION_SPECIES
CO3-2 + 2 H+ = CO2 + H2O
log_k 16.681
delta_h -5.738 kcal
analytical_expression 464.1965 0.09344813 -26986.16 -165.75951 2248628.9
dw 1.92e-9
vm 7.29 0.92 2.07 -1.23 -1.60 # ref. 1 + McBride et al. 2015, JCED 60, 171
2CO2 = (CO2)2 # activity correction for CO2 solubility at high P, T
log_k -1.8
analytical_expression 8.68 -0.0103 -2190
vm 14.58 1.84 4.14 -2.46 -3.20
END

End of simulation.

Reading input data for simulation 2.

PHASES
CO2(g)
CO2 = CO2
log_k -1.468
delta_h -4.776 kcal
analytical_expression 10.5624 -2.3547e-2 -3972.8 0 5.8746e5 1.9194e-5
t_c 304.2 # critical T, K
p_c 72.86 # critical P, atm
omega 0.225 # acentric factor

Ankerite
CaMg0.3Fe0.7(CO3)2 + 2H+ = Ca++ + 0.3Mg++ + 0.7Fe++ + 2HCO3-
log_k 1.54
delta_h 0
analytical_expression -1.8649e+03 -2.9583e-01 1.0468e+05 6.7554e+02 -6.0514e+06
END

End of simulation.

Reading input data for simulation 3.

SOLUTION 1 UW-8B
temp 200
pH 6.8
pe 4
redox pe
units mg/l
density 1
C(4) 1824
Ca 278
Cl 1088
Mg 126
Na 746
S(6) 0.1
K 47.1
F 0.06
B 19.7
Si 95
water 1 # kg
pressure 249 atm
EQUILIBRIUM_PHASES 1 Reservoir
Albite 0 17.11
Alunite 0 1.91
Anhydrite 0 0
Ankerite 0 0
Anorthite 0 19.07
CO2(g) 2.396 1.4 #1.4
Calcite 0 0
Corundum 0 6.56
Dawsonite 0 0
Dolomite 0 0
Enstatite 0 28.44
Fluorapatite 0 0.27

```

Gypsum      0 0
Ilmenite    0 1.09
K-Feldspar  0 15.83
Kaolinite   0 3.06
Magnesite   0 0
Quartz      0 69.09
Siderite    0 0
Zircon      0 0.01
SELECTED_OUTPUT 1
file        D:\20182 SPRING\Thesis PHREEQC\1. Ungaran - UW-8\equilibrium ungaran.sel
reset       false
solution    true
ph          true
pe          true
temperature true
molalities  K+ Na+ Ca+2 Mg+2
             HCO3- SO4-2 Cl- CO3-2
saturation_indices Anhydrite Gypsum Aragonite Calcite
                  Dolomite Magnesite CO2(g)
USER_PUNCH
10 PUNCH description
PRINT
species
false
END

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

Initial solution 1.      UW-8B

WARNING: USER_PUNCH: Headings count does not match number of calls to PUNCH.

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

Elements      Molality      Moles
B              1.830e-03    1.830e-03
C(4)           3.003e-02    3.003e-02
Ca             6.966e-03    6.966e-03
Cl             3.082e-02    3.082e-02
F             3.172e-06    3.172e-06
K             1.210e-03    1.210e-03
Mg            5.206e-03    5.206e-03
Na            3.259e-02    3.259e-02
S(6)          1.046e-06    1.046e-06
Si            1.588e-03    1.588e-03

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

pH            = 6.800
pe            = 4.000
Density (g/cm³) = 0.88413
Volume (L)    = 1.13562
Activity of water = 0.998
Ionic strength (mol/kgw) = 5.105e-02
Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = 1.253e-02
Total CO2 (mol/kg) = 3.003e-02
Temperature (°C) = 200.00
Pressure (atm) = 249.00
Electrical balance (eq) = 1.479e-02
Percent error, 100*(Cat-|An|)/(|Cat+|An|) = 16.71
Iterations    = 8
Total H       = 1.110676e+02
Total O       = 5.560607e+01

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

Phase          SI** log IAP    log K(473 K, 249 atm)
Afwillite      -11.89    26.54    38.43    Ca3Si2O4(OH)6
Akermanite     1.13    26.44    25.31    Ca2MgSi2O7
Anhydrite      -3.57    -10.86    -7.29    CaSO4
Antarcticite   -9.98     -6.23     3.75    CaCl2:6H2O
Anthophyllite  20.68    51.83    31.15    Mg7Si8O22(OH)2
Antigorite     169.71   413.94   244.23    Mg48Si34O85(OH)62
Aphthitalite   -22.90   -26.79    -3.89    NaK3(SO4)2
Aragonite       2.08      1.64    -0.44    CaCO3
Arcanite       -12.21   -14.11    -1.90    K2SO4
Artinite       1.21     12.14    10.93    Mg2CO3(OH)2:3H2O
B              -61.65     5.69    67.34    B
B(g)           -116.38     5.69   122.07    B
B2O3           -9.15     -5.48     3.66    B2O3
Bassanite      -4.23    -10.86    -6.63    CaSO4:0.5H2O
BF3(g)         -30.01    -40.78   -10.77    BF3
Bischofite     -10.39     -6.33     4.05    MgCl2:6H2O
Bloedite       -19.51    -22.22    -2.70    Na2Mg(SO4)2:4H2O
Borax          -17.99     -0.64    17.35    Na2(B4O5(SO4)4):8H2O
Boric acid     -3.78     -2.74     1.03    B(OH)3
Brucite        1.41     10.61     9.20    Mg(OH)2
Burkeite       -30.71   -21.22     9.49    Na6CO3(SO4)2
C              -35.13     2.16    37.29    C
C(g)           -106.35     2.16   108.51    C
Ca             -69.71    16.34    86.05    Ca
Ca(g)          -83.54    16.34    99.88    Ca
Ca2Cl2(OH)2:H2O -21.62     4.50    26.12    Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O -41.32    25.93    67.25    Ca4Cl2(OH)6:13H2O
Calcite        2.23      1.64    -0.59    CaCO3
Carnallite     -15.00   -11.07     3.93    KMgCl3:6H2O
CaSO4:0.5H2O(beta) -4.26   -10.86    -6.60    CaSO4:0.5H2O
Chalcedony     -0.53     -2.81    -2.28    SiO2
Chloromagnesite -16.31    -6.33     9.99    MgCl2
Chrysotile     10.08    26.22    16.15    Mg3Si2O5(OH)4
Cl2(g)         -21.07   -22.56    -1.49    Cl2
CO2(g)         0.46     -1.74    -2.20    CO2
Coesite        -0.89     -2.81    -1.92    SiO2
Colemanite     -16.65     4.98    21.63    Ca2B6O11:5H2O

```

Cristobalite(alpha)	-0.66	-2.81	-2.14	SiO2
Cristobalite(beta)	-0.87	-2.81	-1.94	SiO2
Dicalcium_silicate	-3.69	18.63	22.32	Ca2SiO4
Diopside	4.63	15.72	11.09	CaMgSi2O6
Dolomite	5.95	3.17	-2.78	CaMg(CO3)2
Dolomite-dis	5.21	3.17	-2.03	CaMg(CO3)2
Dolomite-ord	5.96	3.17	-2.79	CaMg(CO3)2
Enstatite	2.38	7.81	5.43	MgSiO3
Epsomite	-8.62	-10.98	-2.36	MgSO4·7H2O
F2(g)	-60.53	-30.98	29.55	F2
Fluorite	-3.86	-14.64	-10.78	CaF2
Forsterite	4.40	18.42	14.02	Mg2SiO4
Foshagite	-6.22	34.46	40.68	Ca4Si3O9(OH)2·0.5H2O
Gaylussite	-7.98	2.90	10.88	CaNa2(CO3)2·5H2O
Glauberite	-16.64	-22.10	-5.47	Na2Ca(SO4)2
Gypsum	-4.61	-10.86	-6.25	CaSO4·2H2O
Gyrolite	-2.92	13.02	15.94	Ca2Si3O7(OH)2·1.5H2O
H2(g)	-18.94	-21.75	-2.81	H2
H2O(g)	1.21	-0.00	-1.21	H2O
Halite	-4.54	-3.30	1.24	NaCl
Hatburite	-15.01	29.35	44.36	Ca3SiO5
HCl(g)	-9.36	-8.47	0.89	HCl
Hexahydrite	-8.91	-10.97	-2.07	MgSO4·6H2O
Hillebrandite	-4.42	18.63	23.05	Ca2SiO3(OH)2·0.17H2O
Huntite	9.71	6.24	-3.47	CaMg3(CO3)4
Hydroboracite	-15.55	4.87	20.42	MgCaB6O11·6H2O
Hydromagnesite	7.52	16.74	9.22	Mg5(CO3)4(OH)2·4H2O
Hydrophilite	-11.04	-6.22	4.82	CaCl2
Ice	-0.88	-0.00	0.88	H2O
K	-38.89	6.55	45.44	K
K(g)	-43.84	6.55	50.39	K
K2CO3·1.5H2O	-14.90	-1.61	13.29	K2CO3·1.5H2O
K2O	-48.95	7.47	56.42	K2O
K3H(SO4)2	-28.34	-31.96	-3.62	K3H(SO4)2
K8H4(CO3)6·3H2O	-52.14	-24.60	27.54	K8H4(CO3)6·3H2O
Kainite	-15.23	-15.71	-0.48	KMgClSO4·3H2O
Kalclinite	-5.63	-5.34	0.28	KHCO3
Kieserite	-10.65	-10.97	-0.32	MgSO4·H2O
KMgCl3	-22.00	-11.06	10.94	KMgCl3
KMgCl3·2H2O	-18.94	-11.07	7.88	KMgCl3·2H2O
KNaCO3·6H2O	-10.10	-0.18	9.92	KNaCO3·6H2O
Lansfordite	-3.03	1.53	4.56	MgCO3·5H2O
Larnite	-4.35	18.63	22.99	Ca2SiO4
Leonite	-20.75	-25.08	-4.34	K2Mg(SO4)2·4H2O
Lime	-9.21	10.72	19.93	CaO
Magnesite	2.76	1.53	-1.23	MgCO3
Mercallite	-16.41	-17.85	-1.44	KHSO4
Merwinite	-2.10	37.16	39.26	MgCa3(SiO4)2
Mg	-57.61	16.23	73.84	Mg
Mg(g)	-67.91	16.23	84.15	Mg
Mg1.25SO4(OH)0.5·0.5H2O	-5.68	-8.32	-2.63	Mg1.25SO4(OH)0.5·0.5H2O
Mg1.5SO4(OH)	-5.16	-5.66	-0.51	Mg1.5SO4(OH)
MgCl2·2H2O	-11.75	-6.33	5.42	MgCl2·2H2O
MgCl2·4H2O	-9.61	-6.33	3.28	MgCl2·4H2O
MgCl2·H2O	-13.23	-6.33	6.90	MgCl2·H2O
MgOHCl	-5.35	2.14	7.49	MgOHCl
MgSO4	-8.28	-10.97	-2.69	MgSO4
Mirabilite	-17.66	-11.25	6.41	Na2SO4·10H2O
Misenite	-110.12	-121.20	-11.08	K8H6(SO4)7
Monohydrocalcite	0.33	1.64	1.31	CaCO3·H2O
Monticellite	2.26	18.53	16.27	CaMgSiO4
Na	-34.78	7.98	42.76	Na
Na(g)	-41.42	7.98	49.40	Na
Na2CO3	-7.02	1.26	8.28	Na2CO3
Na2CO3·7H2O	-12.92	1.26	14.18	Na2CO3·7H2O
Na2O	-34.71	10.34	45.06	Na2O
Na2SiO3	-9.17	7.53	16.71	Na2SiO3
Na3H(SO4)2	-26.76	-27.65	-0.89	Na3H(SO4)2
Na4Ca(SO4)3·2H2O	-27.34	-33.35	-6.01	Na4Ca(SO4)3·2H2O
Na4SiO4	-31.79	17.87	49.67	Na4SiO4
Na6Si2O7	-45.66	25.41	71.07	Na6Si2O7
Nahcolite	-4.51	-3.91	0.60	NaHCO3
Natron	-12.32	1.25	13.58	Na2CO3·10H2O
Natrosilite	-9.28	4.73	14.01	Na2Si2O5
Nesquehonite	-2.73	1.53	4.26	MgCO3·3H2O
O2(g)	-8.37	-11.24	-2.87	O2
Okenite	-3.83	5.11	8.93	CaSi2O4(OH)2·H2O
Oxychloride-Mg	-12.69	12.75	25.43	Mg2Cl(OH)3·4H2O
Pentahydrite	-9.30	-10.97	-1.67	MgSO4·5H2O
Periclase	-1.03	10.61	11.64	MgO
Picromerite	-20.31	-25.09	-4.78	K2Mg(SO4)2·6H2O
Pirssonite	-8.31	2.90	11.21	Na2Ca(CO3)2·2H2O
Polyhalite	-32.38	-46.81	-14.43	K2MgCa2(SO4)4·2H2O
Portlandite	-3.48	10.72	14.20	Ca(OH)2
Pseudowollastonite	-0.26	7.91	8.17	CaSiO3
Quartz	-0.36	-2.81	-2.45	SiO2
Rankinite	-4.34	26.55	30.89	Ca3Si2O7
Sellaite	-3.13	-14.75	-11.62	MgF2
Sepiolite	7.99	25.60	17.61	Mg4Si6O15(OH)2·6H2O
Si	-83.00	8.44	91.43	Si
Si(g)	-124.99	8.44	133.42	Si
SiF4(g)	-33.25	-53.52	-20.28	SiF4
SiO2(am)	-0.98	-2.81	-1.83	SiO2
Starkeyite	-9.75	-10.97	-1.23	MgSO4·4H2O
Sylvite	-5.97	-4.73	1.23	KCl
Syngenite	-17.32	-24.97	-7.66	K2Ca(SO4)2·H2O
Tachyhydrite	-35.35	-18.89	16.46	Mg2CaCl6·12H2O
Talc	11.25	20.61	9.36	Mg3Si4O10(OH)2
Thenardite	-9.51	-11.24	-1.73	Na2SO4
Thermonatrite	-7.81	1.26	9.07	Na2CO3·H2O
Tobermorite-11A	-6.88	36.76	43.64	Ca5Si6H11O22.5
Tobermorite-14A	-9.92	36.75	46.67	Ca5Si6H21O27.5
Tobermorite-9A	-7.28	36.76	44.04	Ca5Si6H6O20
Tremolite	21.69	52.05	30.36	Ca2Mg5Si8O22(OH)2
Tridymite	-0.68	-2.81	-2.13	SiO2
Trona-K	-16.99	-5.52	11.48	K2NaH(CO3)2·2H2O
Wollastonite	-0.21	7.91	8.12	CaSiO3
Xonotlite	-11.34	47.48	58.82	Ca6Si6O17(OH)2

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

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. UW-8B
Using pure phase assemblage 1. Reservoir

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

Phase	SI	log IAP	log K(T, P)	Moles in assemblage		
				Initial	Final	Delta
Albite	-0.00	-2.55	-2.55	1.711e+01	1.710e+01	-6.807e-03
Alunite	-15.34	-35.14	-19.79	1.910e+00	0	-1.910e+00
Anhydrite	0.00	-7.29	-7.29	0.000e+00	3.820e+00	3.820e+00
Ankerite	-1.28	-4.88	-3.59	0.000e+00	0	0.000e+00
Anorthite	-0.00	4.84	4.84	1.907e+01	1.382e+01	-5.245e+00
CO2(g)	-2.30	-4.50	-2.20	1.400e+00	0	-1.400e+00
Calcite	-0.00	-0.59	-0.59	0.000e+00	1.430e+00	1.430e+00
Corundum	0.00	-1.50	-1.50	6.560e+00	1.678e+01	1.022e+01
Dawsonite	-6.45	-7.03	-0.58	0.000e+00	0	0.000e+00
Dolomite	-1.77	-4.55	-2.78	0.000e+00	0	0.000e+00
Enstatite	-0.00	5.43	5.43	2.844e+01	2.845e+01	5.203e-03
Fluorapatite	-0.00	-37.50	-37.50	2.700e-01	2.700e-01	-1.043e-12
Gypsum	-1.04	-7.29	-6.25	0.000e+00	0	0.000e+00
Ilmenite	-0.00	0.96	0.96	1.090e+00	1.090e+00	-4.304e-07
K-Feldspar	-0.00	-3.91	-3.91	1.583e+01	1.774e+01	1.909e+00
Kaolinite	-1.58	-6.40	-4.83	3.060e+00	0	-3.060e+00
Magnesite	-2.73	-3.96	-1.23	0.000e+00	0	0.000e+00
Quartz	0.00	-2.45	-2.45	6.909e+01	7.998e+01	1.089e+01
Siderite	-1.39	-4.43	-3.03	0.000e+00	0	0.000e+00
Zircon	-0.00	-12.14	-12.14	1.000e-02	1.000e-02	-1.900e-11

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

Elements	Molality	Moles
Al	1.846e-05	2.240e-05
B	1.508e-03	1.830e-03
C	6.772e-05	8.218e-05
Ca	2.378e-03	2.886e-03
Cl	2.540e-02	3.082e-02
F	2.614e-06	3.172e-06
Fe	3.547e-07	4.304e-07
K	1.418e-03	1.721e-03
Mg	2.940e-06	3.567e-06
Na	3.246e-02	3.939e-02
P	2.578e-12	3.129e-12
S	3.495e-04	4.242e-04
Si	3.693e-03	4.482e-03
Ti	3.547e-07	4.304e-07
Zr	1.566e-11	1.900e-11

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

pH = 7.166 Charge balance
pe = -1.443 Adjusted to redox equilibrium
Density (g/cm³) = 0.88322
Volume (L) = 1.37694
Activity of water = 0.999
Ionic strength (mol/kgw) = 3.386e-02
Mass of water (kg) = 1.214e+00
Total alkalinity (eq/kg) = 4.141e-04
Total CO2 (mol/kg) = 6.772e-05
Temperature (°C) = 200.00
Pressure (atm) = 249.00
Electrical balance (eq) = 1.479e-02
Percent error, 100*(Cat-|An|)/(|Cat+|An|) = 19.33
Iterations = 17
Total H = 1.347676e+02
Total O = 6.739764e+01

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

Phase	SI**	log IAP	log K(473 K, 249 atm)
Al	-63.90	22.91	86.81
Al(g)	-93.34	22.91	116.25
Al2(SO4)3	-46.23	-57.11	-10.89
Al2(SO4)3:6H2O	-40.07	-57.11	-17.04
Albite	-0.00	-2.55	-2.55
Albite_high	-0.61	-2.55	-1.94
Albite_low	-0.00	-2.55	-2.55
AlF3	-17.55	-39.54	-21.99
Alum-K	-26.28	-33.64	-7.36
Alunite	-15.34	-35.14	-19.79
Amesite-14A	2.21	23.59	21.38
Analcime	-0.30	-0.39	-0.09
Analcime-dehy	-3.93	-0.39	3.54
Anatase	2.00	-6.45	-8.45
Andalusite	-3.24	-3.95	-0.72
Andradite	17.76	28.65	10.89
Anhydrite	0.00	-7.29	-7.29
Ankerite	-1.28	-4.88	-3.59
Annite	7.98	18.32	10.34
Anorthite	-0.00	4.84	4.84

Antarcticite	-10.30	-6.54	3.75	CaCl ₂ ·6H ₂ O
Anthophyllite	4.38	35.53	31.15	Mg ₇ Si ₈ O ₂₂ (OH) ₂
Antigorite	50.49	294.72	244.23	Mg ₄₈ Si ₃₄₀ 85(OH) ₆₂
Aphthitalite	-15.06	-18.95	-3.89	NaK ₃ (SO ₄) ₂
Aragonite	-0.15	-0.59	-0.44	CaCO ₃
Arcanite	-8.25	-10.16	-1.90	K ₂ SO ₄
Artinite	-7.02	3.91	10.93	Mg ₂ CO ₃ (OH) ₂ ·3H ₂ O
B	-46.51	20.83	67.34	B
B(g)	-101.24	20.83	122.07	B
B ₂ O ₃	-9.33	-5.67	3.66	B ₂ O ₃
Baddeleyite	-2.04	-9.69	-7.65	ZrO ₂
Bassanite	-0.66	-7.29	-6.63	CaSO ₄ ·0.5H ₂ O
Beidellite-Ca	-0.90	-8.89	-7.99	Ca _{1.165} Al _{12.33} Si _{13.67} O ₁₀ (OH) ₂
Beidellite-H	-2.33	-10.74	-8.41	H _{3.3} Al _{12.33} Si _{13.67} O ₁₀ (OH) ₂
Beidellite-K	-1.86	-9.36	-7.50	K _{3.3} Al _{12.33} Si _{13.67} O ₁₀ (OH) ₂
Beidellite-Mg	-1.24	-9.44	-8.21	Mg _{1.65} Al _{12.33} Si _{13.67} O ₁₀ (OH) ₂
Beidellite-Na	-1.48	-8.91	-7.43	Na _{1.33} Al _{12.33} Si _{13.67} O ₁₀ (OH) ₂
Berlinite	-11.97	-27.68	-15.72	AlPO ₄
BF ₃ (g)	-30.85	-41.62	-10.77	BF ₃
Bischofite	-13.97	-9.91	4.05	MgCl ₂ ·6H ₂ O
Bloedite	-15.39	-18.09	-2.70	Na ₂ Mg(SO ₄) ₂ ·4H ₂ O
Boehmite	-0.58	-0.75	-0.17	AlO ₂ H
Borax	-17.58	-0.23	17.35	Na ₂ (B ₄ O ₅ (OH) ₄)·8H ₂ O
Boric acid	-3.87	-2.83	1.03	B(OH) ₃
Brucite	-1.33	7.88	9.20	Mg(OH) ₂
Brushite	-22.12	-15.69	6.44	CaHPO ₄ ·2H ₂ O
Burkeite	-25.07	-15.58	9.49	Na ₆ CO ₃ (SO ₄) ₂
C	-17.58	19.71	37.29	C
C(g)	-88.80	19.71	108.51	C
Ca	-59.03	27.02	86.05	Ca
Ca(g)	-72.86	27.02	99.88	Ca
Ca-Al Pyroxene	-3.74	7.29	11.04	CaAl ₂ SiO ₆
Ca ₂ Al ₂ O ₅ ·8H ₂ O	-37.85	20.98	58.83	Ca ₂ Al ₂ O ₅ ·8H ₂ O
Ca ₂ Cl ₂ (OH) ₂ ·2H ₂ O	-21.42	4.70	26.12	Ca ₂ Cl ₂ (OH) ₂ ·2H ₂ O
Ca ₃ Al ₂ O ₆	-26.80	32.23	59.03	Ca ₃ Al ₂ O ₆
Ca ₄ Al ₂ Fe ₂ O ₁₀	-20.65	45.75	66.39	Ca ₄ Al ₂ Fe ₂ O ₁₀
Ca ₄ Al ₂ O ₇ ·13H ₂ O	-62.65	43.47	106.12	Ca ₄ Al ₂ O ₇ ·13H ₂ O
Ca ₄ Al ₂ O ₇ ·19H ₂ O	-58.74	43.47	102.21	Ca ₄ Al ₂ O ₇ ·19H ₂ O
Ca ₄ Cl ₂ (OH) ₆ ·13H ₂ O	-40.06	27.19	67.25	Ca ₄ Cl ₂ (OH) ₆ ·13H ₂ O
CaAl ₂ O ₄	-7.87	9.74	17.62	CaAl ₂ O ₄
CaAl ₂ O ₄ ·10H ₂ O	-27.46	9.74	37.20	CaAl ₂ O ₄ ·10H ₂ O
CaAl ₄ O ₇	-13.15	8.24	21.39	CaAl ₄ O ₇
Calcite	-0.00	-0.59	-0.59	CaCO ₃
Carnallite	-18.55	-14.62	3.93	KMgCl ₃ ·6H ₂ O
CaSO ₄ ·0.5H ₂ O(beta)	-0.69	-7.29	-6.60	CaSO ₄ ·0.5H ₂ O
CaZrO ₃	98.06	1.56	-96.50	CaZrO ₃
Celadonite	1.21	1.51	0.30	KMgAlSi ₄ O ₁₀ (OH) ₂
CH ₄ (g)	-31.29	-34.03	-2.75	CH ₄
Chalcedony	-0.17	-2.45	-2.28	SiO ₂
Chamosite-7A	3.05	10.87	7.82	Fe ₂ Al ₂ SiO ₅ (OH) ₄
Chloromagnesite	-19.90	-9.91	9.99	MgCl ₂
Chrysotile	2.58	18.73	16.15	Mg ₃ Si ₂ O ₅ (OH) ₄
Cl ₂ (g)	-32.07	-33.56	-1.49	Cl ₂
Clinocllore-14A	5.07	30.52	25.46	Mg ₅ Al ₂ Si ₃ O ₁₀ (OH) ₈
Clinocllore-7A	2.49	30.52	28.03	Mg ₅ Al ₂ Si ₃ O ₁₀ (OH) ₈
Clinoptilolite-Ca	3.63	-18.69	-22.32	Ca _{1.7335} Al _{13.45} Fe _{0.17} Si _{14.5330} 36:10.922H ₂ O
Clinoptilolite-dehy-Ca	-15.74	-18.68	-2.95	Ca _{1.7335} Al _{13.45} Fe _{0.17} Si _{14.5330} 36
Clinoptilolite-dehy-K	-25.90	-23.65	2.25	K _{3.467} Al _{13.45} Fe _{0.17} Si _{14.5330} 36
Clinoptilolite-dehy-Na	-21.60	-18.92	2.68	Na _{3.467} Al _{13.45} Fe _{0.17} Si _{14.5330} 36
Clinoptilolite-hy-Ca	3.05	-18.69	-21.74	Ca _{1.7335} Al _{13.45} Fe _{0.17} Si _{14.5330} 36:11.645H ₂ O
Clinoptilolite-hy-K	-4.38	-23.65	-19.27	K _{3.467} Al _{13.45} Fe _{0.17} Si _{14.5330} 36:7.499H ₂ O
Clinoptilolite-hy-Na	-2.31	-18.93	-16.62	Na _{3.467} Al _{13.45} Fe _{0.17} Si _{14.5330} 36:10.877H ₂ O
Clinoptilolite-K	-6.81	-23.66	-16.85	K _{3.467} Al _{13.45} Fe _{0.17} Si _{14.5330} 36:10.922H ₂ O
Clinoptilolite-Na	-2.34	-18.93	-16.59	Na _{3.467} Al _{13.45} Fe _{0.17} Si _{14.5330} 36:10.922H ₂ O
Clinozoisite	2.40	12.89	10.48	Ca ₂ Al ₃ Si ₃ O ₁₂ (OH)
CO(g)	-15.04	-17.84	-2.80	CO
CO ₂ (g)	-2.30	-4.50	-2.20	CO ₂
Coesite	-0.53	-2.45	-1.92	SiO ₂
Colemanite	-16.14	5.49	21.63	Ca ₂ B ₆ O ₁₁ ·5H ₂ O
Cordierite_anhyd	-6.70	0.50	7.19	Mg ₂ Al ₄ Si ₅ O ₁₈
Cordierite_hydr	-5.43	0.49	5.92	Mg ₂ Al ₄ Si ₅ O ₁₈ ·H ₂ O
Corundum	0.00	-1.50	-1.50	Al ₂ O ₃
Cristobalite(alpha)	-0.31	-2.45	-2.14	SiO ₂
Cristobalite(beta)	-0.51	-2.45	-1.94	SiO ₂
Cronstedtite-7A	15.83	14.63	-1.19	Fe ₂ Fe ₂ SiO ₅ (OH) ₄
Daphnite-14A	12.22	28.20	15.97	Fe ₅ Al ₁ Al ₃ Si ₃ O ₁₀ (OH) ₈
Daphnite-7A	9.73	28.20	18.47	Fe ₅ Al ₁ Al ₃ Si ₃ O ₁₀ (OH) ₈
Dawsonite	-6.45	-7.03	-0.58	NaAlCO ₃ (OH) ₂
Diaspore	-0.39	-0.75	-0.36	Al ₂ O ₃
Dicalcium_silicate	-2.28	20.04	22.32	Ca ₂ SiO ₄
Diopside	3.13	14.22	11.09	CaMgSi ₂ O ₆
Dolomite	-1.77	-4.55	-2.78	CaMg(CO ₃) ₂
Dolomite-dis	-2.52	-4.55	-2.03	CaMg(CO ₃) ₂
Dolomite-ord	-1.76	-4.55	-2.79	CaMg(CO ₃) ₂
Enstatite	-0.00	5.43	5.43	MgSiO ₃
Epidote	10.04	14.77	4.73	Ca ₂ FeAl ₂ Si ₃ O ₁₂ OH
Epidote-ord	10.01	14.77	4.76	FeCa ₂ Al ₂ (OH)(SiO ₄) ₃
Epsomite	-8.30	-10.66	-2.36	MgSO ₄ ·7H ₂ O
Ettringite	-33.16	10.35	43.51	Ca ₆ Al ₂ (SO ₄) ₃ (OH) ₁₂ ·26H ₂ O
F ₂ (g)	-71.18	-41.63	29.55	F ₂
Fayalite	3.86	12.37	8.51	Fe ₂ SiO ₄
Fe	-11.29	23.19	34.47	Fe
Fe(OH) ₂	-0.29	7.41	7.70	Fe(OH) ₂
Fe(OH) ₃	1.19	1.13	-0.06	Fe(OH) ₃
Fe ₂ (SO ₄) ₃	-34.01	-53.34	-19.33	Fe ₂ (SO ₄) ₃
FeF ₂	-11.22	-18.45	-7.23	FeF ₂
FeF ₃	-15.37	-37.66	-22.29	FeF ₃
FeO	0.84	7.41	6.57	FeO
Ferrite-Ca	10.16	13.51	3.35	CaFe ₂ O ₄
Ferrite-Dicalcium	-0.16	24.76	24.92	Ca ₂ Fe ₂ O ₅
Ferrite-Mg	8.26	10.14	1.88	MgFe ₂ O ₄
Ferrosillite	1.93	4.96	3.03	FeSiO ₃
FeSO ₄	-7.30	-11.13	-3.83	FeSO ₄
Fluorapatite	-0.00	-37.50	-37.50	Ca ₅ (PO ₄) ₃ F
Fluorite	-3.83	-14.61	-10.78	CaF ₂
Forsterite	-0.72	13.30	14.02	Mg ₂ SiO ₄
Foshagite	-3.04	37.63	40.68	Ca ₄ Si ₃ O ₉ (OH) ₂ ·0.5H ₂ O
Gaylussite	-12.20	-1.32	10.88	CaNa ₂ (CO ₃) ₂ ·5H ₂ O

Gehlenite	-4.44	18.54	22.98	Ca2Al2SiO7
Gibbsite	-1.01	-0.75	0.26	Al(OH)3
Gismondine	-31.07	9.68	40.75	Ca2Al4Si4O16·9H2O
Glauberite	-9.25	-14.72	-5.47	Na2Ca(SO4)2
Goethite	4.64	1.13	-3.51	FeOOH
Greenalite	6.63	17.33	10.70	Fe3Si2O5(OH)4
Grossular	3.78	24.88	21.10	Ca3Al2(SiO4)3
Gypsum	-1.04	-7.29	-6.25	CaSO4·2H2O
Gyrolite	-0.80	15.14	15.94	Ca2Si3O7(OH)2·1.5H2O
H2(g)	-8.79	-11.59	-2.81	H2
H2O(g)	1.21	-0.00	-1.21	H2O
H2S(g)	-26.54	-34.82	-8.28	H2S
Halite	-4.58	-3.34	1.24	NaCl
Hatrurite	-13.08	31.29	44.36	Ca3SiO5
HCl(g)	-9.78	-8.89	0.89	HCl
Hedenbergite	3.54	13.76	10.21	CaFe(SiO3)2
Hematite	11.47	2.26	-9.20	Fe2O3
Hercynite	0.34	5.91	5.57	FeAl2O4
Hexahydrite	-8.60	-10.66	-2.07	MgSO4·6H2O
Hillebrandite	-3.01	20.04	23.05	Ca2SiO3(OH)2·0.17H2O
Huntite	-9.00	-12.47	-3.47	CaMg3(CO3)4
Hydroboracite	-18.30	2.12	20.42	MgCaB6O11·6H2O
Hydromagnesite	-17.19	-7.97	9.22	Mg5(CO3)4(OH)2·4H2O
Hydrophilite	-11.36	-6.54	4.82	CaCl2
Hydroxylapatite	-3.17	-24.57	-21.39	Ca5(OH)(PO4)3
Ice	-0.88	-0.00	0.88	H2O
Illite	-0.78	-5.82	-5.04	K0.6Mg0.25Al1.8Al0.5Si3.5O10(OH)2
Ilmenite	-0.00	0.96	0.96	FeTiO3
Jadeite	-1.64	-0.10	1.55	NaAl(SiO3)2
Jarosite	-5.48	-29.49	-24.00	KFe3(SO4)2(OH)6
Jarosite-Na	-22.33	-28.12	-5.79	NaFe3(SO4)2(OH)6
K	-33.36	12.08	45.44	K
K(g)	-38.31	12.08	50.39	K
K-Feldspar	-0.00	-3.91	-3.91	KAlSi3O8
K2CO3·1.5H2O	-16.75	-3.46	13.29	K2CO3·1.5H2O
K2O	-48.04	8.38	56.42	K2O
K3H(SO4)2	-20.88	-24.50	-3.62	K3H(SO4)2
K8H4(CO3)6·3H2O	-65.03	-37.50	27.54	K8H4(CO3)6·3H2O
Kainite	-14.88	-15.36	-0.48	KMgClSO4·3H2O
KAl(SO4)2	-24.10	-33.63	-9.53	KAl(SO4)2
Kalicanite	-7.93	-7.65	0.28	KHCO3
Kalsilite	-1.93	0.99	2.92	KAlSiO4
Kaolinite	-1.58	-6.40	-4.83	Al2Si2O5(OH)4
Katoite	-46.03	32.23	78.26	Ca3Al2H12O12
Kieserite	-10.34	-10.66	-0.32	MgSO4·H2O
KMgCl3	-25.55	-14.61	10.94	KMgCl3
KMgCl3·2H2O	-22.49	-14.61	7.88	KMgCl3·2H2O
KNaCO3·6H2O	-12.01	-2.09	9.92	KNaCO3·6H2O
Kyanite	-3.24	-3.95	-0.71	Al2SiO5
Lansfordite	-8.52	-3.96	4.56	MgCO3·5H2O
Larnite	-2.94	20.04	22.99	Ca2SiO4
Laumontite	1.20	-0.06	-1.26	CaAl2Si4O12·4H2O
Lawrencite	-12.29	-10.38	1.92	FeCl2
Lawsonite	0.39	4.84	4.45	CaAl2Si2O7(OH)2·H2O
Leonite	-16.48	-20.82	-4.34	K2Mg(SO4)2·4H2O
Lime	-8.68	11.25	19.93	CaO
Magnesite	-2.73	-3.96	-1.23	MgCO3
Magnetite	14.26	9.68	-4.59	Fe3O4
Margarite	-1.11	3.34	4.45	CaAl4Si2O10(OH)2
Maximum Microcline	0.02	-3.91	-3.93	KAlSi3O8
Mayenite	-105.70	124.43	230.13	Ca12Al14O33
Melanterite	-8.51	-11.13	-2.62	FeSO4·7H2O
Mercallite	-12.91	-14.35	-1.44	KHSO4
Merwinite	-2.55	36.71	39.26	MgCa3(SiO4)2
Mesolite	2.40	2.27	-0.13	Na.676Ca.657Al1.99Si3.01O10·2.647H2O
Mg	-50.19	23.65	73.84	Mg
Mg(g)	-60.50	23.65	84.15	Mg
Mg1.25SO4(OH)0.5·0.5H2O	-6.06	-8.69	-2.63	Mg1.25SO4(OH)0.5·0.5H2O
Mg1.5SO4(OH)	-6.21	-6.72	-0.51	Mg1.5SO4(OH)
MgCl2·2H2O	-15.33	-9.91	5.42	MgCl2·2H2O
MgCl2·4H2O	-13.19	-9.91	3.28	MgCl2·4H2O
MgCl2·H2O	-16.81	-9.91	6.90	MgCl2·H2O
MgOHCl	-8.51	-1.02	7.49	MgOHCl
MgSO4	-7.97	-10.66	-2.69	MgSO4
Minnesotaite	7.80	12.43	4.63	Fe3Si4O10(OH)2
Mirabilite	-13.84	-7.43	6.41	Na2SO4·10H2O
Misenite	-85.15	-96.23	-11.08	K8H6(SO4)7
Molysite	-26.29	-25.55	0.74	FeCl3
Monohydrocalcite	-1.90	-0.59	1.31	CaCO3·H2O
Monticellite	0.40	16.67	16.27	CaMgSiO4
Montmor-Ca	0.38	-6.60	-6.98	Ca.165Mg.33Al1.67Si4O10(OH)2
Montmor-K	-0.47	-7.07	-6.60	K.33Mg.33Al1.67Si4O10(OH)2
Montmor-Mg	0.07	-7.16	-7.23	Mg.495Al1.67Si4O10(OH)2
Montmor-Na	-0.16	-6.62	-6.46	Na.33Mg.33Al1.67Si4O10(OH)2
Mordenite	-0.52	-7.84	-7.33	Ca.2895Na.361Al.94Si5.06O12·3.468H2O
Mordenite-dehy	-8.80	-7.84	0.96	Ca.2895Na.361Al.94Si5.06O12
Muscovite	-0.39	-5.41	-5.02	KAl3Si3O10(OH)2
Na	-29.32	13.44	42.76	Na
Na(g)	-35.96	13.44	49.40	Na
Na2CO3	-9.01	-0.73	8.28	Na2CO3
Na2CO3·7H2O	-14.91	-0.73	14.18	Na2CO3·7H2O
Na2O	-33.95	11.11	45.06	Na2O
Na2SiO3	-8.05	8.66	16.71	Na2SiO3
Na3H(SO4)2	-19.52	-20.41	-0.89	Na3H(SO4)2
Na4Ca(SO4)3·2H2O	-16.14	-22.15	-6.01	Na4Ca(SO4)3·2H2O
Na4SiO4	-29.90	19.77	49.67	Na4SiO4
Na6Si2O7	-42.64	28.43	71.07	Na6Si2O7
NaFeO2	-2.82	6.69	9.50	NaFeO2
Nahcolite	-6.88	-6.28	0.60	NaHCO3
Natrolite	-2.17	2.25	4.42	Na2Al2Si3O10·2H2O
Natron	-14.31	-0.73	13.58	Na2CO3·10H2O
Natrosilite	-7.80	6.21	14.01	Na2Si2O5
Nepheeline	-1.88	2.35	4.24	NaAlSiO4
Nesquehonite	-8.23	-3.96	4.26	MgCO3·3H2O
Nontronite-Ca	12.08	-5.12	-17.20	Ca.165Fe2Al.33Si3.67H2O12
Nontronite-H	10.68	-6.98	-17.65	H.33Fe2Al.33Si3.67H2O12
Nontronite-K	11.12	-5.59	-16.71	K.33Fe2Al.33Si3.67H2O12
Nontronite-Mg	11.74	-5.68	-17.41	Mg.165Fe2Al.33Si3.67H2O12

Nontronite-Na	11.49	-5.14	-16.64	Na.33Fe2Al.33Si3.67H2O12
O2 (g)	-28.68	-31.55	-2.87	O2
Okenite	-2.59	6.35	8.93	CaSi2O4 (OH) 2:2H2O
Oxychloride-Mg	-18.58	6.86	25.43	Mg2Cl (OH) 3:4H2O
P	-61.80	12.50	74.31	P
Paragonite	-1.07	-4.05	-2.98	NaAl3Si3O10 (OH) 2
Pargasite	2.08	42.59	40.51	NaCa2Al3Mg4Si6O22 (OH) 2
Pentahydrate	-8.99	-10.66	-1.67	MgSO4:5H2O
Periclase	-3.77	7.88	11.64	MgO
Phlogopite	4.29	19.72	15.42	KAlMg3Si3O10 (OH) 2
Picromerite	-16.04	-20.82	-4.78	K2Mg (SO4) 2:6H2O
Pirssonite	-12.53	-1.32	11.21	Na2Ca (CO3) 2:2H2O
Polyhalite	-20.97	-35.40	-14.43	K2MgCa2 (SO4) 4:2H2O
Portlandite	-2.95	11.25	14.20	Ca (OH) 2
Prehnite	3.59	13.64	10.05	CaAl2Si3O10 (OH) 2
Pseudowollastonite	0.62	8.80	8.17	CaSiO3
Pyrite	-38.81	-58.15	-19.35	FeS2
Pyrophyllite	-2.04	-11.30	-9.26	Al2Si4O10 (OH) 2
Pyrrhotite	-22.27	-27.41	-5.14	FeS
Quartz	0.00	-2.45	-2.45	SiO2
Rankinite	-2.05	28.84	30.89	Ca3Si2O7
Ripidolite-14A	8.11	29.59	21.48	Mg3Fe2Al2Si3O10 (OH) 8
Ripidolite-7A	5.56	29.59	24.04	Mg3Fe2Al2Si3O10 (OH) 8
Rutile	3.08	-6.45	-9.53	TiO2
S	-22.22	-50.59	-28.38	S
S2 (g)	-50.08	-61.49	-11.41	S2
Sanidine_high	-0.46	-3.91	-3.45	KAlSi3O8
Saponite-Ca	5.54	16.24	10.70	Ca.165Mg3Al.33Si3.67O10 (OH) 2
Saponite-H	4.11	14.39	10.28	H.33Mg3Al.33Si3.67O10 (OH) 2
Saponite-K	4.59	15.77	11.18	K.33Mg3Al.33Si3.67O10 (OH) 2
Saponite-Mg	5.19	15.69	10.50	Mg3.165Al.33Si3.67O10 (OH) 2
Saponite-Na	4.95	16.22	11.27	Na.33Mg3Al.33Si3.67O10 (OH) 2
Scolecite	2.28	2.39	0.11	CaAl2Si3O10:3H2O
Sellaite	-6.36	-17.98	-11.62	MgF2
Sepiolite	-0.81	16.80	17.61	Mg4Si6O15 (OH) 2:6H2O
Si	-62.33	29.10	91.43	Si
Si (g)	-104.33	29.10	133.42	Si
Siderite	-1.39	-4.43	-3.03	FeCO3
SiF4 (g)	-33.89	-54.17	-20.28	SiF4
Sillimanite	-3.40	-3.95	-0.56	Al2SiO5
SiO2 (am)	-0.62	-2.45	-1.83	SiO2
Smectite-high-Fe-Mg	3.25	5.15	1.90	Ca.025Na.1K.2Fe.5Fe.2Mg1.15Al1.25Si3.5H2O12
Smectite-low-Fe-Mg	2.20	1.19	-1.01	Ca.02Na.15K.2Fe.29Fe.16Mg.9Al1.25Si3.75H2O12
SO2 (g)	-17.60	-18.56	-0.96	SO2
Spinel	-4.68	6.37	11.05	Al2MgO4
Starkeyite	-9.44	-10.66	-1.23	MgSO4:4H2O
Stilbite	2.85	-6.11	-8.96	Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O
Strengite	-10.06	-25.80	-15.74	FePO4:2H2O
Sylvite	-5.94	-4.70	1.23	KCl
Syngenite	-9.79	-17.45	-7.66	K2Ca (SO4) 2:2H2O
Tachyhydrite	-42.83	-26.37	16.46	Mg2CaCl6:12H2O
Talc	4.47	13.83	9.36	Mg3Si4O10 (OH) 2
Thenardite	-5.70	-7.43	-1.73	Na2SO4
Thermonatrite	-9.80	-0.73	9.07	Na2CO3:H2O
Ti	-124.31	25.10	149.41	Ti
Ti (g)	-199.36	25.10	224.46	Ti
Ti2O3	-40.34	2.88	43.21	Ti2O3
Ti3O5	-38.57	-3.57	35.00	Ti3O5
TiB2	-245.95	66.76	312.70	TiB2
TiC	-137.17	44.81	181.98	TiC
TiCl2	-79.57	-8.46	71.11	TiCl2
TiCl3	-64.75	-25.24	39.51	TiCl3
TiCl4 (g)	-70.30	-42.02	28.28	TiCl4
TiF4 (am)	-45.95	-58.17	-12.21	TiF4
TiO (alpha)	-51.92	9.33	61.24	TiO
TiO (g)	-136.36	9.33	145.68	TiO
Titanite	-717.29	2.35	719.64	CaTiSiO5
Tobermorite-11A	-2.11	41.53	43.64	Ca5Si6H11O22.5
Tobermorite-14A	-5.15	41.53	46.67	Ca5Si6H12O27.5
Tobermorite-9A	-2.51	41.53	44.04	Ca5Si6H6O20
Tremolite	11.91	42.27	30.36	Ca2Mg5Si8O22 (OH) 2
Tridymite	-0.32	-2.45	-2.13	SiO2
Troilite	-22.20	-27.41	-5.21	FeS
Trona-K	-21.21	-9.74	11.48	K2NaH (CO3) 2:2H2O
Vivianite	-26.46	-31.64	-5.18	Fe3 (PO4) 2:8H2O
Wairakite	0.39	-0.06	-0.45	CaAl2Si4O10 (OH) 4
Whitlockite	-4.46	-20.13	-15.67	Ca3 (PO4) 2
Wollastonite	0.67	8.80	8.12	CaSiO3
Wustite	0.71	6.35	5.64	Fe.947O
Xonotlite	-6.05	52.78	58.82	Ca6Si6O17 (OH) 2
Zircon	-0.00	-12.14	-12.14	ZrSiO4
Zoisite	2.37	12.89	10.52	Ca2Al3 (SiO4) 3OH
Zr	-84.76	21.86	106.62	Zr
Zr (g)	-255.03	21.98	277.02	Zr
ZrB2	-186.59	-83.01	103.58	ZrB2
ZrC	-165.34	41.70	207.03	ZrC
ZrCl	-125.66	5.20	130.86	ZrCl
ZrCl2	-107.84	-11.58	96.26	ZrCl2
ZrCl3	-90.78	-28.36	62.42	ZrCl3
ZrCl4	-73.12	-45.14	27.98	ZrCl4
ZrF4 (beta)	-33.53	-61.28	-27.76	ZrF4
ZrF4 (g)	-204.23	-61.28	142.95	ZrF4
ZrH2	-160.39	37.76	198.15	ZrH2

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

End of simulation.

APPENDIX B

KINETIC MODELING RESULT IN UNGARAN FIELD FOR 4 DAYS (0.01 YEAR) AND 1 YEAR TIME STEP

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\llnl.dat

Reading data base.

LLNL AQUEOUS_MODEL_PARAMETERS
NAMED_EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\llnl.dat
SOLUTION_SPECIES
CO3-2 + 2 H+ = CO2 + H2O
log_k 16.681
delta_h -5.738 kcal
analytical_expression 464.1965 0.09344813 -26986.16 -165.75951 2248628.9
dw 1.92e-9
vm 7.29 0.92 2.07 -1.23 -1.60 # ref. 1 + McBride et al. 2015, JCD 60, 171
2CO2 = (CO2)2 # activity correction for CO2 solubility at high P, T
log_k -1.8
analytical_expression 8.68 -0.0103 -2190
vm 14.58 1.84 4.14 -2.46 -3.20
END

End of simulation.

Reading input data for simulation 2.

PHASES
CO2(g)
CO2 = CO2
log_k -1.468
delta_h -4.776 kcal
analytical_expression 10.5624 -2.3547e-2 -3972.8 0 5.8746e5 1.9194e-5
t_c 304.2 # critical T, K
p_c 72.86 # critical P, atm
omega 0.225 # acentric factor
Ankerite
CaMg0.3Fe0.7(CO3)2 + 2H+ = Ca++ + 0.3Mg++ + 0.7Fe++ + 2HCO3-
log_k 1.54
delta_h 0
analytical_expression -1.8649e+03 -2.9583e-01 1.0468e+05 6.7554e+02 -6.0514e+06
END

End of simulation.

Reading input data for simulation 3.

SOLUTION 1 UW-8B
temp 200
pH 6.8
pe 4
redox pe
units mg/l
density 1
C(4) 1824
Ca 278
Cl 1088
Mg 126
Na 746
S(6) 0.1
K 47.1
F 0.06
B 19.7
Si 95
water 1 # kg
pressure 249 atm
EQUILIBRIUM_PHASES 1
CO2(g) 2.396 1.4
RATES
Quartz
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_qtz = SI("Quartz")
30 if (M <= 0 and si_qtz < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_qtz > 0) then SA = 1e-05 #nucleation
60 k_acid = 0
70 k_neut = 10^(-13.99)*EXP(-87.60e+03/8.314*(1.0/TK-1.0/298.15))

```

80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_qtz))
190 moles = r * TIME
200 SAVE moles
end
Anorthite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_anort = SI("Anorthite")
30 if (M <= 0 and si_anort < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_anort > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-3.5)*EXP(-16.60e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.411)
70 k_neut = 10^(-9.82)*EXP(-31.50e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_anort))
190 moles = r * TIME
200 SAVE moles
end
Albite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_alb = SI("Albite")
30 if (M <= 0 and si_alb < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_alb > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-10.16)*EXP(-65.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.457)
70 k_neut = 10^(-12.56)*EXP(-69.80e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-15.60)*EXP(-71.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.572)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_alb))
190 moles = r * TIME
200 SAVE moles
end
K-Feldspar
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_kfeld = SI("K-Feldspar")
30 if (M <= 0 and si_kfeld < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_kfeld > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-10.06)*EXP(-51.70e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.500)
70 k_neut = 10^(-12.41)*EXP(-38.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-21.20)*EXP(-94.10e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.823)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_kfeld))
190 moles = r * TIME
200 SAVE moles
end
Corundum
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_cornd = SI("Corundum")
30 if (M <= 0 and si_cornd < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_cornd > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-12.53)*EXP(-47.61e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.150)
70 k_neut = 10^(-15.70)*EXP(-47.61e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-11.75)*EXP(-47.61e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.550)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_cornd))
190 moles = r * TIME
200 SAVE moles
end
Enstatite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_enst = SI("Enstatite")
30 if (M <= 0 and si_enst < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_enst > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-9.02)*EXP(-80.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.600)
70 k_neut = 10^(-12.72)*EXP(-80.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_enst))
190 moles = r * TIME
200 SAVE moles
end
Ilmenite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_ilmen = SI("Ilmenite")
30 if (M <= 0 and si_ilmen < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_ilmen > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-8.35)*EXP(-37.90e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.421)
70 k_neut = 10^(-11.16)*EXP(-37.90e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_ilmen))
190 moles = r * TIME
200 SAVE moles
end
Fluorapatite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_fluorap = SI("Fluorapatite")
30 if (M <= 0 and si_fluorap < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_fluorap > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-3.73)*EXP(-25.00e+04/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.613)
70 k_neut = 10^(-8.00)*EXP(-25.00e+04/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_fluorap))

```

```

190 moles = r * TIME
200 SAVE moles
end
Kaolinite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_kaol = SI("Kaolinite")
30 if (M <= 0 and si_kaol < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_kaol > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-11.31)*EXP(-65.90e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.777)
70 k_neut = 10^(-13.18)*EXP(-22.20e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-17.05)*EXP(-17.90e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.472)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_kaol))
190 moles = r * TIME
200 SAVE moles
end
Alunite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_alun = SI("Alunite")
30 if (M <= 0 and si_alun < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_alun > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-10.65)*EXP(-32.30e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.133)
70 k_neut = 10^(-12.53)*EXP(-39.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-12.53)*EXP(-39.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.194)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_alun))
190 moles = r * TIME
200 SAVE moles
end
Calcite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_calc = SI("Calcite")
30 if (M <= 0 and si_calc < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_calc > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-0.30)*EXP(-14.40e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.000)
70 k_neut = 10^(-5.81)*EXP(-23.50e+03/8.314*(1.0/TK-1.0/298.15))
80 k_carb = 10^(-3.48)*EXP(-35.40e+03/8.314*(1.0/TK-1.0/298.15))*PR_P("CO2(g)")^(1.000)
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_calc))
190 moles = r * TIME
200 SAVE moles
end
Anhydrite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_anhyd = SI("Anhydrite")
30 if (M <= 0 and si_anhyd < 0) then goto 200
40 SA = PARM(1)*M
50 if (M = 0 and si_anhyd > 0) then SA = 1e-05 #nucleation
60 k_acid = 0
70 k_neut = 10^(-3.19)*EXP(-14.30e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_anhyd))
190 moles = r * TIME
200 SAVE moles
end
Gypsum
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_gyps = SI("Gypsum")
30 if (M <= 0 and si_gyps < 0) then goto 200
40 SA = PARM(1)*M
50 if (M = 0 and si_gyps > 0) then SA = 1e-05 #nucleation
60 k_acid = 0
70 k_neut = 10^(-2.79)*EXP(-0.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_gyps))
190 moles = r * TIME
200 SAVE moles
end
KINETICS 1
Quartz
formula SiO2 1
m 69.09
m0 69.09
parms 2.956
tol 1e-08
Anorthite
formula CaAl2(SiO4)2 1
m 19.07
m0 19.07
parms 5.548
tol 1e-08
Albite
formula NaAlSi3O8 1
m 17.11
m0 17.11
parms 5.26
tol 1e-08
K-Feldspar
formula KAlSi3O8 1
m 15.83
m0 15.83
parms 86.282
tol 1e-08
Corundum
formula Al2O3 1
m 6.56
m0 6.56
parms 377.252

```

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tol 1e-08
Enstatite
formula MgSiO3 1
m 28.44
m0 28.44
parms 933.627
tol 1e-08
Ilmenite
formula FeTiO3 1
m 1.09
m0 1.09
parms 31.101
tol 1e-08
Kaolinite
formula Al2Si2O5(OH)4 1
m 3.06
m0 3.06
parms 5163.2
tol 1e-08
Alunite
formula KAl3(OH)6(SO4)2 1
m 1.91
m0 1.91
parms 10769.46
tol 1e-08
Calcite
formula CaCO3 1
m 0
m0 0
parms 15.0135
tol 1e-08
Anhydrite
formula CaSO4 1
m 0
m0 0
parms 16.578
tol 1e-08
steps 3 30 300 3000 30000 300000 3000000 30000000 300000000 3000000000 30000000000 300000000000
cvscode true
KNOBS
convergence_tolerance 1e-10
INCREMENTAL REACTIONS True
USER_GRAPH 1
-headers Time Quartz Anorthite Albite K-Feldspar Corundum Kaolinite Alunite Calcite Anhydrite
-axis_titles "Log10 Time" "Kin" ""
-initial_solutions false
-connect_simulations true
-plot_concentration_vs x
-start
10 GRAPH_X log10(total_time)
20 GRAPH_Y kin("Quartz"), kin("Anorthite"), kin("Albite"), kin("K-Feldspar"), kin("Corundum"), kin("Kaolinite"),
kin("Alunite"), kin("Calcite"), kin("Anhydrite")
-end
-active true
SELECTED OUTPUT 1
file D:\20182 SPRING\Thesis PHREEQC\1. Ungaran - UW-8\kinetics ungaran.sel
reset false
time true
step true
ph true
pe true
totals C(4)
molalities K+ Na+ Ca+2 Mg+2
HCO3- SO4-2 Cl- CO3-2
kinetic_reactants Quartz Anorthite Albite K-feldspar
Corundum Kaolinite Alunite Calcite
Anhydrite

END
-----
Beginning of initial solution calculations.
-----
Initial solution 1. UW-8B
-----Solution composition-----

```

Elements	Molality	Moles
B	1.830e-03	1.830e-03
C(4)	3.003e-02	3.003e-02
Ca	6.966e-03	6.966e-03
Cl	3.082e-02	3.082e-02
F	3.172e-06	3.172e-06
K	1.210e-03	1.210e-03
Mg	5.206e-03	5.206e-03
Na	3.259e-02	3.259e-02
S(6)	1.046e-06	1.046e-06
Si	1.588e-03	1.588e-03

```

-----Description of solution-----
pH = 6.800
pe = 4.000
Density (g/cm³) = 0.88413
Volume (L) = 1.13562
Activity of water = 0.998
Ionic strength (mol/kgw) = 5.105e-02
Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = 1.253e-02
Total CO2 (mol/kg) = 3.003e-02
Temperature (°C) = 200.00
Pressure (atm) = 249.00
Electrical balance (eq) = 1.479e-02
Percent error, 100*(Cat-[An])/(Cat+[An]) = 16.71
Iterations = 8
Total H = 1.110676e+02
Total O = 5.560607e+01
-----Distribution of species-----

```

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm ³ /mol
OH-	5.069e-05	3.690e-05	-4.295	-4.433	-0.138	(0)
H+	2.002e-07	1.585e-07	-6.699	-6.800	-0.101	0.00
H2O	5.553e+01	9.982e-01	1.744	-0.001	0.000	20.44
B(-5)	0.000e+00					
BH4-	0.000e+00	0.000e+00	-119.979	-120.112	-0.134	(0)
B(3)	1.830e-03					
B(OH)3	1.805e-03	1.805e-03	-2.743	-2.743	0.000	(0)
BO2-	2.257e-05	1.660e-05	-4.646	-4.780	-0.134	(0)
CaB(OH)4+	8.809e-07	6.478e-07	-6.055	-6.189	-0.134	(0)
MgB(OH)4+	8.174e-07	6.011e-07	-6.088	-6.221	-0.134	(0)
NaB(OH)4	3.231e-07	3.231e-07	-6.491	-6.491	0.000	(0)
BF2(OH)2-	2.468e-15	1.815e-15	-14.608	-14.741	-0.134	(0)
B2O(OH)5-	5.775e-18	4.246e-18	-17.238	-17.372	-0.134	(0)
BF4-	9.301e-28	6.840e-28	-27.031	-27.165	-0.134	(0)
BF3OH-	5.458e-40	4.013e-40	-39.263	-39.397	-0.134	(0)
C(4)	3.003e-02					
CO2	1.797e-02	1.819e-02	-1.745	-1.740	0.005	52.92
HCO3-	7.132e-03	5.244e-03	-2.147	-2.280	-0.134	(0)
CaHCO3+	2.405e-03	1.769e-03	-2.619	-2.752	-0.134	(0)
MgHCO3+	1.943e-03	1.429e-03	-2.711	-2.845	-0.134	(0)
CaCO3	4.177e-04	4.177e-04	-3.379	-3.379	0.000	(0)
(CO2)2	4.925e-05	4.983e-05	-4.308	-4.303	0.005	105.85
MgCO3	4.622e-05	4.622e-05	-4.335	-4.335	0.000	(0)
NaHCO3	7.513e-06	7.513e-06	-5.124	-5.124	0.000	(0)
CO3-2	3.743e-06	1.118e-06	-5.427	-5.952	-0.525	(0)
NaCO3-	2.407e-10	1.770e-10	-9.619	-9.752	-0.134	(0)
Ca	6.966e-03					
Ca+2	4.004e-03	1.322e-03	-2.397	-2.879	-0.481	(0)
CaHCO3+	2.405e-03	1.769e-03	-2.619	-2.752	-0.134	(0)
CaCO3	4.177e-04	4.177e-04	-3.379	-3.379	0.000	(0)
CaCl+	1.322e-04	9.722e-05	-3.879	-4.012	-0.134	(0)
CaCl2	4.962e-06	4.962e-06	-5.304	-5.304	0.000	(0)
CaB(OH)4+	8.809e-07	6.478e-07	-6.055	-6.189	-0.134	(0)
CaF+	3.933e-07	2.892e-07	-6.405	-6.539	-0.134	(0)
CaSO4	3.911e-08	3.911e-08	-7.408	-7.408	0.000	(0)
CaOH+	1.822e-09	1.340e-09	-8.739	-8.873	-0.134	(0)
Cl(-1)	3.082e-02					
Cl-	2.962e-02	2.133e-02	-1.528	-1.671	-0.142	(0)
NaCl	6.293e-04	6.293e-04	-3.201	-3.201	0.000	(0)
MgCl+	4.180e-04	3.073e-04	-3.379	-3.512	-0.134	(0)
CaCl+	1.322e-04	9.722e-05	-3.879	-4.012	-0.134	(0)
KCl	1.142e-05	1.142e-05	-4.942	-4.942	0.000	(0)
CaCl2	4.962e-06	4.962e-06	-5.304	-5.304	0.000	(0)
HCl	2.768e-09	2.768e-09	-8.558	-8.558	0.000	(0)
Cl(1)	1.014e-18					
HClO	8.234e-19	8.234e-19	-18.084	-18.084	0.000	(0)
ClO-	1.905e-19	1.401e-19	-18.720	-18.854	-0.134	(0)
Cl(3)	3.391e-30					
ClO2-	3.391e-30	2.493e-30	-29.470	-29.603	-0.134	(0)
HClO2	5.842e-34	5.842e-34	-33.233	-33.233	0.000	(0)
Cl(5)	3.473e-32					
ClO3-	3.473e-32	2.529e-32	-31.459	-31.597	-0.138	(0)
Cl(7)	9.443e-38					
ClO4-	9.443e-38	6.875e-38	-37.025	-37.163	-0.138	(0)
F	3.172e-06					
F-	1.812e-06	1.319e-06	-5.742	-5.880	-0.138	(0)
MgF+	9.199e-07	6.764e-07	-6.036	-6.170	-0.134	(0)
CaF+	3.933e-07	2.892e-07	-6.405	-6.539	-0.134	(0)
NaF	3.083e-08	3.083e-08	-7.511	-7.511	0.000	(0)
HF	1.523e-08	1.523e-08	-7.817	-7.817	0.000	(0)
HF2-	8.979e-15	6.603e-15	-14.047	-14.180	-0.134	(0)
BF2(OH)2-	2.468e-15	1.815e-15	-14.608	-14.741	-0.134	(0)
H2F2	2.563e-19	2.563e-19	-18.591	-18.591	0.000	(0)
BF4-	9.301e-28	6.840e-28	-27.031	-27.165	-0.134	(0)
BF3OH-	5.458e-40	4.013e-40	-39.263	-39.397	-0.134	(0)
SiF6-2	1.234e-40	0.000e+00	-39.909	-40.450	-0.541	(0)
H(0)	3.500e-22					
H2	1.750e-22	1.787e-22	-21.757	-21.748	0.009	(0)
K	1.210e-03					
K+	1.198e-03	8.632e-04	-2.921	-3.064	-0.142	(0)
KCl	1.142e-05	1.142e-05	-4.942	-4.942	0.000	(0)
KSO4-	1.027e-09	7.553e-10	-8.988	-9.122	-0.134	(0)
KOH	2.148e-11	2.148e-11	-10.668	-10.668	0.000	(0)
KHSO4	3.872e-14	3.872e-14	-13.412	-13.412	0.000	(0)
Mg	5.206e-03					
Mg+2	2.796e-03	1.031e-03	-2.553	-2.987	-0.433	(0)
MgHCO3+	1.943e-03	1.429e-03	-2.711	-2.845	-0.134	(0)
MgCl+	4.180e-04	3.073e-04	-3.379	-3.512	-0.134	(0)
MgCO3	4.622e-05	4.622e-05	-4.335	-4.335	0.000	(0)
MgSO4	9.671e-07	9.671e-07	-6.015	-6.015	0.000	(0)
MgF+	9.199e-07	6.764e-07	-6.036	-6.170	-0.134	(0)
MgB(OH)4+	8.174e-07	6.011e-07	-6.088	-6.221	-0.134	(0)
Mg4(OH)4+4	5.174e-23	5.324e-25	-22.286	-24.274	-1.988	(0)
Na	3.259e-02					
Na+	3.194e-02	2.349e-02	-1.496	-1.629	-0.134	(0)
NaCl	6.293e-04	6.293e-04	-3.201	-3.201	0.000	(0)
NaHCO3	7.513e-06	7.513e-06	-5.124	-5.124	0.000	(0)
NaHSiO3	5.940e-06	5.940e-06	-5.226	-5.226	0.000	(0)
NaOH	1.019e-06	1.019e-06	-5.992	-5.992	0.000	(0)
NaB(OH)4	3.231e-07	3.231e-07	-6.491	-6.491	0.000	(0)
NaF	3.083e-08	3.083e-08	-7.511	-7.511	0.000	(0)
NaSO4-	2.192e-09	1.612e-09	-8.659	-8.793	-0.134	(0)
NaCO3-	2.407e-10	1.770e-10	-9.619	-9.752	-0.134	(0)
O(0)	1.120e-11					
O2	5.602e-12	5.723e-12	-11.252	-11.242	0.009	(0)
S(6)	1.046e-06					
MgSO4	9.671e-07	9.671e-07	-6.015	-6.015	0.000	(0)
CaSO4	3.911e-08	3.911e-08	-7.408	-7.408	0.000	(0)
SO4-2	3.613e-08	1.039e-08	-7.442	-7.983	-0.541	(0)
NaSO4-	2.192e-09	1.612e-09	-8.659	-8.793	-0.134	(0)
KSO4-	1.027e-09	7.553e-10	-8.988	-9.122	-0.134	(0)
HSO4-	6.664e-11	4.900e-11	-10.176	-10.310	-0.134	(0)
KHSO4	3.872e-14	3.872e-14	-13.412	-13.412	0.000	(0)
H2SO4	2.487e-23	2.487e-23	-22.604	-22.604	0.000	(0)
Si	1.588e-03					

SiO2	1.560e-03	1.560e-03	-2.807	-2.807	0.000	(0)
HSiO3-	2.215e-05	1.629e-05	-4.655	-4.788	-0.134	(0)
NaHSiO3	5.940e-06	5.940e-06	-5.226	-5.226	0.000	(0)
H6(H2SiO4)4-2	5.264e-11	1.514e-11	-10.279	-10.820	-0.541	(0)
H2SiO4-2	3.064e-12	8.810e-13	-11.514	-12.055	-0.541	(0)
H4(H2SiO4)4-4	4.491e-18	3.020e-20	-17.348	-19.520	-2.172	(0)
SiF6-2	1.234e-40	0.000e+00	-39.909	-40.450	-0.541	(0)

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

Phase	SI**	log IAP	log K(473 K, 249 atm)	
Afwillite	-11.89	26.54	38.43	Ca3Si2O4 (OH) 6
Akermanite	1.13	26.44	25.31	Ca2MgSi2O7
Anhydrite	-3.57	-10.86	-7.29	CaSO4
Antarcticite	-9.98	-6.23	3.75	CaCl2:6H2O
Anthophyllite	20.68	51.83	31.15	Mg7Si8O22 (OH) 2
Antigorite	169.71	413.94	244.23	Mg48Si34O85 (OH) 62
Aphthitalite	-22.90	-26.79	-3.89	NaK3 (SO4) 2
Aragonite	2.08	1.64	-0.44	CaCO3
Arcanite	-12.21	-14.11	-1.90	K2SO4
Artinite	1.21	12.14	10.93	Mg2CO3 (OH) 2:3H2O
B	-61.65	5.69	67.34	B
B(g)	-116.38	5.69	122.07	B
B2O3	-9.15	-5.48	3.66	B2O3
Bassanite	-4.23	-10.86	-6.63	CaSO4:0.5H2O
BF3(g)	-30.01	-40.78	-10.77	BF3
Bischofite	-10.39	-6.33	4.05	MgCl2:6H2O
Bloedite	-19.51	-22.22	-2.70	Na2Mg (SO4) 2:4H2O
Borax	-17.99	-0.64	17.35	Na2 (B4O5 (OH) 4) :8H2O
Boric_acid	-3.78	-2.74	1.03	B (OH) 3
Brucite	1.41	10.61	9.20	Mg (OH) 2
Burkeite	-30.71	-21.22	9.49	Na6CO3 (SO4) 2
C	-35.13	2.16	37.29	C
C(g)	-106.35	2.16	108.51	C
Ca	-69.71	16.34	86.05	Ca
Ca(g)	-83.54	16.34	99.88	Ca
Ca2Cl2 (OH) 2:H2O	-21.62	4.50	26.12	Ca2Cl2 (OH) 2:H2O
Ca4Cl2 (OH) 6:13H2O	-41.32	25.93	67.25	Ca4Cl2 (OH) 6:13H2O
Calcite	2.23	1.64	-0.59	CaCO3
Carnallite	-15.00	-11.07	3.93	KMgCl3:6H2O
CaSO4:0.5H2O (beta)	-4.26	-10.86	-6.60	CaSO4:0.5H2O
Chalcedony	-0.53	-2.81	-2.28	SiO2
Chloromagnesite	-16.31	-6.33	9.99	MgCl2
Chrysotile	10.08	26.22	16.15	Mg3Si2O5 (OH) 4
Cl2(g)	-21.07	-22.56	-1.49	Cl2
CO2(g)	0.46	-1.74	-2.20	CO2
Coesite	-0.89	-2.81	-1.92	SiO2
Colemanite	-16.65	4.98	21.63	Ca2B6O11:5H2O
Cristobalite (alpha)	-0.66	-2.81	-2.14	SiO2
Cristobalite (beta)	-0.87	-2.81	-1.94	SiO2
Dicalcium silicate	-3.69	18.63	22.32	Ca2SiO4
Diopside	4.63	15.72	11.09	CaMgSi2O6
Dolomite	5.95	3.17	-2.78	CaMg (CO3) 2
Dolomite-dis	5.21	3.17	-2.03	CaMg (CO3) 2
Dolomite-ord	5.96	3.17	-2.79	CaMg (CO3) 2
Enstatite	2.38	7.81	5.43	MgSiO3
Epsomite	-8.62	-10.98	-2.36	MgSO4:7H2O
F2(g)	-60.53	-30.98	29.55	F2
Fluorite	-3.86	-14.64	-10.78	CaF2
Forsterite	4.40	18.42	14.02	Mg2SiO4
Foshagite	-6.22	34.46	40.68	Ca4Si3O9 (OH) 2:0.5H2O
Gaylussite	-7.98	2.90	10.88	CaNa2 (CO3) 2:5H2O
Glauberite	-16.64	-22.10	-5.47	Na2Ca (SO4) 2
Gypsum	-4.61	-10.86	-6.25	CaSO4:2H2O
Gyrolite	-2.92	13.02	15.94	Ca2Si3O7 (OH) 2:1.5H2O
H2(g)	-18.94	-21.75	-2.81	H2
H2O(g)	1.21	-0.00	-1.21	H2O
Halite	-4.54	-3.30	1.24	NaCl
Hatrurite	-15.01	29.35	44.36	Ca3SiO5
HCl(g)	-9.36	-8.47	0.89	HCl
Hexahydrite	-8.91	-10.97	-2.07	MgSO4:6H2O
Hillebrandite	-4.42	18.63	23.05	Ca2SiO3 (OH) 2:0.17H2O
Huntite	9.71	6.24	-3.47	CaMg3 (CO3) 4
Hydroboracite	-15.55	4.87	20.42	MgCaB6O11:6H2O
Hydromagnesite	7.52	16.74	9.22	Mg5 (CO3) 4 (OH) 2:4H2O
Hydrophilite	-11.04	-6.22	4.82	CaCl2
Ice	-0.88	-0.00	0.88	H2O
K	-38.89	6.55	45.44	K
K(g)	-43.84	6.55	50.39	K
K2CO3:1.5H2O	-14.90	-1.61	13.29	K2CO3:1.5H2O
K2O	-48.95	7.47	56.42	K2O
K3H (SO4) 2	-28.34	-31.96	-3.62	K3H (SO4) 2
K8H4 (CO3) 6:3H2O	-52.14	-24.60	27.54	K8H4 (CO3) 6:3H2O
Kainite	-15.23	-15.71	-0.48	KMgClSO4:3H2O
Kallicinite	-5.63	-5.34	0.28	KHCO3
Kieserite	-10.65	-10.97	-0.32	MgSO4:H2O
KMgCl3	-22.00	-11.06	10.94	KMgCl3
KMgCl3:2H2O	-18.94	-11.07	7.88	KMgCl3:2H2O
KNaCO3:6H2O	-10.10	-0.18	9.92	KNaCO3:6H2O
Lansfordite	-3.03	1.53	4.56	MgCO3:5H2O
Larnite	-4.35	18.63	22.99	Ca2SiO4
Leonite	-20.75	-25.08	-4.34	K2Mg (SO4) 2:4H2O
Lime	-9.21	10.72	19.93	CaO
Magnesite	2.76	1.53	-1.23	MgCO3
Mercallite	-16.41	-17.85	-1.44	KHSO4
Merwinite	-2.10	37.16	39.26	MgCa3 (SiO4) 2
Mg	-57.61	16.23	73.84	Mg
Mg(g)	-67.91	16.23	84.15	Mg
Mg1.25SO4 (OH) 0.5:0.5H2O	-5.68	-8.32	-2.63	Mg1.25SO4 (OH) 0.5:0.5H2O
Mg1.5SO4 (OH)	-5.16	-5.66	-0.51	Mg1.5SO4 (OH)
MgCl2:2H2O	-11.75	-6.33	5.42	MgCl2:2H2O
MgCl2:4H2O	-9.61	-6.33	3.28	MgCl2:4H2O
MgCl2:7H2O	-13.23	-6.33	6.90	MgCl2:7H2O
MgOHCl	-5.35	2.14	7.49	MgOHCl
MgSO4	-8.28	-10.97	-2.69	MgSO4
Mirabilite	-17.66	-11.25	6.41	Na2SO4:10H2O
Misenite	-110.12	-121.20	-11.08	K8H6 (SO4) 7

Monohydrocalcite	0.33	1.64	1.31	CaCO3:H2O
Monticellite	2.26	18.53	16.27	CaMgSiO4
Na	-34.78	7.98	42.76	Na
Na(g)	-41.42	7.98	49.40	Na
Na2CO3	-7.02	1.26	8.28	Na2CO3
Na2CO3:7H2O	-12.92	1.26	14.18	Na2CO3:7H2O
Na2O	-34.71	10.34	45.06	Na2O
Na2SiO3	-9.17	7.53	16.71	Na2SiO3
Na3H(SO4)2	-26.76	-27.65	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-27.34	-33.35	-6.01	Na4Ca(SO4)3:2H2O
Na4SiO4	-31.79	17.87	49.67	Na4SiO4
Na6Si2O7	-45.66	25.41	71.07	Na6Si2O7
Nahcolite	-4.51	-3.91	0.60	NaHCO3
Natron	-12.32	1.25	13.58	Na2CO3:10H2O
Natrosillite	-9.28	4.73	14.01	Na2Si2O5
Nesquehonite	-2.73	1.53	4.26	MgCO3:3H2O
O2(g)	-8.37	-11.24	-2.87	O2
Okenite	-3.83	5.11	8.93	CaSi2O4(OH)2:H2O
Oxychloride-Mg	-12.69	12.75	25.43	Mg2Cl(OH)3:4H2O
Pentahydrate	-9.30	-10.97	-1.67	MgSO4:5H2O
Periclase	-1.03	10.61	11.64	MgO
Picromerite	-20.31	-25.09	-4.78	K2Mg(SO4)2:6H2O
Pirssonite	-8.31	2.90	11.21	Na2Ca(CO3)2:2H2O
Polyhalite	-32.38	-46.81	-14.43	K2MgCa2(SO4)4:2H2O
Portlandite	-3.48	10.72	14.20	Ca(OH)2
Pseudowollastonite	-0.26	7.91	8.17	CaSiO3
Quartz	-0.36	-2.81	-2.45	SiO2
Rankinite	-4.34	26.55	30.89	Ca3Si2O7
Sellaite	-3.13	-14.75	-11.62	MgF2
Sepiolite	7.99	25.60	17.61	Mg4Si6O15(OH)2:6H2O
Si	-83.00	8.44	91.43	Si
Si(g)	-124.99	8.44	133.42	Si
SiF4(g)	-33.25	-53.52	-20.28	SiF4
SiO2(am)	-0.98	-2.81	-1.83	SiO2
Starkeyite	-9.75	-10.97	-1.23	MgSO4:4H2O
Sylvite	-5.97	-4.73	1.23	KCl
Syngenite	-17.32	-24.97	-7.66	K2Ca(SO4)2:H2O
Tachyhydrite	-35.35	-18.89	16.46	Mg2CaCl6:12H2O
Talc	11.25	20.61	9.36	Mg3Si4O10(OH)2
Thenardite	-9.51	-11.24	-1.73	Na2SO4
Thermonatrite	-7.81	1.26	9.07	Na2CO3:H2O
Tobermorite-11A	-6.88	36.76	43.64	Ca5Si6H11O22.5
Tobermorite-14A	-9.92	36.75	46.67	Ca5Si6H21O27.5
Tobermorite-9A	-7.28	36.76	44.04	Ca5Si6H6O20
Tremolite	21.69	52.05	30.36	Ca2Mg5Si8O22(OH)2
Tridymite	-0.68	-2.81	-2.13	SiO2
Trona-K	-16.99	-5.52	11.48	K2NaH(CO3)2:2H2O
Wollastonite	-0.21	7.91	8.12	CaSiO3
Xonotlite	-11.34	47.48	58.82	Ca6Si6O17(OH)2

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

Beginning of batch-reaction calculations.

TIME STEP 4 DAYS (0.01 YEAR)

Reaction step 8.

WARNING: CNode incomplete at cnode_steps 100. Cell: 0	Time: 1.096027e+05	Cnode calls: 1, continuing...
WARNING: CNode incomplete at cnode_steps 100. Cell: 0	Time: 1.278031e+05	Cnode calls: 2, continuing...
WARNING: CNode incomplete at cnode_steps 100. Cell: 0	Time: 1.357897e+05	Cnode calls: 3, continuing...
WARNING: CNode incomplete at cnode_steps 100. Cell: 0	Time: 1.915437e+05	Cnode calls: 4, continuing...
WARNING: CNode incomplete at cnode_steps 100. Cell: 0	Time: 4.972836e+05	Cnode calls: 5, continuing...

Using solution 1. UW-8B
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

Time step: 3e+07 seconds (Incremented time: 3.33333e+07 seconds)

Rate name	Delta Moles	Total Moles	Reactant	Coefficient
Quartz	1.777e+00	7.607e+01	SiO2	1
Anorthite	-1.595e-01	1.382e+01	CaAl2(SiO4)2	1
Albite	4.407e-03	1.710e+01	NaAlSi3O8	1
K-Feldspar	1.902e-04	1.774e+01	KAlSi3O8	1
Corundum	8.903e-01	1.482e+01	Al2O3	1
Enstatite	3.534e-03	2.845e+01	MgSiO3	1
Ilmenite	2.216e-05	1.090e+00	FeTiO3	1
Kaolinite	-7.332e-01	1.958e+00	Al2Si2O5(OH)4	1
Alunite	-2.168e-19	0.000e+00	KAl3(OH)6(SO4)2	1
Calcite	1.551e-01	1.430e+00	CaCO3	1
Anhydrite	2.922e-03	3.820e+00	CaSO4	1

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

Phase	SI	log IAP	log K(T, P)	Moles in assemblage		
				Initial	Final	Delta
CO2(g)	-2.26	-4.46	-2.20	0.000e+00	0	0.000e+00

-----Solution composition-----		
Elements	Molality	Moles
Al	1.624e-05	1.857e-05
B	1.601e-03	1.830e-03
C	6.952e-05	7.947e-05
Ca	2.932e-03	3.351e-03
Cl	2.696e-02	3.082e-02
F	2.775e-06	3.172e-06
Fe	4.110e-07	4.697e-07

K	1.465e-03	1.674e-03
Mg	3.300e-06	3.771e-06
Na	3.353e-02	3.833e-02
S	3.181e-04	3.635e-04
Si	3.815e-03	4.361e-03
Ti	4.110e-07	4.697e-07

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-----Description of solution-----
pH = 7.107      Charge balance
pe = -1.326     Adjusted to redox equilibrium
Density (g/cm³) = 0.88332
Volume (L) = 1.29692
Activity of water = 0.999
Ionic strength (mol/kgw) = 3.614e-02
Mass of water (kg) = 1.143e+00
Total alkalinity (eq/kg) = 3.760e-04
Total CO2 (mol/kg) = 6.952e-05
Temperature (°C) = 200.00
Pressure (atm) = 249.00
Electrical balance (eq) = 1.479e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 19.42
Iterations = 6693
Total H = 1.269367e+02
Total O = 6.348165e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	9.879e-05	7.483e-05	-4.005	-4.126	-0.121	(0)
H+	9.664e-08	7.820e-08	-7.015	-7.107	-0.092	0.00
H2O	5.553e+01	9.986e-01	1.744	-0.001	0.000	20.44
Al	1.624e-05					
AlO2-	1.508e-05	1.151e-05	-4.822	-4.939	-0.117	(0)
NaAlO2	1.064e-06	1.064e-06	-5.973	-5.973	0.000	(0)
HAIO2	9.803e-08	9.803e-08	-7.009	-7.009	0.000	(0)
Al(OH)2+	6.160e-12	4.701e-12	-11.210	-11.328	-0.117	(0)
AlOH+2	2.448e-16	8.452e-17	-15.611	-16.073	-0.462	(0)
AlF+2	4.348e-21	1.501e-21	-20.362	-20.824	-0.462	(0)
AlF2+	1.385e-21	1.057e-21	-20.859	-20.976	-0.117	(0)
Al+3	5.889e-22	8.487e-23	-21.230	-22.071	-0.841	(0)
AlF3	2.353e-23	2.353e-23	-22.628	-22.628	0.000	(0)
AlSO4+	5.823e-24	4.444e-24	-23.235	-23.352	-0.117	(0)
Al(SO4)2-	2.313e-26	1.765e-26	-25.636	-25.753	-0.117	(0)
AlF4-	1.370e-26	1.046e-26	-25.863	-25.981	-0.117	(0)
Al2(OH)2+4	1.791e-36	3.114e-38	-35.747	-37.507	-1.760	(0)
Al3(OH)4+5	0.000e+00	0.000e+00	-48.759	-51.442	-2.683	(0)
Al13O4(OH)24+7	0.000e+00	0.000e+00	-151.405	-156.666	-5.261	(0)
B(-5)	0.000e+00					
BH4-	0.000e+00	0.000e+00	-79.595	-79.712	-0.117	(0)
B(3)	1.601e-03					
B(OH)3	1.561e-03	1.561e-03	-2.807	-2.807	0.000	(0)
BO2-	3.809e-05	2.907e-05	-4.419	-4.537	-0.117	(0)
CaB(OH)4+	1.128e-06	8.609e-07	-5.948	-6.065	-0.117	(0)
NaB(OH)4	6.051e-07	6.051e-07	-6.218	-6.218	0.000	(0)
MgB(OH)4+	5.938e-10	4.532e-10	-9.226	-9.344	-0.117	(0)
BF2(OH)2-	1.822e-15	1.390e-15	-14.739	-14.857	-0.117	(0)
B2O(OH)5-	8.432e-18	6.436e-18	-17.074	-17.191	-0.117	(0)
BF4-	3.000e-28	2.290e-28	-27.523	-27.640	-0.117	(0)
BF3OH-	2.663e-40	2.033e-40	-39.575	-39.692	-0.117	(0)
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-80.876	-80.876	0.000	(0)
C(-3)	0.000e+00					
C2H6	0.000e+00	0.000e+00	-48.903	-48.903	0.000	(0)
C(-4)	3.470e-35					
CH4	3.470e-35	3.470e-35	-34.460	-34.460	0.000	(0)
C(2)	1.204e-18					
CO	1.204e-18	1.204e-18	-17.919	-17.919	0.000	(0)
C(4)	6.952e-05					
CO2	3.401e-05	3.430e-05	-4.468	-4.465	0.004	52.92
HCO3-	2.628e-05	2.006e-05	-4.580	-4.698	-0.117	(0)
CaHCO3+	6.717e-06	5.127e-06	-5.173	-5.290	-0.117	(0)
CaCO3	2.454e-06	2.454e-06	-5.610	-5.610	0.000	(0)
NaHCO3	3.069e-08	3.069e-08	-7.513	-7.513	0.000	(0)
CO3-2	2.509e-08	8.663e-09	-7.600	-8.062	-0.462	(0)
MgHCO3+	3.078e-09	2.350e-09	-8.512	-8.629	-0.117	(0)
FeHCO3+	1.870e-09	1.427e-09	-8.728	-8.846	-0.117	(0)
(CO2)2	1.758e-10	1.772e-10	-9.755	-9.751	0.004	105.85
MgCO3	1.540e-10	1.540e-10	-9.812	-9.812	0.000	(0)
FeCO3	8.760e-11	8.760e-11	-10.058	-10.058	0.000	(0)
NaCO3-	1.919e-12	1.465e-12	-11.717	-11.834	-0.117	(0)
FeCO3+	4.115e-20	3.141e-20	-19.386	-19.503	-0.117	(0)
Ca	2.932e-03					
Ca+2	2.683e-03	1.002e-03	-2.571	-2.999	-0.428	(0)
CaSO4	1.460e-04	1.460e-04	-3.836	-3.836	0.000	(0)
CaCl+	8.919e-05	6.807e-05	-4.050	-4.167	-0.117	(0)
CaHCO3+	6.717e-06	5.127e-06	-5.173	-5.290	-0.117	(0)
CaCl2	3.210e-06	3.210e-06	-5.493	-5.493	0.000	(0)
CaCO3	2.454e-06	2.454e-06	-5.610	-5.610	0.000	(0)
CaB(OH)4+	1.128e-06	8.609e-07	-5.948	-6.065	-0.117	(0)
CaF+	3.850e-07	2.938e-07	-6.415	-6.532	-0.117	(0)
CaOH+	2.698e-09	2.059e-09	-8.569	-8.686	-0.117	(0)
Cl(-1)	2.696e-02					
Cl-	2.623e-02	1.971e-02	-1.581	-1.705	-0.124	(0)
NaCl	6.209e-04	6.209e-04	-3.207	-3.207	0.000	(0)
CaCl+	8.919e-05	6.807e-05	-4.050	-4.167	-0.117	(0)
KCl	1.327e-05	1.327e-05	-4.877	-4.877	0.000	(0)
CaCl2	3.210e-06	3.210e-06	-5.493	-5.493	0.000	(0)
MgCl+	1.600e-07	1.221e-07	-6.796	-6.913	-0.117	(0)
FeCl+	4.383e-08	3.345e-08	-7.358	-7.476	-0.117	(0)
HCl	1.262e-09	1.262e-09	-8.899	-8.899	0.000	(0)
FeCl2	3.662e-11	3.662e-11	-10.436	-10.436	0.000	(0)
FeCl4-2	3.130e-12	1.050e-12	-11.504	-11.979	-0.474	(0)
FeCl+2	2.615e-19	9.029e-20	-18.582	-19.044	-0.462	(0)
FeCl2+	4.382e-22	3.345e-22	-21.358	-21.476	-0.117	(0)
FeCl4-	2.047e-28	1.562e-28	-27.689	-27.806	-0.117	(0)

Cl(1)	4.982e-29					
HClO	3.432e-29	3.432e-29	-28.464	-28.464	0.000	(0)
ClO-	1.550e-29	1.183e-29	-28.810	-28.927	-0.117	(0)
Cl(3)	0.000e+00					
ClO2-	0.000e+00	0.000e+00	-49.598	-49.715	-0.117	(0)
HClO2	0.000e+00	0.000e+00	-53.652	-53.652	0.000	(0)
Cl(5)	0.000e+00					
ClO3-	0.000e+00	0.000e+00	-61.628	-61.748	-0.121	(0)
Cl(7)	0.000e+00					
ClO4-	0.000e+00	0.000e+00	-77.232	-77.353	-0.121	(0)
F	2.775e-06					
F-	2.335e-06	1.769e-06	-5.632	-5.752	-0.121	(0)
CaF+	3.850e-07	2.938e-07	-6.415	-6.532	-0.117	(0)
NaF	4.414e-08	4.414e-08	-7.355	-7.355	0.000	(0)
HF	1.007e-08	1.007e-08	-7.997	-7.997	0.000	(0)
MgF+	5.108e-10	3.898e-10	-9.292	-9.409	-0.117	(0)
FeF+	7.198e-12	5.494e-12	-11.143	-11.260	-0.117	(0)
HF2-	7.670e-15	5.854e-15	-14.115	-14.233	-0.117	(0)
BF2(OH) 2-	1.822e-15	1.390e-15	-14.739	-14.857	-0.117	(0)
H2F2	1.121e-19	1.121e-19	-18.950	-18.950	0.000	(0)
FeF+2	8.960e-20	3.093e-20	-19.048	-19.510	-0.462	(0)
FeF2+	3.131e-20	2.389e-20	-19.504	-19.622	-0.117	(0)
AlF+2	4.348e-21	1.501e-21	-20.362	-20.824	-0.462	(0)
AlF2+	1.385e-21	1.057e-21	-20.859	-20.976	-0.117	(0)
AlF3	2.353e-23	2.353e-23	-22.628	-22.628	0.000	(0)
AlF4-	1.370e-26	1.046e-26	-25.863	-25.981	-0.117	(0)
BF4-	3.000e-28	2.290e-28	-27.523	-27.640	-0.117	(0)
BF3OH-	2.663e-40	2.033e-40	-39.575	-39.692	-0.117	(0)
SiF6-2	0.000e+00	0.000e+00	-40.067	-40.541	-0.474	(0)
Fe(2)	4.109e-07					
Fe+2	3.632e-07	1.356e-07	-6.440	-6.868	-0.428	(0)
FeCl+	4.383e-08	3.345e-08	-7.358	-7.476	-0.117	(0)
FeHCO3+	1.870e-09	1.427e-09	-8.728	-8.846	-0.117	(0)
FeSO4	1.100e-09	1.100e-09	-8.959	-8.959	0.000	(0)
FeOH+	8.176e-10	6.240e-10	-9.087	-9.205	-0.117	(0)
FeCO3	8.760e-11	8.760e-11	-10.058	-10.058	0.000	(0)
FeCl2	3.662e-11	3.662e-11	-10.436	-10.436	0.000	(0)
FeF+	7.198e-12	5.494e-12	-11.143	-11.260	-0.117	(0)
FeCl4-2	3.130e-12	1.050e-12	-11.504	-11.979	-0.474	(0)
Fe(OH) 2	7.214e-14	7.214e-14	-13.142	-13.142	0.000	(0)
Fe(OH) 3-	5.476e-17	4.180e-17	-16.261	-16.379	-0.117	(0)
Fe(OH) 4-2	1.814e-24	6.083e-25	-23.741	-24.216	-0.474	(0)
Fe(3)	2.356e-11					
Fe(OH) 3	1.967e-11	1.967e-11	-10.706	-10.706	0.000	(0)
Fe(OH) 2+	3.787e-12	2.890e-12	-11.422	-11.539	-0.117	(0)
Fe(OH) 4-	9.424e-14	7.192e-14	-13.026	-13.143	-0.117	(0)
FeOH+2	1.737e-15	5.997e-16	-14.760	-15.222	-0.462	(0)
FeSO4+	6.264e-19	4.781e-19	-18.203	-18.320	-0.117	(0)
FeCl+2	2.615e-19	9.029e-20	-18.582	-19.044	-0.462	(0)
FeF+2	8.960e-20	3.093e-20	-19.048	-19.510	-0.462	(0)
Fe+3	4.428e-20	6.382e-21	-19.354	-20.195	-0.841	(0)
FeCO3+	4.115e-20	3.141e-20	-19.386	-19.503	-0.117	(0)
FeF2+	3.131e-20	2.389e-20	-19.504	-19.622	-0.117	(0)
FeCl2+	4.382e-22	3.345e-22	-21.358	-21.476	-0.117	(0)
Fe(SO4) 2-	3.582e-26	2.734e-26	-25.446	-25.563	-0.117	(0)
Fe2(OH) 2+4	5.567e-28	9.680e-30	-27.254	-29.014	-1.760	(0)
FeCl4-	2.047e-28	1.562e-28	-27.689	-27.806	-0.117	(0)
Fe3(OH) 4+5	2.819e-36	5.845e-39	-35.550	-38.233	-2.683	(0)
H(0)	3.853e-12					
H2	1.927e-12	1.956e-12	-11.715	-11.709	0.007	(0)
K	1.465e-03					
K+	1.445e-03	1.086e-03	-2.840	-2.964	-0.124	(0)
KCl	1.327e-05	1.327e-05	-4.877	-4.877	0.000	(0)
KSO4-	6.132e-06	4.680e-06	-5.212	-5.330	-0.117	(0)
KHSO4	1.184e-10	1.184e-10	-9.927	-9.927	0.000	(0)
KOH	5.479e-11	5.479e-11	-10.261	-10.261	0.000	(0)
Mg	3.300e-06					
MgSO4	2.048e-06	2.048e-06	-5.689	-5.689	0.000	(0)
Mg+2	1.087e-06	4.432e-07	-5.964	-6.353	-0.390	(0)
MgCl+	1.600e-07	1.221e-07	-6.796	-6.913	-0.117	(0)
MgHCO3+	3.078e-09	2.350e-09	-8.512	-8.629	-0.117	(0)
MgB(OH) 4+	5.938e-10	4.532e-10	-9.226	-9.344	-0.117	(0)
MgF+	5.108e-10	3.898e-10	-9.292	-9.409	-0.117	(0)
MgCO3	1.540e-10	1.540e-10	-9.812	-9.812	0.000	(0)
Mg4(OH) 4+4	1.770e-35	3.077e-37	-34.752	-36.512	-1.760	(0)
Na	3.353e-02					
Na+	3.287e-02	2.508e-02	-1.483	-1.601	-0.117	(0)
NaCl	6.209e-04	6.209e-04	-3.207	-3.207	0.000	(0)
NaHSiO3	3.037e-05	3.037e-05	-4.518	-4.518	0.000	(0)
NaSO4-	1.111e-05	8.481e-06	-4.954	-5.072	-0.117	(0)
NaOH	2.207e-06	2.207e-06	-5.656	-5.656	0.000	(0)
NaAlO2	1.064e-06	1.064e-06	-5.973	-5.973	0.000	(0)
NaB(OH) 4	6.051e-07	6.051e-07	-6.218	-6.218	0.000	(0)
NaF	4.414e-08	4.414e-08	-7.355	-7.355	0.000	(0)
NaHCO3	3.069e-08	3.069e-08	-7.513	-7.513	0.000	(0)
NaCO3-	1.919e-12	1.465e-12	-11.717	-11.834	-0.117	(0)
O(0)	9.423e-32					
O2	4.711e-32	4.784e-32	-31.327	-31.320	0.007	(0)
S(-2)	1.255e-28					
HS-	9.623e-29	7.289e-29	-28.017	-28.137	-0.121	(0)
H2S	2.780e-29	2.780e-29	-28.556	-28.556	0.000	(0)
S-2	1.471e-30	5.220e-31	-29.832	-30.282	-0.450	(0)
S2-2	0.000e+00	0.000e+00	-52.784	-53.258	-0.474	(0)
S3-2	0.000e+00	0.000e+00	-74.544	-75.018	-0.474	(0)
S4-2	0.000e+00	0.000e+00	-96.450	-96.924	-0.474	(0)
S5-2	0.000e+00	0.000e+00	-118.495	-118.970	-0.474	(0)
S(2)	9.924e-35					
S2O3-2	4.962e-35	1.664e-35	-34.304	-34.779	-0.474	(0)
HS2O3-	0.000e+00	0.000e+00	-40.754	-40.872	-0.117	(0)
S(3)	0.000e+00					
S2O4-2	0.000e+00	0.000e+00	-41.568	-42.018	-0.450	(0)
S(4)	3.057e-16					
HSO3-	2.930e-16	2.282e-16	-15.524	-15.642	-0.117	(0)
SO3-2	6.466e-18	2.232e-18	-17.189	-17.651	-0.462	(0)
SO2	2.254e-19	2.254e-19	-18.647	-18.647	0.000	(0)
H2SO3	2.230e-23	2.230e-23	-22.652	-22.652	0.000	(0)
S2O6-2	1.517e-33	5.087e-34	-32.819	-33.294	-0.474	(0)
S3O6-2	0.000e+00	0.000e+00	-56.725	-57.199	-0.474	(0)

S406-2	0.000e+00	0.000e+00	-68.212	-68.686	-0.474	(0)
S506-2	0.000e+00	0.000e+00	-102.592	-103.066	-0.474	(0)
S(5)	7.696e-37					
S205-2	3.848e-37	1.291e-37	-36.415	-36.889	-0.474	(0)
S(6)	3.181e-04					
SO4-2	1.526e-04	5.117e-05	-3.817	-4.291	-0.474	(0)
CaSO4	1.460e-04	1.460e-04	-3.836	-3.836	0.000	(0)
NaSO4-	1.111e-05	8.481e-06	-4.954	-5.072	-0.117	(0)
KSO4-	6.132e-06	4.680e-06	-5.212	-5.330	-0.117	(0)
MgSO4	2.048e-06	2.048e-06	-5.689	-5.689	0.000	(0)
HSO4-	1.560e-07	1.191e-07	-6.807	-6.924	-0.117	(0)
FeSO4	1.100e-09	1.100e-09	-8.959	-8.959	0.000	(0)
KHSO4	1.184e-10	1.184e-10	-9.927	-9.927	0.000	(0)
FeSO4+	6.264e-19	4.781e-19	-18.203	-18.320	-0.117	(0)
H2SO4	2.982e-20	2.982e-20	-19.525	-19.525	0.000	(0)
AlSO4+	5.823e-24	4.444e-24	-23.235	-23.352	-0.117	(0)
Fe(SO4)2-	3.582e-26	2.734e-26	-25.446	-25.563	-0.117	(0)
Al(SO4)2-	2.313e-26	1.765e-26	-25.636	-25.753	-0.117	(0)
S(7)	0.000e+00					
S208-2	0.000e+00	0.000e+00	-46.326	-46.801	-0.474	(0)
S(8)	8.382e-35					
HS05-	8.382e-35	6.398e-35	-34.077	-34.194	-0.117	(0)
Si	3.815e-03					
SiO2	3.683e-03	3.683e-03	-2.434	-2.434	0.000	(0)
HSiO3-	1.022e-04	7.798e-05	-3.991	-4.108	-0.117	(0)
NaHSiO3	3.037e-05	3.037e-05	-4.518	-4.518	0.000	(0)
H6(H2SiO4)4-2	5.783e-09	1.939e-09	-8.238	-8.712	-0.474	(0)
H2SiO4-2	2.550e-11	8.553e-12	-10.593	-11.068	-0.474	(0)
H4(H2SiO4)4-4	1.271e-15	1.589e-17	-14.896	-16.799	-1.903	(0)
SiF6-2	0.000e+00	0.000e+00	-40.067	-40.541	-0.474	(0)
Ti	4.110e-07					
Ti(OH)4	4.110e-07	4.110e-07	-6.386	-6.386	0.000	(0)

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

Phase	SI**	log IAP	log K(473 K, 249 atm)
Afwillite	-9.66	28.77	38.43 Ca3Si2O4(OH)6
Akermanite	0.11	25.42	25.31 Ca2MgSi2O7
Al	-64.07	22.74	86.81 Al
Al(g)	-93.51	22.74	116.25 Al
Al2(SO4)3	-46.13	-57.02	-10.89 Al2(SO4)3
Al2(SO4)3·6H2O	-39.97	-57.02	-17.04 Al2(SO4)3·6H2O
Albite	-0.00	-2.55	-2.55 NaAlSi3O8
Albite_high	-0.61	-2.55	-1.94 NaAlSi3O8
Albite_low	-0.00	-2.55	-2.55 NaAlSi3O8
AlF3	-17.34	-39.33	-21.99 AlF3
Alum-K	-26.27	-33.62	-7.36 KAl(SO4)2·12H2O
Alunite	-15.33	-35.12	-19.79 KAl3(OH)6(SO4)2
Amesite-14A	2.18	23.56	21.38 Mg4Al4Si2O10(OH)8
Analcime	-0.31	-0.40	-0.09 Na.96Al.96Si2.04O6·H2O
Analcime-dehy	-3.94	-0.40	3.54 Na.96Al.96Si2.04O6
Anatase	2.06	-6.39	-8.45 TiO2
Andalusite	-3.22	-3.94	-0.72 Al2SiO5
Andradite	17.70	28.59	10.89 Ca3Fe2(SiO4)3
Anhydrite	0.00	-7.29	-7.29 CaSO4
Ankerite	-1.30	-4.89	-3.59 CaMg0.3Fe0.7(CO3)2
Annite	7.79	18.12	10.34 KFe3AlSi3O10(OH)2
Anorthite	0.00	4.84	4.84 CaAl2(SiO4)2
Antarcticite	-10.17	-6.41	3.75 CaCl2·6H2O
Anthophyllite	4.39	35.55	31.15 Mg7Si8O22(OH)2
Antigorite	50.27	294.49	244.23 Mg48Si34O85(OH)62
Aphthalite	-15.19	-19.08	-3.89 NaK3(SO4)2
Aragonite	-0.15	-0.59	-0.44 CaCO3
Arcanite	-8.31	-10.22	-1.90 K2SO4
Artinite	-7.02	3.91	10.93 Mg2CO3(OH)2·3H2O
B	-46.65	20.68	67.34 B
B(g)	-101.39	20.68	122.07 B
B2O3	-9.27	-5.61	3.66 B2O3
Bassanite	-0.66	-7.29	-6.63 CaSO4·0.5H2O
Beidellite-Ca	-0.84	-8.83	-7.99 Ca.165Al2.33Si3.67O10(OH)2
Beidellite-H	-2.27	-10.68	-8.41 H.33Al2.33Si3.67O10(OH)2
Beidellite-K	-1.81	-9.32	-7.50 K.33Al2.33Si3.67O10(OH)2
Beidellite-Mg	-1.18	-9.39	-8.21 Mg.165Al2.33Si3.67O10(OH)2
Beidellite-Na	-1.44	-8.87	-7.43 Na.33Al2.33Si3.67O10(OH)2
BF3(g)	-30.61	-41.38	-10.77 BF3
Bischofite	-13.82	-9.77	4.05 MgCl2·6H2O
Bloedite	-15.43	-18.14	-2.70 Na2Mg(SO4)2·4H2O
Boehmite	-0.58	-0.75	-0.17 AlO2H
Borax	-17.57	-0.22	17.35 Na2(B4O5(OH)4)·8H2O
Boric_acid	-3.84	-2.81	1.03 B(OH)3
Brucite	-1.34	7.86	9.20 Mg(OH)2
Burkeite	-25.26	-15.78	9.49 Na6CO3(SO4)2
C	-17.78	19.52	37.29 C
C(g)	-89.00	19.52	108.51 C
Ca	-59.18	26.87	86.05 Ca
Ca(g)	-73.01	26.87	99.88 Ca
Ca-Al Pyroxene	-3.76	7.28	11.04 CaAl2SiO6
Ca2Al2O5·8H2O	-37.91	20.92	58.83 Ca2Al2O5·8H2O
Ca2Cl2(OH)2·H2O	-21.32	4.80	26.12 Ca2Cl2(OH)2·H2O
Ca3Al2O6	-26.90	32.14	59.03 Ca3Al2O6
Ca4Al2Fe2O10	-20.79	45.60	66.39 Ca4Al2Fe2O10
Ca4Al2O7·13H2O	-62.77	43.35	106.12 Ca4Al2O7·13H2O
Ca4Al2O7·19H2O	-58.86	43.34	102.21 Ca4Al2O7·19H2O
Ca4Cl2(OH)6·13H2O	-40.03	27.22	67.25 Ca4Cl2(OH)6·13H2O
CaAl2O4	-7.91	9.71	17.62 CaAl2O4
CaAl2O4·10H2O	-27.50	9.71	37.20 CaAl2O4·10H2O
CaAl4O7	-13.18	8.21	21.39 CaAl4O7
Calcite	-0.00	-0.59	-0.59 CaCO3
Carnallite	-18.37	-14.44	3.93 KMgCl3·6H2O
CaSO4·0.5H2O(beta)	-0.69	-7.29	-6.60 CaSO4·0.5H2O
Celadonite	1.21	1.51	0.30 KMgAlSi4O10(OH)2
CH4(g)	-31.71	-34.46	-2.75 CH4
Chalcedony	-0.16	-2.43	-2.28 SiO2
Chamosite-7A	2.93	10.75	7.82 Fe2Al2SiO5(OH)4
Chloromagnesite	-19.75	-9.76	9.99 MgCl2
Chrysotile	2.56	18.71	16.15 Mg3Si2O5(OH)4
Cl2(g)	-31.79	-33.28	-1.49 Cl2

Clinochlore-14A	5.03	30.49	25.46	Mg5Al2Si3O10(OH)8
Clinochlore-7A	2.46	30.49	28.03	Mg5Al2Si3O10(OH)8
Clinoptilolite-Ca	3.80	-18.51	-22.32	Ca1.7335Al3.45Fe.017Si14.533036:10.922H2O
Clinoptilolite-dehy-Ca	-15.56	-18.51	-2.95	Ca1.7335Al3.45Fe.017Si14.533036
Clinoptilolite-dehy-K	-25.83	-23.58	2.25	K3.467Al3.45Fe.017Si14.533036
Clinoptilolite-dehy-Na	-21.54	-18.86	2.68	Na3.467Al3.45Fe.017Si14.533036
Clinoptilolite-hy-Ca	3.22	-18.51	-21.74	Ca1.7335Al3.45Fe.017Si14.533036:11.645H2O
Clinoptilolite-hy-K	-4.32	-23.59	-19.27	K3.467Al3.45Fe.017Si14.533036:7.499H2O
Clinoptilolite-hy-Na	-2.24	-18.86	-16.62	Na3.467Al3.45Fe.017Si14.533036:10.877H2O
Clinoptilolite-K	-6.74	-23.59	-16.85	K3.467Al3.45Fe.017Si14.533036:10.922H2O
Clinoptilolite-Na	-2.27	-18.86	-16.59	Na3.467Al3.45Fe.017Si14.533036:10.922H2O
Clinozoisite	2.39	12.87	10.48	Ca2Al3Si3O12(OH)
CO(g)	-15.12	-17.92	-2.80	CO
CO2(g)	-2.26	-4.46	-2.20	CO2
Coesite	-0.52	-2.43	-1.92	SiO2
Colemanite	-16.04	5.59	21.63	Ca2B6O11:5H2O
Cordierite_anhyd	-6.65	0.54	7.19	Mg2Al4Si5O18
Cordierite_hydr	-5.38	0.54	5.92	Mg2Al4Si5O18:H2O
Corundum	0.00	-1.50	-1.50	Al2O3
Cristobalite(alpha)	-0.29	-2.43	-2.14	SiO2
Cristobalite(beta)	-0.50	-2.43	-1.94	SiO2
Cronstedtite-7A	15.70	14.50	-1.19	Fe2Fe2SiO5(OH)4
Daphnite-14A	11.95	27.92	15.97	Fe5AlAlSi3O10(OH)8
Daphnite-7A	9.45	27.92	18.47	Fe5AlAlSi3O10(OH)8
Dawsonite	-6.47	-7.05	-0.58	NaAlCO3(OH)2
Diaspore	-0.39	-0.75	-0.36	AlHO2
Dicalcium_silicate	-2.33	19.99	22.32	Ca2SiO4
Diopside	3.12	14.21	11.09	CaMgSi2O6
Dolomite	-1.76	-4.53	-2.78	CaMg(CO3)2
Dolomite-dis	-2.50	-4.53	-2.03	CaMg(CO3)2
Dolomite-ord	-1.75	-4.53	-2.79	CaMg(CO3)2
Enstatite	-0.00	5.43	5.43	MgSiO3
Epidote	10.02	14.75	4.73	Ca2FeAl2Si3O12OH
Epidote-ord	9.99	14.75	4.76	FeCa2Al2(OH)(SiO4)3
Epsomite	-8.29	-10.65	-2.36	MgSO4:7H2O
Ettringite	-33.25	10.25	43.51	Ca6Al2(SO4)3(OH)12:26H2O
F2(g)	-70.92	-41.38	29.55	F2
Fayalite	3.75	12.26	8.51	Fe2SiO4
Fe	-11.47	23.01	34.47	Fe
Fe(OH)2	-0.35	7.34	7.70	Fe(OH)2
Fe(OH)3	1.19	1.12	-0.06	Fe(OH)3
Fe2(SO4)3	-33.93	-53.26	-19.33	Fe2(SO4)3
FeF2	-11.14	-18.37	-7.23	FeF2
FeF3	-15.16	-37.45	-22.29	FeF3
FeO	0.78	7.35	6.57	FeO
Ferrite-Ca	10.11	13.46	3.35	CaFe2O4
Ferrite-Dicalcium	-0.24	24.68	24.92	Ca2Fe2O5
Ferrite-Mg	8.23	10.11	1.88	MgFe2O4
Ferrosillite	1.88	4.91	3.03	FeSiO3
FeSO4	-7.33	-11.16	-3.83	FeSO4
Fluorite	-3.72	-14.50	-10.78	CaF2
Forsterite	-0.74	13.29	14.02	Mg2SiO4
Foshagite	-3.12	37.55	40.68	Ca4Si3O9(OH)2:0.5H2O
Gaylussite	-12.27	-1.38	10.88	CaNa2(CO3)2:5H2O
Gehlenite	-4.49	18.49	22.98	Ca2Al2SiO7
Gibbsite	-1.01	-0.75	0.26	Al(OH)3
Gismondine	-31.07	9.68	40.75	Ca2Al4Si4O16:9H2O
Glauberite	-9.31	-14.78	-5.47	Na2Ca(SO4)2
Goethite	4.63	1.12	-3.51	FeOOH
Greenalite	6.46	17.17	10.70	Fe3Si2O5(OH)4
Grossular	3.74	24.84	21.10	Ca3Al2(SiO4)3
Gypsum	-1.04	-7.29	-6.25	CaSO4:2H2O
Gyrolite	-0.81	15.12	15.94	Ca2Si3O7(OH)2:1.5H2O
H2(g)	-8.90	-11.71	-2.81	H2
H2O(g)	1.21	-0.00	-1.21	H2O
H2S(g)	-26.97	-35.24	-8.28	H2S
Halite	-4.54	-3.31	1.24	NaCl
Hatrurite	-13.16	31.21	44.36	Ca3SiO5
HCl(g)	-9.70	-8.81	0.89	HCl
Hedenbergite	3.48	13.69	10.21	CaFe(SiO3)2
Hematite	11.45	2.25	-9.20	Fe2O3
Hercynite	0.27	5.84	5.57	FeAl2O4
Hexahydrite	-8.58	-10.65	-2.07	MgSO4:6H2O
Hillebrandite	-3.06	19.99	23.05	Ca2SiO3(OH)2:0.17H2O
Huntite	-8.95	-12.42	-3.47	CaMg3(CO3)4
Hydroboracite	-18.18	2.24	20.42	MgCaB6O11:6H2O
Hydromagnesite	-17.14	-7.92	9.22	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-11.23	-6.41	4.82	CaCl2
Ice	-0.88	-0.00	0.88	H2O
Illite	-0.76	-5.80	-5.04	K0.6Mg0.25Al1.8Al0.5Si3.5O10(OH)2
Ilmenite	-0.00	0.96	0.96	FeTiO3
Jadeite	-1.66	-0.11	1.55	NaAl(SiO3)2
Jarosite	-5.49	-29.49	-24.00	KFe3(SO4)2(OH)6
Jarosite-Na	-22.34	-28.13	-5.79	NaFe3(SO4)2(OH)6
K	-33.47	11.97	45.44	K
K(g)	-38.42	11.97	50.39	K
K-Feldspar	-0.00	-3.91	-3.91	KAlSi3O8
K2CO3:1.5H2O	-16.81	-3.52	13.29	K2CO3:1.5H2O
K2O	-48.13	8.28	56.42	K2O
K3H(SO4)2	-20.96	-24.58	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-65.23	-37.69	27.54	K8H4(CO3)6:3H2O
Kainite	-14.83	-15.32	-0.48	KMgClSO4:3H2O
KAl(SO4)2	-24.09	-33.62	-9.53	KAl(SO4)2
Kalincinite	-7.95	-7.66	0.28	KHCO3
Kalsilite	-1.96	0.96	2.92	KAlSiO4
Kaolinite	-1.54	-6.37	-4.83	Al2Si2O5(OH)4
Katoite	-46.13	32.13	78.26	Ca3Al2H12O12
Kieserite	-10.32	-10.64	-0.32	MgSO4:H2O
KMgCl3	-25.37	-14.43	10.94	KMgCl3
KMgCl3:2H2O	-22.31	-14.43	7.88	KMgCl3:2H2O
KNaCO3:6H2O	-12.08	-2.16	9.92	KNaCO3:6H2O
Kyanite	-3.23	-3.94	-0.71	Al2SiO5
Lansfordite	-8.50	-3.95	4.56	MgCO3:5H2O
Larnite	-2.99	19.99	22.99	Ca2SiO4
Laumontite	1.23	-0.03	-1.26	CaAl2Si4O12:4H2O
Lawrencite	-12.20	-10.28	1.92	FeCl2
Lawsonite	0.39	4.84	4.45	CaAl2Si2O7(OH)2:H2O
Leonite	-16.53	-20.87	-4.34	K2Mg(SO4)2:4H2O

Lime	-8.72	11.21	19.93	CaO
Magnesite	-2.72	-3.94	-1.23	MgCO3
Magnetite	14.18	9.59	-4.59	Fe3O4
Margarite	-1.11	3.34	4.45	CaAl4Si2O10(OH)2
Maximum Microcline	0.02	-3.91	-3.93	KAlSi3O8
Mayenite	-106.09	124.04	230.13	Ca12Al14O33
Melanterite	-8.54	-11.16	-2.62	FeSO4·7H2O
Mercallite	-12.92	-14.36	-1.44	KHSO4
Merwinite	-2.63	36.63	39.26	MgCa3(SiO4)2
Mesolite	2.40	2.27	-0.13	Na.676Ca.657Al1.99Si3.01O10:2.647H2O
Mg	-50.32	23.52	73.84	Mg
Mg(g)	-60.63	23.52	84.15	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-6.05	-8.68	-2.63	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-6.21	-6.71	-0.51	Mg1.5SO4(OH)
MgCl2:2H2O	-15.18	-9.77	5.42	MgCl2:2H2O
MgCl2:4H2O	-13.05	-9.77	3.28	MgCl2:4H2O
MgCl2:H2O	-16.67	-9.76	6.90	MgCl2:H2O
MgOHCl	-8.45	-0.95	7.49	MgOHCl
MgSO4	-7.96	-10.64	-2.69	MgSO4
Minnesotaite	7.67	12.30	4.63	Fe3Si4O10(OH)2
Mirabilite	-13.91	-7.50	6.41	Na2SO4:10H2O
Misenite	-85.32	-96.39	-11.08	K8H6(SO4)7
Molysite	-26.06	-25.31	0.74	FeCl3
Monohydrocalcite	-1.90	-0.59	1.31	CaCO3:H2O
Monticellite	0.37	16.64	16.27	CaMgSiO4
Montmor-Ca	0.43	-6.55	-6.98	Ca.165Mg.33Al1.67Si4O10(OH)2
Montmor-K	-0.43	-7.03	-6.60	K.33Mg.33Al1.67Si4O10(OH)2
Montmor-Mg	0.12	-7.10	-7.23	Mg.495Al1.67Si4O10(OH)2
Montmor-Na	-0.12	-6.58	-6.46	Na.33Mg.33Al1.67Si4O10(OH)2
Mordenite	-0.46	-7.79	-7.33	Ca.2895Na.361Al.94Si5.06O12:3.468H2O
Mordenite-dehy	-8.75	-7.79	0.96	Ca.2895Na.361Al.94Si5.06O12
Muscovite	-0.39	-5.41	-5.02	KAl3Si3O10(OH)2
Na	-29.42	13.34	42.76	Na
Na(g)	-36.07	13.34	49.40	Na
Na2CO3	-9.07	-0.79	8.28	Na2CO3
Na2CO3:7H2O	-14.97	-0.80	14.18	Na2CO3:7H2O
Na2O	-34.04	11.01	45.06	Na2O
Na2SiO3	-8.13	8.58	16.71	Na2SiO3
Na3H(SO4)2	-19.60	-20.49	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.27	-22.28	-6.01	Na4Ca(SO4)3:2H2O
Na4SiO4	-30.08	19.59	49.67	Na4SiO4
Na6Si2O7	-42.90	28.17	71.07	Na6Si2O7
NaFeO2	-2.87	6.63	9.50	NaFeO2
Nahcolite	-6.90	-6.30	0.60	NaHCO3
Natrolite	-2.22	2.21	4.42	Na2Al2Si3O10:2H2O
Natron	-14.37	-0.80	13.58	Na2CO3:10H2O
Natrosilite	-7.86	6.14	14.01	Na2Si2O5
Nepheline	-1.92	2.32	4.24	NaAlSiO4
Nesquehonite	-8.21	-3.95	4.26	MgCO3:3H2O
Nontronite-Ca	12.12	-5.08	-17.20	Ca.165Fe2Al.33Si3.67H2O12
Nontronite-H	10.72	-6.93	-17.65	H.33Fe2Al.33Si3.67H2O12
Nontronite-K	11.15	-5.56	-16.71	K.33Fe2Al.33Si3.67H2O12
Nontronite-Mg	11.78	-5.63	-17.41	Mg.165Fe2Al.33Si3.67H2O12
Nontronite-Na	11.52	-5.11	-16.64	Na.33Fe2Al.33Si3.67H2O12
O2(g)	-28.45	-31.32	-2.87	O2
Okenite	-2.59	6.35	8.93	CaSi2O4(OH)2:2H2O
Oxychloride-Mg	-18.53	6.90	25.43	Mg2Cl(OH)3:4H2O
Paragonite	-1.07	-4.05	-2.98	NaAl3Si3O10(OH)2
Pargasite	2.00	42.51	40.51	NaCa2Al3Mg4Si6O22(OH)2
Pentahydrate	-8.98	-10.65	-1.67	MgSO4:5H2O
Periclase	-3.78	7.86	11.64	MgO
Phlogopite	4.24	19.67	15.42	KAlMg3Si3O10(OH)2
Picromerite	-16.09	-20.87	-4.78	K2Mg(SO4)2:6H2O
Pirssonite	-12.59	-1.38	11.21	Na2Ca(CO3)2:2H2O
Polyhalite	-21.02	-35.45	-14.43	K2MgCa2(SO4)4:2H2O
Portlandite	-2.98	11.21	14.20	Ca(OH)2
Prehnite	3.57	13.62	10.05	Ca2Al2Si3O10(OH)2
Pseudowollastonite	0.61	8.78	8.17	CaSiO3
Pyrite	-39.61	-58.96	-19.35	FeS2
Pyrophyllite	-1.98	-11.24	-9.26	Al2Si4O10(OH)2
Pyrrhotite	-22.76	-27.90	-5.14	FeS
Quartz	0.02	-2.43	-2.45	SiO2
Rankinite	-2.12	28.77	30.89	Ca3Si2O7
Ripidolite-14A	7.98	29.46	21.48	Mg3Fe2Al2Si3O10(OH)8
Ripidolite-7A	5.42	29.46	24.04	Mg3Fe2Al2Si3O10(OH)8
Rutile	3.15	-6.39	-9.53	TiO2
S	-22.53	-50.90	-28.38	S
S2(g)	-50.70	-62.12	-11.41	S2
Sanidine_high	-0.46	-3.91	-3.45	KAlSi3O8
Saponite-Ca	5.54	16.25	10.70	Ca.165Mg3Al.33Si3.67O10(OH)2
Saponite-H	4.12	14.40	10.28	H.33Mg3Al.33Si3.67O10(OH)2
Saponite-K	4.58	15.76	11.18	K.33Mg3Al.33Si3.67O10(OH)2
Saponite-Mg	5.20	15.69	10.50	Mg3.165Al.33Si3.67O10(OH)2
Saponite-Na	4.95	16.21	11.27	Na.33Mg3Al.33Si3.67O10(OH)2
Scolecite	2.30	2.41	0.11	CaAl2Si3O10:3H2O
Sellaite	-6.24	-17.86	-11.62	MgF2
Sepiolite	-0.78	16.83	17.61	Mg4Si6O15(OH)2:6H2O
Si	-62.55	28.89	91.43	Si
Si(g)	-104.54	28.89	133.42	Si
Siderite	-1.43	-4.46	-3.03	FeCO3
SiF4(g)	-33.59	-53.87	-20.28	SiF4
Sillimanite	-3.38	-3.94	-0.56	Al2SiO5
SiO2(am)	-0.60	-2.43	-1.83	SiO2
Smectite-high-Fe-Mg	3.23	5.14	1.90	Ca.025Na.1K.2Fe.5Fe.2Mg1.15Al1.25Si3.5H2O12
Smectite-low-Fe-Mg	2.21	1.20	-1.01	Ca.02Na.15K.2Fe.29Fe.16Mg.9Al1.25Si3.75H2O12
SO2(g)	-17.68	-18.65	-0.96	SO2
Spinel	-4.69	6.36	11.05	Al2MgO4
Starkeyite	-9.42	-10.65	-1.23	MgSO4:4H2O
Stilbite	2.92	-6.04	-8.96	Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O
Sylvite	-5.90	-4.67	1.23	KCl
Syngenite	-9.85	-17.51	-7.66	K2Ca(SO4)2:2H2O
Tachyhydrite	-42.41	-25.94	16.46	Mg2CaCl6:12H2O
Talc	4.48	13.84	9.36	Mg3Si4O10(OH)2
Thénardite	-5.76	-7.49	-1.73	Na2SO4
Thermonatrite	-9.86	-0.79	9.07	Na2CO3:H2O
Ti	-124.48	24.94	149.41	Ti
Ti(g)	-199.53	24.94	224.46	Ti
Ti2O3	-40.32	2.89	43.21	Ti2O3

Ti3O5	-38.49	-3.50	35.00	Ti3O5
TiB2	-246.40	66.30	312.70	TiB2
TiC	-137.53	44.45	181.98	TiC
TiCl2	-79.46	-8.35	71.11	TiCl2
TiCl3	-64.50	-24.99	39.51	TiCl3
TiCl4(g)	-69.91	-41.63	28.28	TiCl4
TiF4(am)	-45.61	-57.82	-12.21	TiF4
TiO(alpha)	-51.97	9.27	61.24	TiO
TiO(g)	-136.41	9.27	145.68	TiO
Titanite	-717.25	2.39	719.64	CaTiSiO5
Tobermorite-11A	-2.18	41.46	43.64	Ca5Si6H11O22.5
Tobermorite-14A	-5.21	41.46	46.67	Ca5Si6H21O27.5
Tobermorite-9A	-2.58	41.46	44.04	Ca5Si6H6O20
Tremolite	11.90	42.25	30.36	Ca2Mg5Si8O22(OH)2
Tridymite	-0.31	-2.43	-2.13	SiO2
Troilite	-22.69	-27.90	-5.21	FeS
Trona-K	-21.29	-9.82	11.48	K2NaH(CO3)2·2H2O
Wairakite	0.42	-0.03	-0.45	CaAl2Si4O10(OH)4
Wollastonite	0.66	8.78	8.12	CaSiO3
Wustite	0.66	6.30	5.64	Fe.9470
Xonotlite	-6.14	52.68	58.82	Ca6Si6O17(OH)2
Zoisite	2.35	12.87	10.52	Ca2Al3(SiO4)3OH

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

TIME STEP 1 YEAR

Reaction step 10.

WARNING: CCode incomplete at cvcode_steps 100. Cell: 0 Time: 1.751660e+08 Ccode calls: 1, continuing...

WARNING: CCode incomplete at cvcode_steps 100. Cell: 0 Time: 1.372354e+09 Ccode calls: 2, continuing...

Using solution 1. UW-8B
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

Time step: 3e+09 seconds (Incremented time: 3.33333e+09 seconds)

Rate name	Delta Moles	Total Moles	Reactant	Coefficient
Quartz	1.706e-01	7.998e+01	SiO2	1
Anorthite	2.126e-05	1.382e+01	CaAl2(SiO4)2	1
Albite	-4.318e-05	1.710e+01	NaAlSi3O8	1
K-Feldspar	-1.919e-06	1.774e+01	KAlSi3O8	1
Corundum	8.528e-02	1.678e+01	Al2O3	1
Enstatite	7.591e-09	2.845e+01	MgSiO3	1
Ilmenite	1.659e-09	1.090e+00	FeTiO3	1
Kaolinite	-8.528e-02	0.000e+00	Al2Si2O5(OH)4	1
Alunite	-0.000e+00	0.000e+00	KAl3(OH)6(SO4)2	1
Calcite	-1.286e-07	1.430e+00	CaCO3	1
Anhydrite	-2.846e-06	3.820e+00	CaSO4	1

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

Phase	SI	log IAP	log K(T, P)	Initial	Moles in assemblage Final	Delta
CO2(g)	-2.30	-4.50	-2.20	0.000e+00	0	0.000e+00

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

Elements	Molality	Moles
Al	1.846e-05	2.240e-05
B	1.508e-03	1.830e-03
C	6.772e-05	8.218e-05
Ca	2.378e-03	2.886e-03
Cl	2.540e-02	3.082e-02
F	2.614e-06	3.172e-06
Fe	3.547e-07	4.304e-07
K	1.418e-03	1.721e-03
Mg	2.940e-06	3.567e-06
Na	3.246e-02	3.939e-02
S	3.495e-04	4.242e-04
Si	3.693e-03	4.482e-03
Ti	3.547e-07	4.304e-07

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

pH	=	7.166	Charge balance
pe	=	-1.445	Adjusted to redox equilibrium
Density (g/cm³)	=	0.88322	
Volume (L)	=	1.37694	
Activity of water	=	0.999	
Ionic strength (mol/kgw)	=	3.386e-02	
Mass of water (kg)	=	1.214e+00	
Total alkalinity (eq/kg)	=	4.141e-04	
Total CO2 (mol/kg)	=	6.772e-05	
Temperature (°C)	=	200.00	
Pressure (atm)	=	249.00	
Electrical balance (eq)	=	1.479e-02	
Percent error, 100*(Cat- An)/(Cat+ An)	=	19.33	
Iterations	=	1134	
Total H	=	1.347676e+02	
Total O	=	6.739764e+01	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	1.124e-04	8.576e-05	-3.949	-4.067	-0.118	(0)
H+	8.399e-08	6.824e-08	-7.076	-7.166	-0.090	0.00
H2O	5.553e+01	9.989e-01	1.744	-0.000	0.000	20.44

A1	1.846e-05					
AlO2-	1.717e-05	1.319e-05	-4.765	-4.880	-0.114	(0)
NaAlO2	1.189e-06	1.189e-06	-5.925	-5.925	0.000	(0)
HAIO2	9.803e-08	9.803e-08	-7.009	-7.009	0.000	(0)
Al (OH) 2+	5.339e-12	4.103e-12	-11.273	-11.387	-0.114	(0)
AlOH+2	1.816e-16	6.435e-17	-15.741	-16.191	-0.451	(0)
AlF+2	2.740e-21	9.710e-22	-20.562	-21.013	-0.451	(0)
AlF2+	8.663e-22	6.656e-22	-21.062	-21.177	-0.114	(0)
Al+3	3.764e-22	5.639e-23	-21.424	-22.249	-0.824	(0)
AlF3	1.443e-23	1.443e-23	-22.841	-22.841	0.000	(0)
AlSO4+	4.686e-24	3.601e-24	-23.329	-23.444	-0.114	(0)
Al (SO4) 2-	2.270e-26	1.744e-26	-25.644	-25.758	-0.114	(0)
AlF4-	8.123e-27	6.242e-27	-26.090	-26.205	-0.114	(0)
Al2 (OH) 2+4	9.439e-37	1.805e-38	-36.025	-37.743	-1.718	(0)
Al3 (OH) 4+5	0.000e+00	0.000e+00	-49.116	-51.738	-2.622	(0)
Al1304 (OH) 24+7	0.000e+00	0.000e+00	-151.940	-157.080	-5.140	(0)
B (-5)	0.000e+00					
BH4-	0.000e+00	0.000e+00	-79.095	-79.209	-0.114	(0)
B (3)	1.508e-03					
B (OH) 3	1.466e-03	1.466e-03	-2.834	-2.834	0.000	(0)
BO2-	4.070e-05	3.127e-05	-4.390	-4.505	-0.114	(0)
CaB (OH) 4+	9.885e-07	7.595e-07	-6.005	-6.119	-0.114	(0)
NaB (OH) 4	6.349e-07	6.349e-07	-6.197	-6.197	0.000	(0)
MgB (OH) 4+	5.014e-10	3.853e-10	-9.300	-9.414	-0.114	(0)
BF2 (OH) 2-	1.405e-15	1.080e-15	-14.852	-14.967	-0.114	(0)
B2O (OH) 5-	8.460e-18	6.500e-18	-17.073	-17.187	-0.114	(0)
BF4-	1.670e-28	1.283e-28	-27.777	-27.892	-0.114	(0)
BF3OH-	1.745e-40	1.341e-40	-39.758	-39.873	-0.114	(0)
C (-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-80.233	-80.233	0.000	(0)
C (-3)	0.000e+00					
C2H6	0.000e+00	0.000e+00	-48.142	-48.142	0.000	(0)
C (-4)	9.545e-35					
CH4	9.545e-35	9.545e-35	-34.020	-34.020	0.000	(0)
C (2)	1.467e-18					
CO	1.467e-18	1.467e-18	-17.834	-17.834	0.000	(0)
C (4)	6.772e-05					
CO2	3.160e-05	3.185e-05	-4.500	-4.497	0.003	52.92
HCO3-	2.778e-05	2.134e-05	-4.556	-4.671	-0.114	(0)
CaHCO3+	5.822e-06	4.474e-06	-5.235	-5.349	-0.114	(0)
CaCO3	2.454e-06	2.454e-06	-5.610	-5.610	0.000	(0)
NaHCO3	3.185e-08	3.185e-08	-7.497	-7.497	0.000	(0)
CO3-2	2.981e-08	1.056e-08	-7.526	-7.976	-0.451	(0)
MgHCO3+	2.571e-09	1.976e-09	-8.590	-8.704	-0.114	(0)
FeHCO3+	1.749e-09	1.344e-09	-8.757	-8.872	-0.114	(0)
(CO2) 2	1.516e-10	1.528e-10	-9.819	-9.816	0.003	105.85
MgCO3	1.484e-10	1.484e-10	-9.829	-9.829	0.000	(0)
FeCO3	9.450e-11	9.450e-11	-10.025	-10.025	0.000	(0)
NaCO3-	2.267e-12	1.742e-12	-11.644	-11.759	-0.114	(0)
FeCO3+	3.359e-20	2.581e-20	-19.474	-19.588	-0.114	(0)
Ca	2.378e-03					
Ca+2	2.151e-03	8.214e-04	-2.667	-3.085	-0.418	(0)
CaSO4	1.460e-04	1.460e-04	-3.836	-3.836	0.000	(0)
CaCl+4	6.901e-05	5.303e-05	-4.161	-4.275	-0.114	(0)
CaHCO3+	5.822e-06	4.474e-06	-5.235	-5.349	-0.114	(0)
CaCO3	2.454e-06	2.454e-06	-5.610	-5.610	0.000	(0)
CaCl2	2.376e-06	2.376e-06	-5.624	-5.624	0.000	(0)
CaB (OH) 4+	9.885e-07	7.595e-07	-6.005	-6.119	-0.114	(0)
CaF+	3.053e-07	2.346e-07	-6.515	-6.630	-0.114	(0)
CaOH+	2.519e-09	1.935e-09	-8.599	-8.713	-0.114	(0)
Cl (-1)	2.540e-02					
Cl-	2.473e-02	1.872e-02	-1.607	-1.728	-0.121	(0)
NaCl	5.753e-04	5.753e-04	-3.240	-3.240	0.000	(0)
CaCl+	6.901e-05	5.303e-05	-4.161	-4.275	-0.114	(0)
KCl	1.230e-05	1.230e-05	-4.910	-4.910	0.000	(0)
CaCl2	2.376e-06	2.376e-06	-5.624	-5.624	0.000	(0)
MgCl+	1.193e-07	9.165e-08	-6.923	-7.038	-0.114	(0)
FeCl+	3.659e-08	2.811e-08	-7.437	-7.551	-0.114	(0)
HCl	1.046e-09	1.046e-09	-8.981	-8.981	0.000	(0)
FeCl2	2.923e-11	2.923e-11	-10.534	-10.534	0.000	(0)
FeCl4-2	2.194e-12	7.564e-13	-11.659	-12.121	-0.462	(0)
FeCl+2	1.631e-19	5.781e-20	-18.787	-19.238	-0.451	(0)
FeCl2+	2.648e-22	2.034e-22	-21.577	-21.692	-0.114	(0)
FeCl4-	1.116e-28	8.575e-29	-27.952	-28.067	-0.114	(0)
Cl (1)	3.284e-29					
HClO	2.168e-29	2.168e-29	-28.664	-28.664	0.000	(0)
ClO-	1.115e-29	8.569e-30	-28.953	-29.067	-0.114	(0)
Cl (3)	0.000e+00					
ClO2-	0.000e+00	0.000e+00	-49.859	-49.974	-0.114	(0)
HClO2	0.000e+00	0.000e+00	-53.970	-53.970	0.000	(0)
Cl (5)	0.000e+00					
ClO3-	0.000e+00	0.000e+00	-62.007	-62.124	-0.118	(0)
Cl (7)	0.000e+00					
ClO4-	0.000e+00	0.000e+00	-77.729	-77.847	-0.118	(0)
F	2.614e-06					
F-	2.257e-06	1.722e-06	-5.646	-5.764	-0.118	(0)
CaF+	3.053e-07	2.346e-07	-6.515	-6.630	-0.114	(0)
NaF	4.191e-08	4.191e-08	-7.378	-7.378	0.000	(0)
HF	8.556e-09	8.556e-09	-8.068	-8.068	0.000	(0)
MgF+	3.903e-10	2.999e-10	-9.409	-9.523	-0.114	(0)
FeF+	6.158e-12	4.732e-12	-11.211	-11.325	-0.114	(0)
HF2-	6.302e-15	4.842e-15	-14.201	-14.315	-0.114	(0)
BF2 (OH) 2-	1.405e-15	1.080e-15	-14.852	-14.967	-0.114	(0)
H2F2	8.093e-20	8.093e-20	-19.092	-19.092	0.000	(0)
FeF+2	5.727e-20	2.030e-20	-19.242	-19.693	-0.451	(0)
FeF2+	1.986e-20	1.526e-20	-19.702	-19.816	-0.114	(0)
AlF+2	2.740e-21	9.710e-22	-20.562	-21.013	-0.451	(0)
AlF2+	8.663e-22	6.656e-22	-21.062	-21.177	-0.114	(0)
AlF3	1.443e-23	1.443e-23	-22.841	-22.841	0.000	(0)
AlF4-	8.123e-27	6.242e-27	-26.090	-26.205	-0.114	(0)
BF4-	1.670e-28	1.283e-28	-27.777	-27.892	-0.114	(0)
BF3OH-	1.745e-40	1.341e-40	-39.758	-39.873	-0.114	(0)
SiF6-2	0.000e+00	0.000e+00	-40.401	-40.864	-0.462	(0)
Fe (2)	3.546e-07					
Fe+2	3.142e-07	1.199e-07	-6.503	-6.921	-0.418	(0)
FeCl+	3.659e-08	2.811e-08	-7.437	-7.551	-0.114	(0)
FeHCO3+	1.749e-09	1.344e-09	-8.757	-8.872	-0.114	(0)
FeSO4	1.186e-09	1.186e-09	-8.926	-8.926	0.000	(0)

FeOH+	8.234e-10	6.327e-10	-9.084	-9.199	-0.114	(0)
FeCO3	9.450e-11	9.450e-11	-10.025	-10.025	0.000	(0)
FeCl2	2.923e-11	2.923e-11	-10.534	-10.534	0.000	(0)
FeF+	6.158e-12	4.732e-12	-11.211	-11.325	-0.114	(0)
FeCl4-2	2.194e-12	7.564e-13	-11.659	-12.121	-0.462	(0)
Fe (OH) 2	8.382e-14	8.382e-14	-13.077	-13.077	0.000	(0)
Fe (OH) 3-	7.244e-17	5.566e-17	-16.140	-16.254	-0.114	(0)
Fe (OH) 4-2	2.693e-24	9.284e-25	-23.570	-24.032	-0.462	(0)
Fe (3)	2.340e-11					
Fe (OH) 3	1.996e-11	1.996e-11	-10.700	-10.700	0.000	(0)
Fe (OH) 2+	3.330e-12	2.558e-12	-11.478	-11.592	-0.114	(0)
Fe (OH) 4-	1.088e-13	8.362e-14	-12.963	-13.078	-0.114	(0)
FeOH+2	1.307e-15	4.632e-16	-14.884	-15.334	-0.451	(0)
FeSO4+	5.114e-19	3.929e-19	-18.291	-18.406	-0.114	(0)
FeCl+2	1.631e-19	5.781e-20	-18.787	-19.238	-0.451	(0)
FeF+2	5.727e-20	2.030e-20	-19.242	-19.693	-0.451	(0)
FeCO3+	3.359e-20	2.581e-20	-19.474	-19.588	-0.114	(0)
Fe+3	2.871e-20	4.301e-21	-19.542	-20.366	-0.824	(0)
FeF2+	1.986e-20	1.526e-20	-19.702	-19.816	-0.114	(0)
FeCl2+	2.648e-22	2.034e-22	-21.577	-21.692	-0.114	(0)
Fe (SO4) 2-	3.566e-26	2.740e-26	-25.448	-25.562	-0.114	(0)
Fe2 (OH) 2+4	3.020e-28	5.775e-30	-27.520	-29.238	-1.718	(0)
FeCl4-	1.116e-28	8.575e-29	-27.952	-28.067	-0.114	(0)
Fe3 (OH) 4+5	1.292e-36	3.087e-39	-35.889	-38.511	-2.622	(0)
H (0)	5.060e-12					
H2	2.530e-12	2.566e-12	-11.597	-11.591	0.006	(0)
K	1.418e-03					
K+	1.399e-03	1.059e-03	-2.854	-2.975	-0.121	(0)
KCl	1.230e-05	1.230e-05	-4.910	-4.910	0.000	(0)
KSO4-	7.244e-06	5.566e-06	-5.140	-5.254	-0.114	(0)
KHSO4	1.229e-10	1.229e-10	-9.911	-9.911	0.000	(0)
KOH	6.124e-11	6.124e-11	-10.213	-10.213	0.000	(0)
Mg	2.940e-06					
MgSO4	1.974e-06	1.974e-06	-5.705	-5.705	0.000	(0)
Mg+2	8.429e-07	3.502e-07	-6.074	-6.456	-0.382	(0)
MgCl+	1.193e-07	9.165e-08	-6.923	-7.038	-0.114	(0)
MgHCO3+	2.571e-09	1.976e-09	-8.590	-8.704	-0.114	(0)
MgB (OH) 4+	5.014e-10	3.853e-10	-9.300	-9.414	-0.114	(0)
MgF+	3.903e-10	2.999e-10	-9.409	-9.523	-0.114	(0)
MgCO3	1.484e-10	1.484e-10	-9.829	-9.829	0.000	(0)
Mg4 (OH) 4+4	1.082e-35	2.069e-37	-34.966	-36.684	-1.718	(0)
Na	3.246e-02					
Na+	3.184e-02	2.446e-02	-1.497	-1.611	-0.114	(0)
NaCl	5.753e-04	5.753e-04	-3.240	-3.240	0.000	(0)
NaHSiO3	3.270e-05	3.270e-05	-4.485	-4.485	0.000	(0)
NaSO4-	1.313e-05	1.009e-05	-4.882	-4.996	-0.114	(0)
NaOH	2.467e-06	2.467e-06	-5.608	-5.608	0.000	(0)
NaAlO2	1.189e-06	1.189e-06	-5.925	-5.925	0.000	(0)
NaB (OH) 4	6.349e-07	6.349e-07	-6.197	-6.197	0.000	(0)
NaF	4.191e-08	4.191e-08	-7.378	-7.378	0.000	(0)
NaHCO3	3.185e-08	3.185e-08	-7.497	-7.497	0.000	(0)
NaCO3-	2.267e-12	1.742e-12	-11.644	-11.759	-0.114	(0)
O (0)	5.480e-32					
O2	2.740e-32	2.779e-32	-31.562	-31.556	0.006	(0)
S (-2)	3.829e-28					
HS-	3.012e-28	2.298e-28	-27.521	-27.639	-0.118	(0)
H2S	7.648e-29	7.648e-29	-28.116	-28.116	0.000	(0)
S-2	5.184e-30	1.866e-30	-29.285	-29.725	-0.439	(0)
S2-2	0.000e+00	0.000e+00	-51.916	-52.379	-0.462	(0)
S3-2	0.000e+00	0.000e+00	-73.355	-73.817	-0.462	(0)
S4-2	0.000e+00	0.000e+00	-94.939	-95.402	-0.462	(0)
S5-2	0.000e+00	0.000e+00	-116.664	-117.126	-0.462	(0)
S (2)	3.239e-34					
S2O3-2	1.619e-34	5.583e-35	-33.791	-34.253	-0.462	(0)
HS2O3-	0.000e+00	0.000e+00	-40.291	-40.405	-0.114	(0)
S (3)	0.000e+00					
S2O4-2	0.000e+00	0.000e+00	-41.171	-41.610	-0.439	(0)
S (4)	4.251e-16					
HSO3-	4.147e-16	3.186e-16	-15.382	-15.497	-0.114	(0)
SO3-2	1.008e-17	3.571e-18	-16.997	-17.447	-0.451	(0)
SO2	2.746e-19	2.746e-19	-18.561	-18.561	0.000	(0)
H2SO3	2.717e-23	2.717e-23	-22.566	-22.566	0.000	(0)
S2O6-2	2.192e-33	7.557e-34	-32.659	-33.122	-0.462	(0)
S3O6-2	0.000e+00	0.000e+00	-56.243	-56.706	-0.462	(0)
S4O6-2	0.000e+00	0.000e+00	-67.409	-67.871	-0.462	(0)
S5O6-2	0.000e+00	0.000e+00	-101.467	-101.930	-0.462	(0)
S (5)	1.459e-36					
S2O5-2	7.295e-37	2.515e-37	-36.137	-36.599	-0.462	(0)
S (6)	3.495e-04					
SO4-2	1.810e-04	6.241e-05	-3.742	-4.205	-0.462	(0)
CaSO4	1.460e-04	1.460e-04	-3.836	-3.836	0.000	(0)
NaSO4-	1.313e-05	1.009e-05	-4.882	-4.996	-0.114	(0)
KSO4-	7.244e-06	5.566e-06	-5.140	-5.254	-0.114	(0)
MgSO4	1.974e-06	1.974e-06	-5.705	-5.705	0.000	(0)
HSO4-	1.649e-07	1.267e-07	-6.783	-6.897	-0.114	(0)
FeSO4	1.186e-09	1.186e-09	-8.926	-8.926	0.000	(0)
KHSO4	1.229e-10	1.229e-10	-9.911	-9.911	0.000	(0)
FeSO4+	5.114e-19	3.929e-19	-18.291	-18.406	-0.114	(0)
H2SO4	2.769e-20	2.769e-20	-19.558	-19.558	0.000	(0)
AlSO4+	4.686e-24	3.601e-24	-23.329	-23.444	-0.114	(0)
Fe (SO4) 2-	3.566e-26	2.740e-26	-25.448	-25.562	-0.114	(0)
Al (SO4) 2-	2.270e-26	1.744e-26	-25.644	-25.758	-0.114	(0)
S (7)	0.000e+00					
S2O8-2	0.000e+00	0.000e+00	-46.402	-46.865	-0.462	(0)
S (8)	6.754e-35					
HSO5-	6.754e-35	5.190e-35	-34.170	-34.285	-0.114	(0)
Si	3.693e-03					
SiO2	3.549e-03	3.549e-03	-2.450	-2.450	0.000	(0)
HSiO3-	1.121e-04	8.612e-05	-3.950	-4.065	-0.114	(0)
NaHSiO3	3.270e-05	3.270e-05	-4.485	-4.485	0.000	(0)
H6 (H2SiO4) 4-2	6.373e-09	2.197e-09	-8.196	-8.658	-0.462	(0)
H2SiO4-2	3.140e-11	1.082e-11	-10.503	-10.966	-0.462	(0)
H4 (H2SiO4) 4-4	1.692e-15	2.365e-17	-14.772	-16.626	-1.855	(0)
SiF6-2	0.000e+00	0.000e+00	-40.401	-40.864	-0.462	(0)
Ti	3.547e-07					
Ti (OH) 4	3.547e-07	3.547e-07	-6.450	-6.450	0.000	(0)

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

Phase	SI**	log IAP	log K(473 K, 249 atm)	
Afwillite	-9.59	28.84	38.43	Ca3Si2O4 (OH) 6
Akermanite	0.16	25.47	25.31	Ca2MgSi2O7
Al	-63.90	22.92	86.81	Al
Al (g)	-93.33	22.92	116.25	Al
Al2 (SO4) 3	-46.23	-57.11	-10.89	Al2 (SO4) 3
Al2 (SO4) 3:6H2O	-40.07	-57.11	-17.04	Al2 (SO4) 3:6H2O
Albite	0.00	-2.55	-2.55	NaAlSi3O8
Albite_high	-0.61	-2.55	-1.94	NaAlSi3O8
Albite_low	-0.00	-2.55	-2.55	NaAlSi3O8
AlF3	-17.55	-39.54	-21.99	AlF3
Alum-K	-26.28	-33.64	-7.36	KAl (SO4) 2:12H2O
Alunite	-15.34	-35.14	-19.79	KAl3 (OH) 6 (SO4) 2
Amesite-14A	2.21	23.59	21.38	Mg4Al4Si2O10 (OH) 8
Analcime	-0.30	-9.72	-0.09	Na.96Al.96Si2.04O6:H2O
Analcime-dehy	-3.93	-0.39	3.54	Na.96Al.96Si2.04O6
Anatase	2.00	-6.45	-8.45	TiO2
Andalusite	-3.24	-3.95	-0.72	Al2SiO5
Andradite	17.76	28.65	10.89	Ca3Fe2 (SiO4) 3
Anhydrite	0.00	-7.29	-7.29	CaSO4
Ankerite	-1.28	-4.88	-3.59	CaMg0.3Fe0.7 (CO3) 2
Annite	7.98	18.32	10.34	KFe3AlSi3O10 (OH) 2
Anorthite	0.00	4.84	4.84	CaAl2 (SiO4) 2
Antarcticite	-10.30	-6.54	3.75	CaCl2:6H2O
Anthophyllite	4.38	35.53	31.15	Mg7Si8O22 (OH) 2
Antigorite	50.49	294.72	244.23	Mg48Si34O85 (OH) 62
Aphthitalite	-15.06	-18.95	-3.89	NaK3 (SO4) 2
Aragonite	-0.15	-0.59	-0.44	CaCO3
Arcanite	-8.25	-10.16	-1.90	K2SO4
Artinite	-7.02	3.91	10.93	Mg2CO3 (OH) 2:3H2O
B	-46.50	20.83	67.34	B
B (g)	-101.24	20.83	122.07	B
B2O3	-9.33	-5.67	3.66	B2O3
Bassanite	-0.66	-7.29	-6.63	CaSO4:0.5H2O
Beidellite-Ca	-0.90	-8.89	-7.99	Ca.165Al2.33Si3.67O10 (OH) 2
Beidellite-H	-2.33	-10.74	-8.41	H.33Al2.33Si3.67O10 (OH) 2
Beidellite-K	-1.86	-9.36	-7.50	K.33Al2.33Si3.67O10 (OH) 2
Beidellite-Mg	-1.24	-9.44	-8.21	Mg.165Al2.33Si3.67O10 (OH) 2
Beidellite-Na	-1.48	-8.91	-7.43	Na.33Al2.33Si3.67O10 (OH) 2
BF3 (g)	-30.85	-41.62	-10.77	BF3
Bischofite	-13.97	-9.91	4.05	MgCl2:6H2O
Bloedit	-15.39	-18.09	-2.70	Na2Mg (SO4) 2:4H2O
Boehmite	-0.58	-0.75	-0.17	AlO2H
Borax	-17.58	-0.23	17.35	Na2 (B4O5 (OH) 4) :8H2O
Boric_acid	-3.87	-2.83	1.03	B (OH) 3
Brucite	-1.33	7.88	9.20	Mg (OH) 2
Burkeite	-25.07	-15.58	9.49	Na6CO3 (SO4) 2
C	-17.57	19.72	37.29	C
C (g)	-88.79	19.72	108.51	C
Ca	-59.03	27.02	86.05	Ca
Ca (g)	-72.86	27.02	99.88	Ca
Ca-Al Pyroxene	-3.74	7.29	11.04	CaAl2SiO6
Ca2Al2O5:8H2O	-37.85	20.98	58.83	Ca2Al2O5:8H2O
Ca2Cl2 (OH) 2:H2O	-21.42	4.70	26.12	Ca2Cl2 (OH) 2:H2O
Ca3Al2O6	-26.80	32.23	59.03	Ca3Al2O6
Ca4Al2Fe2O10	-20.65	45.74	66.39	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-62.65	43.47	106.12	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-58.74	43.47	102.21	Ca4Al2O7:19H2O
Ca4Cl2 (OH) 6:13H2O	-40.06	27.19	67.25	Ca4Cl2 (OH) 6:13H2O
CaAl2O4	-7.87	9.74	17.62	CaAl2O4
CaAl2O4:10H2O	-27.46	9.74	37.20	CaAl2O4:10H2O
CaAl4O7	-13.15	8.24	21.39	CaAl4O7
Calcite	-0.00	-0.59	-0.59	CaCO3
Carnallite	-18.55	-14.62	3.93	KMgCl3:6H2O
CaSO4:0.5H2O (beta)	-0.69	-7.29	-6.60	CaSO4:0.5H2O
Celadonite	1.21	1.51	0.30	KMgAlSi4O10 (OH) 2
CH4 (g)	-31.28	-34.02	-2.75	CH4
Chalcedony	-0.17	-2.45	-2.28	SiO2
Chamosite-7A	3.05	10.87	7.82	Fe2Al2SiO5 (OH) 4
Chloromagnesite	-19.90	-9.91	9.99	MgCl2
Chrysotile	2.58	18.73	16.15	Mg3Si2O5 (OH) 4
Cl2 (g)	-32.07	-33.56	-1.49	Cl2
Clinochlore-14A	5.07	30.52	25.46	Mg5Al2Si3O10 (OH) 8
Clinochlore-7A	2.49	30.52	28.03	Mg5Al2Si3O10 (OH) 8
Clinoptilolite-Ca	3.63	-18.69	-22.32	Ca1.7335Al3.45Fe.017Si14.533036:10.922H2O
Clinoptilolite-dehy-Ca	-15.74	-18.68	-2.95	Ca1.7335Al3.45Fe.017Si14.533036
Clinoptilolite-dehy-K	-25.90	-23.65	2.25	K3.467Al3.45Fe.017Si14.533036
Clinoptilolite-dehy-Na	-21.60	-18.92	2.68	Na3.467Al3.45Fe.017Si14.533036
Clinoptilolite-hy-Ca	3.05	-18.69	-21.74	Ca1.7335Al3.45Fe.017Si14.533036:11.645H2O
Clinoptilolite-hy-K	-4.38	-23.65	-19.27	K3.467Al3.45Fe.017Si14.533036:7.499H2O
Clinoptilolite-hy-Na	-2.31	-18.93	-16.62	Na3.467Al3.45Fe.017Si14.533036:10.877H2O
Clinoptilolite-K	-6.81	-23.66	-16.85	K3.467Al3.45Fe.017Si14.533036:10.922H2O
Clinoptilolite-Na	-2.34	-18.93	-16.59	Na3.467Al3.45Fe.017Si14.533036:10.922H2O
Clinoroisite	2.40	12.89	10.48	Ca2Al3Si3O12 (OH)
CO (g)	-15.04	-17.83	-2.80	CO
CO2 (g)	-2.30	-4.50	-2.20	CO2
Coesite	-0.53	-2.45	-1.92	SiO2
Colemanite	-16.14	5.49	21.63	Ca2B6O11:5H2O
Cordierite_anhyd	-6.70	0.50	7.19	Mg2Al4Si5O18
Cordierite_hydr	-5.43	0.49	5.92	Mg2Al4Si5O18:H2O
Corundum	0.00	-1.50	-1.50	Al2O3
Cristobalite (alpha)	-0.31	-2.45	-2.14	SiO2
Cristobalite (beta)	-0.51	-2.45	-1.94	SiO2
Cronstedtite-7A	15.83	14.63	-1.19	Fe2Fe2SiO5 (OH) 4
Daphnite-14A	12.22	28.20	15.97	Fe5AlAlSi3O10 (OH) 8
Daphnite-7A	9.73	28.20	18.47	Fe5AlAlSi3O10 (OH) 8
Dawsonite	-6.45	-7.03	-0.58	NaAlCO3 (OH) 2
Diaspore	-0.39	-0.75	-0.36	AlHO2
Dicalcium_silicate	-2.28	20.04	22.32	Ca2SiO4
Diopside	3.13	14.22	11.09	CaMgSi2O6
Dolomite	-1.77	-4.55	-2.78	CaMg (CO3) 2
Dolomite-dis	-2.52	-4.55	-2.03	CaMg (CO3) 2
Dolomite-ord	-1.76	-4.55	-2.79	CaMg (CO3) 2
Enstatite	-0.00	5.43	5.43	MgSiO3
Epidote	10.04	14.77	4.73	Ca2FeAl2Si3O12OH
Epidote-ord	10.01	14.77	4.76	FeCa2Al2 (OH) (SiO4) 3

Epsomite	-8.30	-10.66	-2.36	MgSO4:7H2O
Etringite	-33.16	10.35	43.51	Ca6Al2(SO4)3(OH)12:26H2O
F2(g)	-71.18	-41.64	29.55	F2
Payalite	3.86	12.37	8.51	Fe2SiO4
Fe	-11.29	23.19	34.47	Fe
Fe(OH)2	-0.29	7.41	7.70	Fe(OH)2
Fe(OH)3	1.19	1.13	-0.06	Fe(OH)3
Fe2(SO4)3	-34.02	-53.35	-19.33	Fe2(SO4)3
FeF2	-11.22	-18.45	-7.23	FeF2
FeF3	-15.37	-37.66	-22.29	FeF3
FeO	0.84	7.41	6.57	FeO
Ferrite-Ca	10.15	13.51	3.35	CaFe2O4
Ferrite-Dicalcium	-0.17	24.75	24.92	Ca2Fe2O5
Ferrite-Mg	8.26	10.14	1.88	MgFe2O4
Ferrosillite	1.93	4.96	3.03	FeSiO3
FeSO4	-7.30	-11.13	-3.83	FeSO4
Fluorite	-3.83	-14.61	-10.78	CaF2
Forsterite	-0.72	13.30	14.02	Mg2SiO4
Foshagite	-3.04	37.63	40.68	Ca4Si3O9(OH)2:0.5H2O
Gaylussite	-12.20	-1.32	10.88	CaNa2(CO3)2:5H2O
Gehlenite	-4.44	18.54	22.98	Ca2Al2SiO7
Gibbsite	-1.01	-0.75	0.26	Al(OH)3
Gismondine	-31.07	9.68	40.75	Ca2Al4Si4O16:9H2O
Glauberite	-9.25	-14.72	-5.47	Na2Ca(SO4)2
Goethite	4.64	1.13	-3.51	FeOOH
Greenalite	6.63	17.33	10.70	Fe3Si2O5(OH)4
Grossular	3.78	24.88	21.10	Ca3Al2(SiO4)3
Gypsum	-1.04	-7.29	-6.25	CaSO4:2H2O
Gyrolite	-0.80	15.14	15.94	Ca2Si3O7(OH)2:1.5H2O
H2(g)	-8.78	-11.59	-2.81	H2
H2O(g)	1.21	-0.00	-1.21	H2O
H2S(g)	-26.53	-34.80	-8.28	H2S
Hallite	-4.58	-3.34	1.24	NaCl
Hatrurite	-13.08	31.29	44.36	Ca3SiO5
HCl(g)	-9.78	-8.89	0.89	HCl
Hedenbergite	3.54	13.76	10.21	CaFe(SiO3)2
Hematite	11.47	2.26	-9.20	Fe2O3
Hercynite	0.34	5.91	5.57	FeAl2O4
Hexahydrite	-8.60	-10.66	-2.07	MgSO4:6H2O
Hillebrandite	-3.01	20.04	23.05	Ca2SiO3(OH)2:0.17H2O
Huntite	-9.00	-12.47	-3.47	CaMg3(CO3)4
Hydroboracite	-18.30	2.12	20.42	MgCaB6O11:6H2O
Hydromagnesite	-17.19	-7.97	9.22	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-11.36	-6.54	4.82	CaCl2
Ice	-0.88	-0.00	0.88	H2O
Illite	-0.78	-5.82	-5.04	K0.6Mg0.25Al1.8Al0.5Si3.5O10(OH)2
Ilmenite	-0.00	0.96	0.96	FeTiO3
Jadeite	-1.64	-0.10	1.55	NaAl(SiO3)2
Jarosite	-5.49	-29.49	-24.00	KFe3(SO4)2(OH)6
Jarosite-Na	-22.34	-28.13	-5.79	NaFe3(SO4)2(OH)6
K	-33.36	12.08	45.44	K
K(g)	-38.31	12.08	50.39	K
K-Feldspar	0.00	-3.91	-3.91	KAlSi3O8
K2CO3:1.5H2O	-16.75	-3.46	13.29	K2CO3:1.5H2O
K2O	-48.04	8.38	56.42	K2O
K3H(SO4)2	-20.88	-24.50	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-65.03	-37.50	27.54	K8H4(CO3)6:3H2O
Kainite	-14.88	-15.36	-0.48	KMgClSO4:3H2O
KAl(SO4)2	-24.10	-33.63	-9.53	KAl(SO4)2
Kalichinite	-7.93	-7.65	0.28	KHCO3
Kalsilite	-1.93	0.99	2.92	KAlSiO4
Kaolinite	-1.58	-6.40	-4.83	Al2Si2O5(OH)4
Katoite	-46.03	32.23	78.26	Ca3Al2H12O12
Kieserite	-10.34	-10.66	-0.32	MgSO4:H2O
KMgCl3	-25.55	-14.61	10.94	KMgCl3
KMgCl3:2H2O	-22.49	-14.61	7.88	KMgCl3:2H2O
KNaCO3:6H2O	-12.01	-2.09	9.92	KNaCO3:6H2O
Kyanite	-3.24	-3.95	-0.71	Al2SiO5
Lansfordite	-8.52	-3.96	4.56	MgCO3:5H2O
Larnite	-2.94	20.04	22.99	Ca2SiO4
Laumontite	1.20	-0.06	-1.26	CaAl2Si4O12:4H2O
Lawrencite	-12.29	-10.38	1.92	FeCl2
Lawsonite	0.39	4.84	4.45	CaAl2Si2O7(OH)2:H2O
Leonite	-16.48	-20.82	-4.34	K2Mg(SO4)2:4H2O
Lime	-8.68	11.25	19.93	CaO
Magnesite	-2.73	-3.96	-1.23	MgCO3
Magnetite	14.26	9.67	-4.59	Fe3O4
Margarite	-1.11	3.34	4.45	CaAl4Si2O10(OH)2
Maximum Microcline	0.02	-3.91	-3.93	KAlSi3O8
Mayenite	-105.70	124.43	230.13	Ca12Al14O33
Melanterite	-8.51	-11.13	-2.62	FeSO4:7H2O
Mercurite	-12.91	-14.35	-1.44	KHSO4
Merwinite	-2.55	36.71	39.26	MgCa3(SiO4)2
Mesolite	2.40	2.27	-0.13	Na.676Ca.657Al1.99Si3.01O10:2.647H2O
Mg	-50.19	23.65	73.84	Mg
Mg(g)	-60.49	23.65	84.15	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-6.06	-8.69	-2.63	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-6.21	-6.72	-0.51	Mg1.5SO4(OH)
MgCl2:2H2O	-15.33	-9.91	5.42	MgCl2:2H2O
MgCl2:4H2O	-13.19	-9.91	3.28	MgCl2:4H2O
MgCl2:H2O	-16.81	-9.91	6.90	MgCl2:H2O
MgOHCl	-8.51	-1.02	7.49	MgOHCl
MgSO4	-7.97	-10.66	-2.69	MgSO4
Minnesotaite	7.80	12.43	4.63	Fe3Si4O10(OH)2
Mirabilite	-13.84	-7.43	6.41	Na2SO4:10H2O
Misenite	-85.15	-96.23	-11.08	K8H6(SO4)7
Molysite	-26.29	-25.55	0.74	FeCl3
Monohydrocalcite	-1.90	-0.59	1.31	CaCO3:H2O
Monticellite	0.40	16.67	16.27	CaMgSiO4
Montmor-Ca	0.38	-6.60	-6.98	Ca.165Mg.33Al1.67Si4O10(OH)2
Montmor-K	-0.47	-7.07	-6.60	K.33Mg.33Al1.67Si4O10(OH)2
Montmor-Mg	0.07	-7.16	-7.23	Mg.495Al1.67Si4O10(OH)2
Montmor-Na	-0.16	-6.62	-6.46	Na.33Mg.33Al1.67Si4O10(OH)2
Mordenite	-0.52	-7.84	-7.33	Ca.2895Na.361Al.948Si5.06O12:3.468H2O
Mordenite-dehy	-8.80	-7.84	0.96	Ca.2895Na.361Al.948Si5.06O12
Muscovite	-0.39	-5.41	-5.02	KAl3Si3O10(OH)2
Na	-29.31	13.44	42.76	Na
Na(g)	-35.96	13.44	49.40	Na

Na2CO3	-9.01	-0.73	8.28	Na2CO3
Na2CO3:7H2O	-14.91	-0.73	14.18	Na2CO3:7H2O
Na2O	-33.95	11.11	45.06	Na2O
Na2SiO3	-8.05	8.66	16.71	Na2SiO3
Na3H(SO4)2	-19.52	-20.41	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.14	-22.15	-6.01	Na4Ca(SO4)3:2H2O
Na4SiO4	-29.90	19.77	49.67	Na4SiO4
Na6Si2O7	-42.64	28.43	71.07	Na6Si2O7
NaFeO2	-2.82	6.68	9.50	NaFeO2
Nahcolite	-6.88	-6.28	0.60	NaHCO3
Natrolite	-2.17	2.25	4.42	Na2Al2Si3O10:2H2O
Natron	-14.31	-0.73	13.58	Na2CO3:10H2O
Natrosilite	-7.80	6.21	14.01	Na2Si2O5
Nepheline	-1.88	2.35	4.24	NaAlSiO4
Nesquehonite	-8.23	-3.96	4.26	MgCO3:3H2O
Nontronite-Ca	12.07	-5.12	-17.20	Ca.165Fe2Al.33Si3.67H2O12
Nontronite-H	10.67	-6.98	-17.65	H.33Fe2Al.33Si3.67H2O12
Nontronite-K	11.11	-5.60	-16.71	K.33Fe2Al.33Si3.67H2O12
Nontronite-Mg	11.74	-5.68	-17.41	Mg.165Fe2Al.33Si3.67H2O12
Nontronite-Na	11.49	-5.15	-16.64	Na.33Fe2Al.33Si3.67H2O12
O2(g)	-28.69	-31.56	-2.87	O2
Okenite	-2.59	6.35	8.93	CaSi2O4(OH)2:2H2O
Oxychloride-Mg	-18.58	6.86	25.43	Mg2Cl(OH)3:4H2O
Paragonite	-1.07	-4.05	-2.98	NaAl3Si3O10(OH)2
Pargasite	2.08	42.59	40.51	NaCa2Al3Mg4Si6O22(OH)2
Pentahydrate	-8.99	-10.66	-1.67	MgSO4:5H2O
Periclase	-3.77	7.88	11.64	MgO
Phlogopite	4.29	19.72	15.42	KAlMg3Si3O10(OH)2
Picromerite	-16.04	-20.82	-4.78	K2Mg(SO4)2:6H2O
Pirssonite	-12.53	-1.32	11.21	Na2Ca(CO3)2:2H2O
Polyhalite	-20.97	-35.40	-14.43	K2MgCa2(SO4)4:2H2O
Portlandite	-2.95	11.25	14.20	Ca(OH)2
Prehnite	3.59	13.64	10.05	Ca2Al2Si3O10(OH)2
Pseudowollastonite	0.62	8.80	8.17	CaSiO3
Pyrite	-38.78	-58.13	-19.35	FeS2
Pyrophyllite	-2.04	-11.30	-9.26	Al2Si4O10(OH)2
Pyrrhotite	-22.26	-27.39	-5.14	FeS
Quartz	0.00	-2.45	-2.45	SiO2
Rankinite	-2.05	28.84	30.89	Ca3Si2O7
Ripidolite-14A	8.11	29.59	21.48	Mg3Fe2Al2Si3O10(OH)8
Ripidolite-7A	5.56	29.59	24.04	Mg3Fe2Al2Si3O10(OH)8
Rutile	3.08	-6.45	-9.53	TiO2
S	-22.21	-50.58	-28.38	S
S2(g)	-50.06	-61.47	-11.41	S2
Sanidine_high	-0.46	-3.91	-3.45	KAlSi3O8
Saponite-Ca	5.54	16.24	10.70	Ca.165Mg3Al.33Si3.67O10(OH)2
Saponite-H	4.11	14.39	10.28	H.33Mg3Al.33Si3.67O10(OH)2
Saponite-K	4.59	15.77	11.18	K.33Mg3Al.33Si3.67O10(OH)2
Saponite-Mg	5.19	15.69	10.50	Mg3.165Al.33Si3.67O10(OH)2
Saponite-Na	4.95	16.22	11.27	Na.33Mg3Al.33Si3.67O10(OH)2
Scolecite	2.28	2.39	0.11	CaAl2Si3O10:3H2O
Sellaite	-6.36	-17.98	-11.62	MgF2
Sepiolite	-0.81	16.80	17.61	Mg4Si6O15(OH)2:6H2O
Si	-62.33	29.11	91.43	Si
Si(g)	-104.32	29.11	133.42	Si
Siderite	-1.39	-4.43	-3.03	FeCO3
SiF4(g)	-33.89	-54.17	-20.28	SiF4
Sillimanite	-3.40	-3.95	-0.56	Al2SiO5
SiO2(am)	-0.62	-2.45	-1.83	SiO2
Smectite-high-Fe-Mg	3.25	5.15	1.90	Ca.025Na.1K.2Fe.5Fe.2Mg1.15Al1.25Si3.5H2O12
Smectite-low-Fe-Mg	2.20	1.19	-1.01	Ca.02Na.15K.2Fe.29Fe.16Mg.9Al1.25Si3.75H2O12
SO2(g)	-17.60	-18.56	-0.96	SO2
Spinel	-4.68	6.37	11.05	Al2MgO4
Starkeyite	-9.44	-10.66	-1.23	MgSO4:4H2O
Stilbite	2.85	-6.11	-8.96	Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O
Sylvite	-5.94	-4.70	1.23	KCl
Syngenite	-9.79	-17.45	-7.66	K2Ca(SO4)2:2H2O
Tachyhydrite	-42.83	-26.37	16.46	Mg2CaCl6:12H2O
Talc	4.47	13.83	9.36	Mg3Si4O10(OH)2
Thenardite	-5.70	-7.43	-1.73	Na2SO4
Thermonatrite	-9.80	-0.73	9.07	Na2CO3:H2O
Ti	-124.30	25.11	149.41	Ti
Ti(g)	-199.36	25.11	224.46	Ti
Ti2O3	-40.33	2.88	43.21	Ti2O3
Ti3O5	-38.57	-3.57	35.00	Ti3O5
TiB2	-245.93	66.77	312.70	TiB2
TiC	-137.16	44.83	181.98	TiC
TiCl2	-79.57	-8.46	71.11	TiCl2
TiCl3	-64.75	-25.24	39.51	TiCl3
TiCl4(g)	-70.30	-42.02	28.28	TiCl4
TiF4(am)	-45.95	-58.17	-12.21	TiF4
TiO(alpha)	-51.91	9.33	61.24	TiO
TiO(g)	-136.36	9.33	145.68	TiO
Titanite	-717.29	2.35	719.64	CaTiSiO5
Tobermorite-11A	-2.11	41.53	43.64	Ca5Si6H11O22.5
Tobermorite-14A	-5.15	41.53	46.67	Ca5Si6H21O27.5
Tobermorite-9A	-2.51	41.53	44.04	Ca5Si6H6O20
Tremolite	11.91	42.27	30.36	Ca2Mg5Si8O22(OH)2
Tridymite	-0.32	-2.45	-2.13	SiO2
Troilite	-22.19	-27.39	-5.21	FeS
Trona-K	-21.21	-9.74	11.48	K2NaH(CO3)2:2H2O
Wairakite	0.39	-0.06	-0.45	CaAl2Si4O10(OH)4
Wollastonite	0.67	8.80	8.12	CaSiO3
Wustite	0.71	6.35	5.64	Fe.947O
Xenotlite	-6.05	52.78	58.82	Ca6Si6O17(OH)2
Zoisite	2.37	12.89	10.52	Ca2Al3(SiO4)3OH

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

End of simulation.

APPENDIX C

EQUILIBRIUM MODELING RESULT IN BATURRADEN FIELD

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\llnl.dat

Reading data base.

LLNL AQUEOUS_MODEL_PARAMETERS
NAMED_EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\llnl.dat
SOLUTION_SPECIES
CO3-2 + 2 H+ = CO2 + H2O
log_k 16.681
delta_h -5.738 kcal
analytical_expression 464.1965 0.09344813 -26986.16 -165.75951 2248628.9
dw 1.92e-9
vm 7.29 0.92 2.07 -1.23 -1.60 # ref. 1 + McBride et al. 2015, JCEd 60, 171
2CO2 = (CO2)2 # activity correction for CO2 solubility at high P, T
log_k -1.8
analytical_expression 8.68 -0.0103 -2190
vm 14.58 1.84 4.14 -2.46 -3.20
END

End of simulation.

Reading input data for simulation 2.

PHASES
CO2(g)
CO2 = CO2
log_k -1.468
delta_h -4.776 kcal
analytical_expression 10.5624 -2.3547e-2 -3972.8 0 5.8746e5 1.9194e-5
t_c 304.2 # critical T, K
p_c 72.86 # critical P, atm
omega 0.225 # acentric factor
Ankerite
CaMg0.3Fe0.7(CO3)2 + 2H+ = Ca++ + 0.3Mg++ + 0.7Fe++ + 2HCO3-
log_k 1.54
delta_h 0
analytical_expression -1.8649e+03 -2.9583e-01 1.0468e+05 6.7554e+02 -6.0514e+06
END

End of simulation.

Reading input data for simulation 3.

SOLUTION 1 Pancuran 3
temp 200
pH 6
pe 4
redox pe
units ppm
density 1
C(4) 695.4
Ca 196.5
Cl 724
Mg 185
Na 377
S(6) 600
K 76.7
B 3.97
Li 0.58
Si 163.75
water 1 # kg
pressure 194 atm
EQUILIBRIUM_PHASES 1 Reservoir
Albite 0 25.16
Anhydrite 0 0
Ankerite 0 0
Anorthite 0 23.38
Aragonite 0 0
CO2(g) 2.288 1.2
Calcite 0 0
Dawsonite 0 0
Diopside 0 8.08
Dolomite 0 0
Enstatite 0 29.35
Gypsum 0 0

```

Ilmenite 0 1.33
K-Feldspar 0 8.08
Kaolinite 0 2.95
Magnesite 0 0
Montmor-Na 0 2.08
Quartz 0 18.12
Siderite 0 0
Zircon 0 0
SELECTED_OUTPUT 1
file D:\20182 SPRING\Thesis PHREEQC\2. Baturaden\baturaden_output_equil.sel
reset false
solution true
ph true
pe true
temperature true
molalities K+ Na+ Ca+2 Mg+2
HCO3- SO4-2 Cl- CO3-2
saturation_indices Anhydrite Gypsum Aragonite Calcite
Dolomite Magnesite CO2(g)
USER_PUNCH
10 PUNCH description
PRINT
species false
END
-----
Beginning of initial solution calculations.
-----
Initial solution 1. Pancuran 3
WARNING: USER_PUNCH: Headings count does not match number of calls to PUNCH.
-----Solution composition-----
Elements Molality Moles
B 3.683e-04 3.683e-04
C(4) 1.143e-02 1.143e-02
Ca 4.918e-03 4.918e-03
Cl 2.048e-02 2.048e-02
K 1.968e-03 1.968e-03
Li 8.381e-05 8.381e-05
Mg 7.635e-03 7.635e-03
Na 1.645e-02 1.645e-02
S(6) 6.266e-03 6.266e-03
Si 2.734e-03 2.734e-03
-----Description of solution-----
pH = 6.000
pe = 4.000
Density (g/cm³) = 0.87966
Volume (L) = 1.14007
Activity of water = 0.999
Ionic strength (mol/kgw) = 3.196e-02
Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = 9.343e-04
Total CO2 (mol/kg) = 1.143e-02
Temperature (°C) = 200.00
Pressure (atm) = 194.00
Electrical balance (eq) = 9.655e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 18.69
Iterations = 9
Total H = 1.110527e+02
Total O = 5.558076e+01
-----Saturation indices-----
Phase SI** log IAP log K(473 K, 194 atm)
Afwillite -16.01 22.50 38.50 Ca3Si2O4(OH)6
Akermanite -3.19 22.15 25.35 Ca2MgSi2O7
Anhydrite 0.43 -6.86 -7.29 CaSO4
Antarcticite -10.26 -6.43 3.83 CaCl2·6H2O
Anthophyllite 10.26 41.51 31.25 Mg7Si8O22(OH)2
Antigorite 92.93 338.13 245.21 Mg48Si34O85(OH)62
Aphthitalite -14.64 -18.53 -3.89 NaK3(SO4)2
Aragonite 0.29 -0.15 -0.44 CaCO3
Arcanite -7.82 -9.73 -1.90 K2SO4
Artinite -2.63 8.36 11.00 Mg2CO3(OH)2·3H2O
B -59.90 7.42 67.32 B
B(g) -114.64 7.42 122.05 B
B2O3 -10.49 -6.87 3.63 B2O3
Bassanite -0.24 -6.86 -6.62 CaSO4·0.5H2O
Bischofite -10.91 -6.78 4.13 MgCl2·6H2O
Bloedite -12.43 -15.08 -2.65 Na2Mg(SO4)2·4H2O
Borax -22.96 -5.55 17.42 Na2(B4O5(OH)4)·8H2O
Boric acid -4.47 -3.43 1.03 B(OH)3
Brucite -0.37 8.86 9.23 Mg(OH)2
Burkeite -26.40 -16.91 9.49 Na6CO3(SO4)2
C -32.17 5.11 37.28 C
C(g) -103.39 5.11 108.50 C
Ca -69.62 16.44 86.06 Ca
Ca(g) -83.45 16.44 99.90 Ca
Ca2Cl2(OH)2·2H2O -23.38 2.78 26.16 Ca2Cl2(OH)2·2H2O
Ca4Cl2(OH)6·13H2O -46.29 21.19 67.49 Ca4Cl2(OH)6·13H2O
Calcite 0.44 -0.15 -0.59 CaCO3
Carnallite -15.43 -11.43 4.01 KMgCl3·6H2O
CaSO4·0.5H2O(beta) -0.26 -6.86 -6.60 CaSO4·0.5H2O
Chalcedony -0.29 -2.56 -2.28 SiO2
Chloromagnesite -16.76 -6.78 9.99 MgCl2
Chrysotile 5.25 21.45 16.21 Mg3Si2O5(OH)4
Cl2(g) -21.36 -22.87 -1.51 Cl2
CO2(g) 0.19 -1.98 -2.17 CO2
Coesite -0.65 -2.56 -1.92 SiO2
Colemanite -23.79 -2.19 21.60 Ca2B6O11·5H2O
Cristobalite(alpha) -0.42 -2.56 -2.14 SiO2
Cristobalite(beta) -0.63 -2.56 -1.94 SiO2

```

Dicalcium_silicate	-6.49	15.86	22.34	Ca2SiO4
Diopside	1.83	12.94	11.12	CaMgSi2O6
Dolomite	2.13	-0.65	-2.78	CaMg (CO3) 2
Dolomite-dis	1.39	-0.65	-2.03	CaMg (CO3) 2
Dolomite-ord	2.14	-0.65	-2.79	CaMg (CO3) 2
Enstatite	0.86	6.30	5.44	MgSiO3
Epsomite	-4.94	-7.21	-2.27	MgSO4·7H2O
Forsterite	1.11	15.16	14.05	Mg2SiO4
Foshagite	-11.60	29.15	40.74	Ca4Si3O9 (OH) 2·0.5H2O
Gaylussite	-12.26	-1.32	10.94	CaNa2 (CO3) 2·5H2O
Glauberite	-9.26	-14.73	-5.47	Na2Ca (SO4) 2
Gypsum	-0.63	-6.86	-6.23	CaSO4·2H2O
Gyrolite	-5.27	10.73	15.99	Ca2Si3O7 (OH) 2·1.5H2O
H2 (g)	-17.34	-20.15	-2.81	H2
H2O (g)	1.13	-0.00	-1.13	H2O
Halite	-4.96	-3.72	1.24	NaCl
Hatruite	-19.34	25.07	44.40	Ca3SiO5
HCl (g)	-8.71	-7.82	0.89	HCl
Hexahydrite	-5.22	-7.21	-1.99	MgSO4·6H2O
Hillebrandite	-7.24	15.85	23.09	Ca2SiO3 (OH) 2·0.17H2O
Huntite	1.83	-1.64	-3.47	CaMg3 (CO3) 4
Hydroboracite	-22.94	-2.54	20.41	MgCaB6O11·6H2O
Hydromagnesite	-2.43	6.87	9.30	Mg5 (CO3) 4 (OH) 2·4H2O
Hydrophilite	-11.24	-6.43	4.82	CaCl2
Ice	-0.89	-0.00	0.89	H2O
K	-38.66	6.79	45.45	K
K (g)	-43.61	6.79	50.40	K
K2CO3·1.5H2O	-16.33	-3.02	13.31	K2CO3·1.5H2O
K2O	-50.09	6.34	56.43	K2O
K3H (SO4) 2	-19.01	-22.63	-3.62	K3H (SO4) 2
K8H4 (CO3) 6·3H2O	-58.38	-30.80	27.58	K8H4 (CO3) 6·3H2O
Kainite	-11.41	-11.86	-0.44	KMgClSO4·3H2O
Kalicinite	-6.47	-6.19	0.28	KHCO3
Kieserite	-6.90	-7.21	-0.31	MgSO4·H2O
KMgCl3	-22.36	-11.43	10.94	KMgCl3
KMgCl3·2H2O	-19.33	-11.43	7.90	KMgCl3·2H2O
KNaCO3·6H2O	-12.09	-2.09	9.99	KNaCO3·6H2O
Lansfordite	-5.12	-0.50	4.62	MgCO3·5H2O
Larnite	-7.15	15.86	23.01	Ca2SiO4
Leonite	-12.65	-16.94	-4.29	K2Mg (SO4) 2·4H2O
Li	-40.28	5.44	45.72	Li
Li (g)	-52.25	5.44	57.69	Li
Lime	-10.73	9.21	19.94	CaO
Magnesite	0.73	-0.50	-1.23	MgCO3
Mercallite	-11.46	-12.90	-1.44	KHSO4
Merwinite	-7.95	31.36	39.31	MgCa3 (SiO4) 2
Mg	-57.76	16.09	73.85	Mg
Mg (g)	-68.07	16.09	84.16	Mg
Mg1.25SO4 (OH) 0.5·0.5H2O	-2.37	-4.99	-2.62	Mg1.25SO4 (OH) 0.5·0.5H2O
Mg1.5SO4 (OH)	-2.28	-2.78	-0.50	Mg1.5SO4 (OH)
MgCl2·2H2O	-12.22	-6.78	5.44	MgCl2·2H2O
MgCl2·4H2O	-10.11	-6.78	3.33	MgCl2·4H2O
MgCl2·H2O	-13.69	-6.78	6.91	MgCl2·H2O
MgOHCl	-6.46	1.04	7.51	MgOHCl
MgSO4	-4.52	-7.21	-2.69	MgSO4
Mirabilite	-14.41	-7.88	6.53	Na2SO4·10H2O
Misenite	-76.05	-87.12	-11.08	K8H6 (SO4) 7
Monohydrocalcite	-1.47	-0.15	1.32	CaCO3·H2O
Monticellite	-0.79	15.51	16.29	CaMgSiO4
Na	-35.05	7.71	42.76	Na
Na (g)	-41.70	7.71	49.41	Na
Na2CO3	-9.44	-1.16	8.28	Na2CO3
Na2CO3·7H2O	-15.43	-1.17	14.26	Na2CO3·7H2O
Na2O	-36.87	8.19	45.07	Na2O
Na2SiO3	-11.09	5.63	16.72	Na2SiO3
Na3H (SO4) 2	-18.95	-19.85	-0.89	Na3H (SO4) 2
Na4Ca (SO4) 3·2H2O	-16.62	-22.61	-5.98	Na4Ca (SO4) 3·2H2O
Na4SiO4	-35.87	13.83	49.69	Na4SiO4
Na6Si2O7	-51.65	19.46	71.10	Na6Si2O7
Nahcolite	-5.86	-5.26	0.60	NaHCO3
Natron	-14.87	-1.17	13.70	Na2CO3·10H2O
Natrosilite	-10.95	3.07	14.02	Na2Si2O5
Nesquehonite	-4.80	-0.50	4.30	MgCO3·3H2O
O2 (g)	-11.60	-14.47	-2.87	O2
Okenite	-4.89	4.08	8.97	CaSi2O4 (OH) 2·H2O
Oxychloride-Mg	-15.62	9.90	25.52	Mg2Cl (OH) 3·4H2O
Pentahydrite	-5.60	-7.21	-1.61	MgSO4·5H2O
Periclase	-2.79	8.86	11.65	MgO
Picromerite	-12.23	-16.94	-4.71	K2Mg (SO4) 2·6H2O
Pirssonite	-12.55	-1.31	11.23	Na2Ca (CO3) 2·2H2O
Polyhalite	-16.25	-30.65	-14.40	K2MgCa2 (SO4) 4·2H2O
Portlandite	-5.01	9.21	14.22	Ca (OH) 2
Pseudowollastonite	-1.54	6.65	8.19	CaSiO3
Quartz	-0.11	-2.56	-2.45	SiO2
Rankinite	-8.42	22.50	30.93	Ca3Si2O7
Sepiolite	2.31	20.06	17.75	Mg4Si6O15 (OH) 2·6H2O
Si	-79.53	11.90	91.43	Si
Si (g)	-121.52	11.90	133.42	Si
SiO2 (am)	-0.73	-2.56	-1.83	SiO2
Starkeyite	-6.03	-7.21	-1.18	MgSO4·4H2O
Sylvite	-5.88	-4.65	1.23	KCl
Syngenite	-8.94	-16.59	-7.64	K2Ca (SO4) 2·H2O
Tachyhydrite	-36.60	-19.99	16.61	Mg2CaCl6·12H2O
Talc	6.92	16.33	9.41	Mg3Si4O10 (OH) 2
Thenardite	-6.14	-7.87	-1.73	Na2SO4
Thermonatrite	-10.25	-1.16	9.08	Na2CO3·H2O
Tobermorite-11A	-13.11	30.66	43.77	Ca5Si6H11O22.5
Tobermorite-14A	-16.21	30.66	46.87	Ca5Si6H21O27.5
Tobermorite-9A	-13.48	30.66	44.14	Ca5Si6H6O20
Tremolite	11.75	42.21	30.46	Ca2Mg5Si8O22 (OH) 2
Tridymite	-0.44	-2.56	-2.13	SiO2
Trona-K	-19.78	-8.28	11.50	K2NaH (CO3) 2·2H2O
Wollastonite	-1.49	6.65	8.14	CaSiO3
Xonotlite	-19.03	39.87	58.91	Ca6Si6O17 (OH) 2

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

Beginning of batch-reaction calculations.

Reaction step 1.

WARNING: Element Zr is contained in Zircon (which has 0.0 mass),
but is not in solution or other phases.
Using solution 1. Pancuran 3
Using pure phase assemblage 1. Reservoir

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

Phase	SI	log IAP	log K(T, P)	Moles in assemblage		
				Initial	Final	Delta
Albite	-0.00	-2.52	-2.52	2.516e+01	2.579e+01	6.325e-01
Anhydrite	-2.71	-10.00	-7.29	0.000e+00	0	0.000e+00
Ankerite	-0.25	-3.84	-3.59	0.000e+00	0	0.000e+00
Anorthite	-0.00	4.89	4.89	2.338e+01	1.133e+00	-2.225e+01
Aragonite	-0.83	-1.27	-0.44	0.000e+00	0	0.000e+00
CO2(g)	-1.37	-3.54	-2.17	1.200e+00	0	-1.200e+00
Calcite	-0.68	-1.27	-0.59	0.000e+00	0	0.000e+00
Dawsonite	-0.97	-1.53	-0.56	0.000e+00	0	0.000e+00
Diopside	-0.00	11.12	11.12	8.080e+00	2.973e+01	2.165e+01
Dolomite	-0.00	-2.78	-2.78	0.000e+00	6.050e-01	6.050e-01
Enstatite	0.00	5.44	5.44	2.935e+01	7.792e+00	-2.156e+01
Gypsum	-3.78	-10.01	-6.23	0.000e+00	0	0.000e+00
Ilmenite	-0.00	0.95	0.95	1.330e+00	1.330e+00	-2.090e-08
K-Feldspar	-0.00	-3.89	-3.89	8.080e+00	8.079e+00	-1.382e-03
Kaolinite	-0.00	-4.77	-4.77	2.950e+00	2.660e+01	2.365e+01
Magnesite	-0.28	-1.51	-1.23	0.000e+00	0	0.000e+00
Montmor-Na	-1.14	-7.55	-6.41	2.080e+00	0	-2.080e+00
Quartz	-1.52	-3.97	-2.45	1.812e+01	0	-1.812e+01
Siderite	-0.00	-3.03	-3.03	0.000e+00	1.903e-08	1.903e-08
Zircon		Element not present.		0.000e+00	0	0.000e+00

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

Elements	Molality	Moles
Al	1.548e-01	2.872e-02
B	1.986e-03	3.683e-04
C	7.782e-03	1.443e-03
Ca	1.119e-06	2.075e-07
Cl	1.104e-01	2.048e-02
Fe	1.012e-08	1.876e-09
K	1.806e-02	3.349e-03
Li	4.519e-04	8.381e-05
Mg	5.386e-06	9.989e-07
Na	3.794e-01	7.037e-02
S	3.379e-02	6.266e-03
Si	3.746e-04	6.948e-05
Ti	1.127e-07	2.090e-08

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

pH = 8.537 Charge balance
pe = -3.195 Adjusted to redox equilibrium
Density (g/cm³) = 0.90074
Volume (L) = 0.21134
Activity of water = 0.989
Ionic strength (mol/kgw) = 3.319e-01
Mass of water (kg) = 1.855e-01
Total alkalinity (eq/kg) = 6.324e-01
Total CO2 (mol/kg) = 7.782e-03
Temperature (°C) = 200.00
Pressure (atm) = 194.00
Electrical balance (eq) = 9.655e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 8.50
Iterations = 23
Total H = 2.059863e+01
Total O = 1.038660e+01

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

Phase	SI**	log IAP	log K(473 K, 194 atm)	
Afwillite	-17.52	20.99	38.50	Ca3Si2O4(OH) 6
Akermanite	-4.58	20.76	25.35	Ca2MgSi2O7
Al	-60.41	26.42	86.83	Al
Al(g)	-89.84	26.42	116.26	Al
Al2(SO4)3	-44.88	-55.77	-10.89	Al2(SO4) 3
Al2(SO4)3:6H2O	-38.83	-55.80	-16.97	Al2(SO4) 3:6H2O
Albite	-0.00	-2.52	-2.52	NaAlSi3O8
Albite_high	-0.61	-2.52	-1.92	NaAlSi3O8
Albite_low	-0.00	-2.52	-2.52	NaAlSi3O8
Alum-K	-24.12	-31.33	-7.21	KAl(SO4) 2:12H2O
Alunite	-8.38	-28.10	-19.72	KAl3(OH) 6(SO4) 2
Amesite-14A	14.50	36.05	21.55	Mg4Al4Si2O10(OH) 8
Analcime	0.97	0.91	-0.06	Na.96Al.96Si2.04O6:H2O
Analcime-dehy	-2.65	0.92	3.56	Na.96Al.96Si2.04O6
Anatase	1.53	-6.94	-8.47	TiO2
Andalusite	-0.10	-0.78	-0.68	Al2SiO5
Andradite	8.52	19.48	10.97	Ca3Fe2(SiO4) 3
Anhydrite	-2.71	-10.00	-7.29	CaSO4
Ankerite	-0.25	-3.84	-3.59	CaMg0.3Fe0.7(CO3) 2
Annite	9.36	19.77	10.41	KFe3AlSi3O10(OH) 2
Anorthite	-0.00	4.89	4.89	CaAl2(SiO4) 2
Antarcticite	-13.83	-10.00	3.83	CaCl2:6H2O
Anthophyllite	2.84	34.09	31.25	Mg7Si8O22(OH) 2
Antigorite	71.29	316.50	245.21	Mg48Si34O85(OH) 62
Aphthitalite	-9.31	-12.19	-3.89	NaK3(SO4) 2
Aragonite	-0.83	-1.27	-0.44	CaCO3
Arcanite	-4.87	-6.78	-1.90	K2SO4
Artinite	-3.11	7.88	11.00	Mg2CO3(OH) 2:3H2O
B	-45.48	21.84	67.32	B
B(g)	-100.21	21.84	122.05	B

B2O3	-9.60	-5.98	3.63	B2O3
Bassanite	-3.38	-10.01	-6.62	CaSO4·0.5H2O
Beidellite-Ca	-1.34	-9.28	-7.93	Ca _{1.165} Al _{2.33} Si _{3.67} O ₁₀ (OH) ₂
Beidellite-H	-2.52	-10.87	-8.35	H _{3.3} Al _{2.33} Si _{3.67} O ₁₀ (OH) ₂
Beidellite-K	-1.30	-8.75	-7.44	K _{3.3} Al _{2.33} Si _{3.67} O ₁₀ (OH) ₂
Beidellite-Mg	-1.17	-9.32	-8.15	Mg _{1.165} Al _{2.33} Si _{3.67} O ₁₀ (OH) ₂
Beidellite-Na	-0.93	-8.30	-7.37	Na _{3.3} Al _{2.33} Si _{3.67} O ₁₀ (OH) ₂
Bischofite	-14.37	-10.24	4.13	MgCl ₂ ·6H ₂ O
Bloedite	-11.66	-14.31	-2.65	Na ₂ Mg(SO ₄) ₂ ·4H ₂ O
Boehmite	1.74	1.59	-0.15	Al ₂ O ₃ H
Borax	-13.82	3.60	17.42	Na ₂ (B ₄ O ₅ (OH) ₄):8H ₂ O
Boric_acid	-4.03	-3.00	1.03	B(OH) ₃
Brucite	0.18	9.41	9.23	Mg(OH) ₂
Burkeite	-12.91	-3.42	9.49	Na ₆ CO ₃ (SO ₄) ₂
C	-15.09	22.19	37.28	C
C(g)	-86.31	22.19	108.50	C
Ca	-59.86	26.20	86.06	Ca
Ca(g)	-73.69	26.20	99.90	Ca
Ca-Al Pyroxene	-2.22	8.86	11.09	CaAl ₂ SiO ₆
Ca ₂ Al ₂ O ₅ ·8H ₂ O	-36.54	22.45	58.99	Ca ₂ Al ₂ O ₅ ·8H ₂ O
Ca ₂ Cl ₂ (OH) ₂ ·2H ₂ O	-26.49	-0.33	26.16	Ca ₂ Cl ₂ (OH) ₂ ·2H ₂ O
Ca ₃ Al ₂ O ₆	-26.97	32.14	59.11	Ca ₃ Al ₂ O ₆
Ca ₄ Al ₂ Fe ₂ O ₁₀	-22.28	44.24	66.51	Ca ₄ Al ₂ Fe ₂ O ₁₀
Ca ₄ Al ₂ O ₇ ·13H ₂ O	-64.64	41.72	106.37	Ca ₄ Al ₂ O ₇ ·13H ₂ O
Ca ₄ Al ₂ O ₇ ·19H ₂ O	-60.83	41.69	102.53	Ca ₄ Al ₂ O ₇ ·19H ₂ O
Ca ₄ Cl ₂ (OH) ₆ ·13H ₂ O	-48.59	18.90	67.49	Ca ₄ Cl ₂ (OH) ₆ ·13H ₂ O
CaAl ₂ O ₄	-4.83	12.84	17.67	CaAl ₂ O ₄
CaAl ₂ O ₄ ·10H ₂ O	-24.58	12.79	37.37	CaAl ₂ O ₄ ·10H ₂ O
CaAl ₄ O ₇	-5.45	16.02	21.48	CaAl ₄ O ₇
Calcite	-0.68	-1.27	-0.59	CaCO ₃
Carnallite	-17.62	-13.61	4.01	KMgCl ₃ ·6H ₂ O
CaSO ₄ ·0.5H ₂ O(beta)	-3.41	-10.01	-6.60	CaSO ₄ ·0.5H ₂ O
Celadonite	1.20	1.55	0.35	KMgAlSi ₄ O ₁₀ (OH) ₂
CH ₄ (g)	-27.25	-30.02	-2.78	CH ₄
Chalcedony	-1.69	-3.97	-2.28	SiO ₂
Chamosite-7A	7.07	14.98	7.91	Fe ₂ Al ₂ SiO ₅ (OH) ₄
Chloromagnesite	-20.20	-10.21	9.99	MgCl ₂
Chrysotile	4.07	20.28	16.21	Mg ₃ Si ₂ O ₅ (OH) ₄
Cl ₂ (g)	-34.67	-36.18	-1.51	Cl ₂
Clinocllore-14A	12.70	38.30	25.61	Mg ₅ Al ₂ Si ₃ O ₁₀ (OH) ₈
Clinocllore-7A	10.12	38.30	28.18	Mg ₅ Al ₂ Si ₃ O ₁₀ (OH) ₈
Clinoptilolite-Ca	-13.44	-35.54	-22.09	Ca _{1.7335} Al _{3.45} Fe _{0.1781} Si _{14.5330} 36:10.922H ₂ O
Clinoptilolite-dehy-Ca	-32.62	-35.48	-2.86	Ca _{1.7335} Al _{3.45} Fe _{0.1781} Si _{14.5330} 36
Clinoptilolite-dehy-K	-32.23	-29.89	2.33	K _{3.467} Al _{3.45} Fe _{0.1781} Si _{14.5330} 36
Clinoptilolite-dehy-Na	-27.93	-25.17	2.77	Na _{3.467} Al _{3.45} Fe _{0.1781} Si _{14.5330} 36
Clinoptilolite-hy-Ca	-14.03	-35.54	-21.51	Ca _{1.7335} Al _{3.45} Fe _{0.1781} Si _{14.5330} 36:11.645H ₂ O
Clinoptilolite-hy-K	-10.84	-29.93	-19.09	K _{3.467} Al _{3.45} Fe _{0.1781} Si _{14.5330} 36:7.499H ₂ O
Clinoptilolite-hy-Na	-8.82	-25.22	-16.40	Na _{3.467} Al _{3.45} Fe _{0.1781} Si _{14.5330} 36:10.877H ₂ O
Clinoptilolite-K	-13.32	-29.95	-16.63	K _{3.467} Al _{3.45} Fe _{0.1781} Si _{14.5330} 36:10.922H ₂ O
Clinoptilolite-Na	-8.85	-25.22	-16.37	Na _{3.467} Al _{3.45} Fe _{0.1781} Si _{14.5330} 36:10.922H ₂ O
Clinzoisite	1.59	12.16	10.57	Ca ₂ Al ₃ Si ₃ O ₁₂ (OH)
CO(g)	-13.33	-16.13	-2.80	CO
CO ₂ (g)	-1.37	-3.54	-2.17	CO ₂
Coesite	-2.06	-3.97	-1.92	SiO ₂
Colemanite	-20.26	1.34	21.60	Ca ₂ B ₆ O ₁₁ ·5H ₂ O
Cordierite_anhyd	-1.96	5.33	7.29	Mg ₂ Al ₄ Si ₅ O ₁₈
Cordierite_hydr	-0.70	5.33	6.03	Mg ₂ Al ₄ Si ₅ O ₁₈ ·H ₂ O
Corundum	4.65	3.19	-1.47	Al ₂ O ₃
Cristobalite(alpha)	-1.83	-3.97	-2.14	SiO ₂
Cristobalite(beta)	-2.03	-3.97	-1.94	SiO ₂
Cronstedtite-7A	15.35	14.25	-1.11	Fe ₂ Fe ₂ SiO ₅ (OH) ₄
Daphnite-14A	14.57	30.69	16.12	Fe ₅ Al ₁ Al ₃ Si ₃ O ₁₀ (OH) ₈
Daphnite-7A	12.07	30.69	18.61	Fe ₅ Al ₁ Al ₃ Si ₃ O ₁₀ (OH) ₈
Dawsonite	-0.97	-1.53	-0.56	NaAlCO ₃ (OH) ₂
Diaspore	1.93	1.59	-0.33	Al ₂ HO ₂
Dicalcium_silicate	-7.02	15.33	22.34	Ca ₂ SiO ₄
Diopside	-0.00	11.12	11.12	CaMgSi ₂ O ₆
Dolomite	-0.00	-2.78	-2.78	CaMg(CO ₃) ₂
Dolomite-dis	-0.74	-2.78	-2.03	CaMg(CO ₃) ₂
Dolomite-ord	0.01	-2.78	-2.79	CaMg(CO ₃) ₂
Enstatite	0.00	5.44	5.44	MgSiO ₃
Epidote	6.98	11.79	4.81	Ca ₂ FeAl ₂ Si ₃ O ₁₂ OH
Epidote-ord	6.95	11.79	4.85	FeCa ₂ Al ₂ (OH)(SiO ₄) ₃
Epsomite	-8.00	-10.28	-2.27	MgSO ₄ ·7H ₂ O
Etringite	-42.00	1.97	43.98	Ca ₆ Al ₂ (SO ₄) ₃ (OH) ₁₂ ·26H ₂ O
Eucryptite	-1.09	2.61	3.70	LiAlSiO ₄
Fayalite	3.27	11.80	8.53	Fe ₂ SiO ₄
Fe	-10.05	24.44	34.49	Fe
Fe(OH) ₂	0.16	7.88	7.72	Fe(OH) ₂
Fe(OH) ₃	1.24	1.22	-0.02	Fe(OH) ₃
Fe ₂ (SO ₄) ₃	-37.17	-56.51	-19.33	Fe ₂ (SO ₄) ₃
FeO	1.31	7.89	6.58	FeO
Ferrite-Ca	8.70	12.10	3.40	CaFe ₂ O ₄
Ferrite-Dicalcium	-3.23	21.75	24.98	Ca ₂ Fe ₂ O ₅
Ferrite-Mg	9.93	11.86	1.93	MgFe ₂ O ₄
Ferrosilite	0.87	3.91	3.04	FeSiO ₃
FeSO ₄	-7.94	-11.77	-3.83	FeSO ₄
Forsterite	0.80	14.85	14.05	Mg ₂ SiO ₄
Foshagite	-14.07	26.67	40.74	Ca ₄ Si ₃ O ₉ (OH) ₂ ·0.5H ₂ O
Gaylussite	-7.55	3.39	10.94	CaNa ₂ (CO ₃) ₂ ·5H ₂ O
Gehlenite	-4.52	18.51	23.04	Ca ₂ Al ₂ SiO ₇
Gibbsite	1.29	1.59	0.30	Al(OH) ₃
Gismondine	-31.22	9.74	40.96	Ca ₂ Al ₄ Si ₄ O ₁₆ ·9H ₂ O
Glauberite	-8.59	-14.05	-5.47	Na ₂ Ca(SO ₄) ₂
Goethite	4.71	1.22	-3.49	FeOOH
Greenalite	4.94	15.71	10.77	Fe ₃ Si ₂ O ₅ (OH) ₄
Grossular	-0.96	20.22	21.17	Ca ₃ Al ₂ (SiO ₄) ₃
Gypsum	-3.78	-10.01	-6.23	CaSO ₄ ·2H ₂ O
Gyrolite	-8.62	7.37	15.99	Ca ₂ Si ₃ O ₇ (OH) ₂ ·2:1.5H ₂ O
H ₂ (g)	-8.02	-10.83	-2.81	H ₂
H ₂ O(g)	1.13	-0.00	-1.13	H ₂ O
H ₂ S(g)	-24.55	-32.83	-8.28	H ₂ S
Halite	-3.25	-2.01	1.24	NaCl
Hatrunite	-19.43	24.98	44.40	Ca ₃ SiO ₅
HCl(g)	-10.70	-9.81	0.89	HCl
Hedenbergite	-0.64	9.59	10.24	CaFe(SiO ₃) ₂
Hematite	11.62	2.45	-9.17	Fe ₂ O ₃
Hercynite	5.45	11.08	5.62	FeAl ₂ O ₄

Hexahydrite	-8.28	-10.27	-1.99	MgSO ₄ ·6H ₂ O
Hillebrandite	-7.77	15.32	23.09	Ca ₂ SiO ₃ (OH) 2:0.17H ₂ O
Huntite	-2.32	-5.79	-3.47	CaMg ₃ (CO ₃) ₄
Hydroboracite	-19.31	1.10	20.41	MgCaB ₆ O ₁₁ ·6H ₂ O
Hydromagnesite	-5.94	3.35	9.30	Mg ₅ (CO ₃) ₄ (OH) 2:4H ₂ O
Hydrophilite	-14.79	-9.97	4.82	CaCl ₂
Ice	-0.90	-0.00	0.89	H ₂ O
Illite	0.95	-4.03	-4.98	K _{0.6} Mg _{0.25} Al _{1.8} Al _{0.5} Si _{3.5} O ₁₀ (OH) 2
Ilmenite	-0.00	0.95	0.95	FeTiO ₃
Jadeite	-0.12	1.45	1.57	NaAl(SiO ₃) ₂
Jarosite	-5.27	-29.20	-23.93	KFe ₃ (SO ₄) ₂ (OH) 6
Jarosite-Na	-22.13	-27.84	-5.71	NaFe ₃ (SO ₄) ₂ (OH) 6
K	-30.73	14.71	45.45	K
K (g)	-35.68	14.71	50.40	K
K-Feldspar	-0.00	-3.89	-3.89	KAlSi ₃ O ₈
K ₂ CO ₃ ·1.5H ₂ O	-11.36	1.95	13.31	K ₂ CO ₃ ·1.5H ₂ O
K ₂ O	-43.56	12.87	56.43	K ₂ O
K ₃ H(SO ₄) ₂	-16.37	-20.00	-3.62	K ₃ H(SO ₄) ₂
K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O	-41.61	-14.04	27.58	K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O
Kainite	-13.19	-13.63	-0.44	KMgClSO ₄ ·3H ₂ O
KAl(SO ₄) ₂	-21.74	-31.27	-9.53	KAl(SO ₄) ₂
Kalifornite	-4.77	-4.48	0.28	KHCO ₃
Kalsilite	1.12	4.06	2.94	KAlSiO ₄
Kaolinite	-0.00	-4.77	-4.77	Al ₂ Si ₂ O ₅ (OH) 4
Katoite	-46.30	32.11	78.41	Ca ₃ Al ₂ H ₁₂ O ₁₂
Kieserite	-9.94	-10.25	-0.31	MgSO ₄ ·H ₂ O
KMgCl ₃	-24.52	-13.59	10.94	KMgCl ₃
KMgCl ₃ ·2H ₂ O	-21.50	-13.59	7.90	KMgCl ₃ ·2H ₂ O
KNaCO ₃ ·6H ₂ O	-6.70	3.29	9.99	KNaCO ₃ ·6H ₂ O
Kyanite	-0.11	-0.78	-0.67	Al ₂ SiO ₅
Lansfordite	-6.15	-1.53	4.62	MgCO ₃ ·5H ₂ O
Larnite	-7.68	15.33	23.01	Ca ₂ SiO ₄
Laumontite	-1.91	-3.07	-1.16	CaAl ₂ Si ₄ O ₁₂ ·4H ₂ O
Lawrencite	-13.65	-11.73	1.92	FeCl ₂
Lawsonite	0.36	4.88	4.53	CaAl ₂ Si ₂ O ₇ (OH) 2:·H ₂ O
Leonite	-12.75	-17.04	-4.29	K ₂ Mg(SO ₄) ₂ ·4H ₂ O
Li	-32.45	13.27	45.72	Li
Li (g)	-44.42	13.27	57.69	Li
Lime	-10.29	9.65	19.94	CaO
Magnesite	-0.28	-1.51	-1.23	MgCO ₃
Magnetite	14.88	10.34	-4.54	Fe ₃ O ₄
Margarite	3.53	8.08	4.55	CaAl ₄ Si ₂ O ₁₀ (OH) 2
Maximum Microcline	0.02	-3.89	-3.91	KAlSi ₃ O ₈
Mayenite	-92.43	138.11	230.54	Ca ₁₂ Al ₁₄ O ₃₃
Melanterite	-9.27	-11.80	-2.53	FeSO ₄ ·7H ₂ O
Mercallite	-11.78	-13.22	-1.44	KHSO ₄
Merwinite	-8.90	30.41	39.31	MgCa ₃ (SiO ₄) ₂
Mesolite	2.87	2.82	-0.05	Na ₆ Fe ₆ Ca ₆ Si ₁₁ O ₃₀ ·2.647H ₂ O
Mg	-47.89	25.96	73.85	Mg
Mg (g)	-58.20	25.96	84.16	Mg
Mg _{1.25} SO ₄ (OH) 0.5:0.5H ₂ O	-5.27	-7.88	-2.62	Mg _{1.25} SO ₄ (OH) 0.5:0.5H ₂ O
Mg _{1.5} SO ₄ (OH)	-5.04	-5.54	-0.50	Mg _{1.5} SO ₄ (OH)
MgCl ₂ ·2H ₂ O	-15.66	-10.22	5.44	MgCl ₂ ·2H ₂ O
MgCl ₂ ·4H ₂ O	-13.56	-10.23	3.33	MgCl ₂ ·4H ₂ O
MgCl ₂ ·H ₂ O	-17.13	-10.22	6.91	MgCl ₂ ·H ₂ O
MgOHCl	-7.91	-0.40	7.51	MgOHCl
MgSO ₄	-7.55	-10.24	-2.69	MgSO ₄
Minnesotaite	3.09	7.77	4.68	Fe ₃ Si ₄ O ₁₀ (OH) 2
Mirabilite	-10.63	-4.10	6.53	Na ₂ SO ₄ ·10H ₂ O
Misenite	-75.01	-86.09	-11.08	K ₈ H ₆ (SO ₄) ₇
Molysite	-28.95	-28.21	0.74	FeCl ₃
Monohydrocalcite	-2.60	-1.27	1.32	CaCO ₃ ·H ₂ O
Monticellite	-1.21	15.09	16.29	CaMgSiO ₄
Montmor-Ca	-1.61	-8.54	-6.93	Ca _{1.65} Mg _{0.33} Al _{1.67} Si ₄ O ₁₀ (OH) 2
Montmor-K	-1.45	-8.00	-6.55	K _{0.33} Mg _{0.33} Al _{1.67} Si ₄ O ₁₀ (OH) 2
Montmor-Mg	-1.40	-8.57	-7.18	Mg _{0.495} Al _{1.67} Si ₄ O ₁₀ (OH) 2
Montmor-Na	-1.14	-7.55	-6.41	Na _{0.33} Mg _{0.33} Al _{1.67} Si ₄ O ₁₀ (OH) 2
Mordenite	-5.75	-13.01	-7.26	Ca _{0.2895} Na _{0.361} Al _{0.945} Si _{5.060} O ₁₂ ·3.468H ₂ O
Mordenite-dehy	-13.97	-12.99	0.98	Ca _{0.2895} Na _{0.361} Al _{0.945} Si _{5.060} O ₁₂
Muscovite	4.24	-0.70	-4.95	KAl ₃ Si ₃ O ₁₀ (OH) 2
Na	-26.69	16.08	42.76	Na
Na (g)	-33.33	16.08	49.41	Na
Na ₂ CO ₃	-3.60	4.68	8.28	Na ₂ CO ₃
Na ₂ CO ₃ ·7H ₂ O	-9.61	4.65	14.26	Na ₂ CO ₃ ·7H ₂ O
Na ₂ O	-29.47	15.60	45.07	Na ₂ O
Na ₂ SiO ₃	-5.09	11.63	16.72	Na ₂ SiO ₃
Na ₃ H(SO ₄) ₂	-15.01	-15.91	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ ·2H ₂ O	-12.13	-18.11	-5.98	Na ₄ Ca(SO ₄) ₃ ·2H ₂ O
Na ₄ SiO ₄	-22.46	27.23	49.69	Na ₄ SiO ₄
Na ₆ Si ₂ O ₇	-32.24	38.86	71.10	Na ₆ Si ₂ O ₇
NaFeO ₂	-0.50	9.03	9.53	NaFeO ₂
Nahcolite	-3.72	-3.12	0.60	NaHCO ₃
Natrolite	2.37	6.86	4.50	Na ₂ Al ₂ Si ₃ O ₁₀ ·2H ₂ O
Natron	-9.06	4.64	13.70	Na ₂ CO ₃ ·10H ₂ O
Natrosilite	-6.36	7.66	14.02	Na ₂ Si ₂ O ₅
Nepheline	1.16	5.42	4.26	NaAlSi ₃ O ₈
Nesquehonite	-5.82	-1.52	4.30	MgCO ₃ ·3H ₂ O
Nontronite-Ca	7.13	-10.01	-17.14	Ca _{0.165} Fe ₂ Al _{1.33} Si _{3.67} H ₂ O ₁₂
Nontronite-H	5.99	-11.61	-17.59	H _{0.33} Fe ₂ Al _{1.33} Si _{3.67} H ₂ O ₁₂
Nontronite-K	7.17	-9.48	-16.65	K _{0.33} Fe ₂ Al _{1.33} Si _{3.67} H ₂ O ₁₂
Nontronite-Mg	7.30	-10.05	-17.36	Mg _{0.165} Fe ₂ Al _{1.33} Si _{3.67} H ₂ O ₁₂
Nontronite-Na	7.55	-9.03	-16.58	Na _{0.33} Fe ₂ Al _{1.33} Si _{3.67} H ₂ O ₁₂
O ₂ (g)	-30.24	-33.11	-2.87	O ₂
Okenite	-7.28	1.70	8.97	CaSi ₂ O ₄ (OH) 2:·H ₂ O
Oxychloride-Mg	-16.54	8.98	25.52	Mg ₂ Cl(OH) 3:4H ₂ O
Paragonite	3.57	0.66	-2.91	NaAl ₃ Si ₃ O ₁₀ (OH) 2
Pargasite	5.02	45.68	40.66	NaCa ₂ Al ₃ Mg ₄ Si ₆ O ₂₂ (OH) 2
Pentahydrite	-8.66	-10.27	-1.61	MgSO ₄ ·5H ₂ O
Periclase	-2.24	9.41	11.65	MgO
Petalite	-2.16	-9.31	-7.14	LiAlSi ₄ O ₁₀
Phlogopite	8.84	24.34	15.50	KAlMg ₃ Si ₃ O ₁₀ (OH) 2
Picromerite	-12.34	-17.05	-4.71	K ₂ Mg(SO ₄) ₂ ·6H ₂ O
Pirssonite	-7.83	3.40	11.23	Na ₂ Ca(CO ₃) ₂ ·2H ₂ O
Polysilite	-22.64	-37.04	-14.40	K ₂ MgCa ₂ (SO ₄) ₄ ·2H ₂ O
Portlandite	-4.58	9.64	14.22	Ca(OH) ₂
Prehnite	0.44	10.56	10.12	Ca ₂ Al ₂ Si ₃ O ₁₀ (OH) 2
Pseudowollastonite	-2.51	5.68	8.19	CaSiO ₃
Pyrite	-35.10	-54.46	-19.36	FeS ₂

Pyrophyllite	-3.49	-12.71	-9.21	Al2Si4O10(OH)2
Pyrrhotite	-19.80	-24.93	-5.14	FeS
Quartz	-1.52	-3.97	-2.45	SiO2
Rankinite	-9.92	21.00	30.93	Ca3Si2O7
Ripidolite-14A	13.63	35.26	21.63	Mg3Fe2Al2Si3O10(OH)8
Ripidolite-7A	11.07	35.26	24.19	Mg3Fe2Al2Si3O10(OH)8
Rutile	2.62	-6.94	-9.56	TiO2
S	-20.99	-49.37	-28.39	S
S2(g)	-47.62	-59.06	-11.44	S2
Sanidine_high	-0.46	-3.89	-3.43	KAlSi3O8
Saponite-Ca	5.00	15.77	10.76	Ca.165Mg3Al.33Si3.67O10(OH)2
Saponite-H	3.84	14.17	10.34	H.33Mg3Al.33Si3.67O10(OH)2
Saponite-K	5.06	16.30	11.24	K.33Mg3Al.33Si3.67O10(OH)2
Saponite-Mg	5.17	15.73	10.55	Mg3.165Al.33Si3.67O10(OH)2
Saponite-Na	5.42	16.75	11.33	Na.33Mg3Al.33Si3.67O10(OH)2
Scolecite	0.71	0.91	0.20	CaAl2Si3O10:3H2O
Sepiolite	-3.98	13.77	17.75	Mg4Si6O15(OH)2:6H2O
Si	-62.30	29.13	91.43	Si
Si(g)	-104.29	29.13	133.42	Si
Siderite	-0.00	-3.03	-3.03	FeCO3
Sillimanite	-0.26	-0.78	-0.52	Al2SiO5
SiO2(am)	-2.14	-3.97	-1.83	SiO2
Smectite-high-Fe-Mg	3.44	5.40	1.96	Ca.025Na.1K.2Fe.5Fe.2Mg1.15Al1.25Si3.5H2O12
Smectite-low-Fe-Mg	1.65	0.69	-0.96	Ca.02Na.15K.2Fe.29Fe.16Mg.9Al1.25Si3.75H2O12
SO2(g)	-17.93	-18.89	-0.96	SO2
Spinel	1.50	12.60	11.10	Al2MgO4
Spodumene	-1.27	-1.36	-0.09	LiAlSi2O6
Starkeyite	-9.08	-10.26	-1.18	MgSO4:4H2O
Stilbite	-3.91	-12.72	-8.81	Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O
Sylvite	-4.61	-3.37	1.23	KCl
Syngenite	-9.14	-16.79	-7.64	K2Ca(SO4)2:2H2O
Tachyhydrite	-47.07	-30.45	16.61	Mg2CaCl6:12H2O
Talc	2.93	12.34	9.41	Mg3Si4O10(OH)2
Thenardite	-2.32	-4.05	-1.73	Na2SO4
Thermonatrite	-4.40	4.68	9.08	Na2CO3:H2O
Ti	-123.22	26.17	149.39	Ti
Ti(g)	-198.27	26.17	224.44	Ti
Ti2O3	-40.49	2.68	43.16	Ti2O3
Ti3O5	-39.18	-4.26	34.92	Ti3O5
TiB2	-242.79	69.85	312.64	TiB2
TiC	-133.59	48.36	181.95	TiC
TiCl2	-81.08	-10.01	71.07	TiCl2
TiCl3	-67.56	-28.09	39.47	TiCl3
TiCl4(g)	-74.41	-46.18	28.23	TiCl4
TiO(alpha)	-51.60	9.61	61.22	TiO
TiO(g)	-136.05	9.61	145.66	TiO
Titanite	-720.89	-1.26	719.63	CaTiSiO5
Tobermorite-11A	-19.38	24.39	43.77	Ca5Si6H11O22.5
Tobermorite-14A	-22.50	24.36	46.87	Ca5Si6H21O27.5
Tobermorite-9A	-19.74	24.40	44.14	Ca5Si6H6O20
Tremolite	4.11	34.57	30.46	Ca2Mg5Si8O22(OH)2
Tridymite	-1.84	-3.97	-2.13	SiO2
Troilite	-19.73	-24.93	-5.21	FeS
Trona-K	-12.67	-1.17	11.50	K2NaH(CO3)2:2H2O
Wairakite	-2.69	-3.06	-0.37	CaAl2Si4O10(OH)4
Wollastonite	-2.46	5.68	8.14	CaSiO3
Wustite	1.11	6.76	5.65	Fe.947O
Xonotlite	-24.85	34.06	58.91	Ca6Si6O17(OH)2
Zoisite	1.56	12.16	10.60	Ca2Al3(SiO4)3OH

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

End of simulation.

APPENDIX D

KINETIC MODELING RESULT IN BATURRADEN FIELD FOR 10 HOURS (0.001 YEAR) AND 10 YEARS TIME STEP

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\llnl.dat

Reading data base.

```
LLNL AQUEOUS MODEL PARAMETERS
NAMED EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END
```

Reading input data for simulation 1.

```
DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\llnl.dat
SOLUTION_SPECIES
CO3-2 + 2 H+ = CO2 + H2O
  log_k 16.681
  delta_h -5.738 kcal
  analytical_expression 464.1965 0.09344813 -26986.16 -165.75951 2248628.9
  dw 1.92e-9
  vm 7.29 0.92 2.07 -1.23 -1.60 # ref. 1 + McBride et al. 2015, JCED 60, 171
2CO2 = (CO2)2 # activity correction for CO2 solubility at high P, T
  log_k -1.8
  analytical_expression 8.68 -0.0103 -2190
  vm 14.58 1.84 4.14 -2.46 -3.20
END
```

End of simulation.

Reading input data for simulation 2.

```
PHASES
CO2(g)
  CO2 = CO2
  log_k -1.468
  delta_h -4.776 kcal
  analytical_expression 10.5624 -2.3547e-2 -3972.8 0 5.8746e5 1.9194e-5
  t_c 304.2 # critical T, K
  p_c 72.86 # critical P, atm
  omega 0.225 # acentric factor
Ankerite
  CaMg0.3Fe0.7(CO3)2 + 2H+ = Ca++ + 0.3Mg++ + 0.7Fe++ + 2HCO3-
  log_k 1.54
  delta_h 0
  analytical_expression -1.8649e+03 -2.9583e-01 1.0468e+05 6.7554e+02 -6.0514e+06
END
```

End of simulation.

Reading input data for simulation 3.

```
SOLUTION 1 P-3
temp 200
pH 6
pe 4
redox pe
units ppm
density 1
C(4) 695.4
Ca 196.5
Cl 724
Mg 185
Na 377
S(6) 600
K 76.7
B 3.97
Li 0.58
Si 163.75
water 1 # kg
pressure 194 atm
EQUILIBRIUM PHASES 1
CO2(g) - 2.288 1.2
RATES
Quartz
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_qtz = SI("Quartz")
30 if (M <= 0 and si_qtz < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_qtz > 0) then SA = 1e-05 #nucleation
60 k_acid = 0
70 k_neut = 10^(-13.99)*EXP(-87.60e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
```

```

90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_qtz))
190 moles = r * TIME
200 SAVE moles
end
Anorthite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_anort = SI("Anorthite")
30 if (M <= 0 and si_anort < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_anort > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-3.5)*EXP(-16.60e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.411)
70 k_neut = 10^(-9.82)*EXP(-31.50e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_anort))
190 moles = r * TIME
200 SAVE moles
end
Albite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_alb = SI("Albite")
30 if (M <= 0 and si_alb < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_alb > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-10.16)*EXP(-65.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.457)
70 k_neut = 10^(-12.56)*EXP(-69.80e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-15.60)*EXP(-71.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.572)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_alb))
190 moles = r * TIME
200 SAVE moles
end
K-Feldspar
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_kfeld = SI("K-Feldspar")
30 if (M <= 0 and si_kfeld < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_kfeld > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-10.06)*EXP(-51.70e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.500)
70 k_neut = 10^(-12.41)*EXP(-38.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-21.20)*EXP(-94.10e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.823)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_kfeld))
190 moles = r * TIME
200 SAVE moles
end
Diopside
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_diopsi = SI("Diopside")
30 if (M <= 0 and si_diopsi < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_diopsi > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-6.36)*EXP(-96.10e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.710)
70 k_neut = 10^(-11.11)*EXP(-40.60e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_diopsi))
190 moles = r * TIME
200 SAVE moles
end
Enstatite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_enst = SI("Enstatite")
30 if (M <= 0 and si_enst < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_enst > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-9.02)*EXP(-80.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.600)
70 k_neut = 10^(-12.72)*EXP(-80.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_enst))
190 moles = r * TIME
200 SAVE moles
end
Ilmenite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_ilmen = SI("Ilmenite")
30 if (M <= 0 and si_ilmen < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_ilmen > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-8.35)*EXP(-37.90e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.421)
70 k_neut = 10^(-11.16)*EXP(-37.90e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_ilmen))
190 moles = r * TIME
200 SAVE moles
end
Kaolinite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_kaol = SI("Kaolinite")
30 if (M <= 0 and si_kaol < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_kaol > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-11.31)*EXP(-65.90e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.777)
70 k_neut = 10^(-13.18)*EXP(-22.20e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-17.05)*EXP(-17.90e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.472)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_kaol))
190 moles = r * TIME

```

```

200 SAVE moles
end
Montmor-Na
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_montna = SI("Montmor-Na")
30 if (M <= 0 and si_montna < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_montna > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-12.71)*EXP(-48.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.220)
70 k_neut = 10^(-14.41)*EXP(-48.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-14.41)*EXP(-48.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.130)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_montna))
190 moles = r * TIME
200 SAVE moles
end
Calcite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_calc = SI("Calcite")
30 if (M <= 0 and si_calc < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_calc > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-0.30)*EXP(-14.40e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.000)
70 k_neut = 10^(-5.81)*EXP(-23.50e+03/8.314*(1.0/TK-1.0/298.15))
80 k_carb = 10^(-3.48)*EXP(-35.40e+03/8.314*(1.0/TK-1.0/298.15))*PR_P("CO2(g)")^(1.000)
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_calc))
190 moles = r * TIME
200 SAVE moles
end
Dolomite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_dolo = SI("Dolomite")
30 if (M <= 0 and si_dolo < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_dolo > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-3.76)*EXP(-56.70e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.500)
70 k_neut = 10^(-8.60)*EXP(-95.30e+03/8.314*(1.0/TK-1.0/298.15))
80 k_carb = 10^(-5.37)*EXP(-45.70e+03/8.314*(1.0/TK-1.0/298.15))*PR_P("CO2(g)")^(0.500)
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_dolo))
190 moles = r * TIME
200 SAVE moles
end
Siderite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_side = SI("Siderite")
30 if (M <= 0 and si_side < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_side > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-3.76)*EXP(-56.70e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.500)
70 k_neut = 10^(-8.60)*EXP(-95.30e+03/8.314*(1.0/TK-1.0/298.15))
80 k_carb = 10^(-5.37)*EXP(-45.70e+03/8.314*(1.0/TK-1.0/298.15))*PR_P("CO2(g)")^(0.500)
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_side))
190 moles = r * TIME
200 SAVE moles
end
Ankerite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_anke = SI("Ankerite")
30 if (M <= 0 and si_anke < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_anke > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-3.76)*EXP(-56.70e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.500)
70 k_neut = 10^(-8.60)*EXP(-95.30e+03/8.314*(1.0/TK-1.0/298.15))
80 k_carb = 10^(-5.37)*EXP(-45.70e+03/8.314*(1.0/TK-1.0/298.15))*PR_P("CO2(g)")^(0.500)
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_anke))
190 moles = r * TIME
200 SAVE moles
end
KINETICS 1
Quartz
formula SiO2 1
m 18.12
m0 18.12
parms 2.956
tol 1e-09
Anorthite
formula CaAl2(SiO4)2 1
m 23.38
m0 23.38
parms 5.548
tol 1e-09
Albite
formula NaAlSi3O8 1
m 25.16
m0 25.16
parms 5.26
tol 1e-09
K-Feldspar
formula KAlSi3O8 1
m 8.08
m0 8.08
parms 86.282
tol 1e-09
Diopside
formula CaMgSi2O6 1
m 8.08
m0 8.08
parms 3.974
tol 1e-09

```

```

Enstatite
  formula  MgSiO3  1
  m        29.35
  m0       29.35
  parms    933.627
  tol      1e-09
Kaolinite
  formula  Al2Si2O5(OH)4  1
  m        2.95
  m0       2.95
  parms    5163.2
  tol      1e-09
Montmor-Na
  formula  Na.33Mg.33Al1.67Si4O10(OH)2  1
  m        2.08
  m0       2.08
  parms    5866.72
  tol      1e-09
Dolomite
  formula  CaMg(CO3)2  1
  m        0
  m0       0
  parms    17.149
  tol      1e-09
Siderite
  formula  FeCO3  1
  m        0
  m0       0
  parms    15.062
  tol      1e-09
steps      3 30 300 3000 30000 300000 3000000 30000000 300000000 3000000000 30000000000 300000000000
cvscode true
KNOBS
convergence tolerance 1e-10
INCREMENTAL_REACTIONS True
USER_GRAPH 1
  -headings      Time Quartz Anorthite Albite K-Feldspar Diopside Enstatite Kaolinite Montmor-Na Calcite Dolomite
  -axis_titles   "Log10 Time" "kin" ""
  -initial_solutions false
  -connect_simulations true
  -plot_concentration_vs x
  -start
10 GRAPH X log10(total_time)
20 GRAPH Y kin("Quartz"), kin("Anorthite"), kin("Albite"), kin("K-Feldspar"), kin("Diopside"), kin("Enstatite"),
kin("Kaolinite"), kin("Montmor-Na"), kin("Calcite"), kin("Dolomite"), kin("Siderite")
  -end
  -active      true
SELECTED_OUTPUT 1
  file        D:\20182 SPRING\Thesis PHREEQC\2. Baturaden\kin baturaden.sel
  reset       false
  time        true
  step        true
  ph          true
  pe          true
  totals      C(4) Si
  molalities  K+ Na+ Ca+2 Mg+2
              HCO3- SO4-2 Cl- CO3-2
  kinetic_reactants  Quartz Anorthite Albite K-Feldspar
                    Diopside Enstatite Kaolinite Montmor-Na
                    Calcite Dolomite Siderite
END
-----
Beginning of initial solution calculations.
-----
Initial solution 1.      P-3
-----Solution composition-----

```

Elements	Molality	Moles
B	3.683e-04	3.683e-04
C(4)	1.143e-02	1.143e-02
Ca	4.918e-03	4.918e-03
Cl	2.048e-02	2.048e-02
K	1.968e-03	1.968e-03
Li	8.381e-05	8.381e-05
Mg	7.635e-03	7.635e-03
Na	1.645e-02	1.645e-02
S(6)	6.266e-03	6.266e-03
Si	2.734e-03	2.734e-03

```

-----Description of solution-----
pH = 6.000
pe = 4.000
Density (g/cm³) = 0.87966
Volume (L) = 1.14007
Activity of water = 0.999
Ionic strength (mol/kgw) = 3.196e-02
Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = 9.343e-04
Total CO2 (mol/kg) = 1.143e-02
Temperature (°C) = 200.00
Pressure (atm) = 194.00
Electrical balance (eq) = 9.655e-03
Percent error, 100*(Cat-|An|)/(|Cat+|An|) = 18.69
Iterations = 9
Total H = 1.110527e+02
Total O = 5.558076e+01
-----Distribution of species-----

```

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	7.410e-06	5.687e-06	-5.130	-5.245	-0.115	(0)

H+	1.226e-06	1.000e-06	-5.911	-6.000	-0.089	0.00
H2O	5.553e+01	9.989e-01	1.744	-0.000	0.000	20.53
B(-5)	0.000e+00					
BH4-	0.000e+00	0.000e+00	-115.055	-115.167	-0.112	(0)
B(3)	3.683e-04					
B(OH)3	3.676e-04	3.676e-04	-3.435	-3.435	0.000	(0)
BO2-	7.126e-07	5.507e-07	-6.147	-6.259	-0.112	(0)
CaB(OH)4+	3.230e-08	2.496e-08	-7.491	-7.603	-0.112	(0)
MgB(OH)4+	1.722e-08	1.331e-08	-7.764	-7.876	-0.112	(0)
NaB(OH)4	5.405e-09	5.405e-09	-8.267	-8.267	0.000	(0)
B2O(OH)5-	3.610e-20	2.790e-20	-19.443	-19.554	-0.112	(0)
C(4)	1.143e-02					
CO2	1.048e-02	1.056e-02	-1.979	-1.976	0.003	53.80
HCO3-	5.660e-04	4.374e-04	-3.247	-3.359	-0.112	(0)
CaHCO3+	2.344e-04	1.812e-04	-3.630	-3.742	-0.112	(0)
MgHCO3+	1.088e-04	8.408e-05	-3.963	-4.075	-0.112	(0)
(CO2)2	1.668e-05	1.681e-05	-4.778	-4.775	0.003	107.59
CaCO3	6.781e-06	6.781e-06	-5.169	-5.169	0.000	(0)
MgCO3	4.310e-07	4.310e-07	-6.366	-6.366	0.000	(0)
NaHCO3	3.340e-07	3.340e-07	-6.476	-6.476	0.000	(0)
CO3-2	4.076e-08	1.477e-08	-7.390	-7.830	-0.441	(0)
NaCO3-	1.613e-12	1.247e-12	-11.792	-11.904	-0.112	(0)
Ca	4.918e-03					
Ca+2	4.169e-03	1.623e-03	-2.380	-2.790	-0.410	(0)
CaSO4	3.945e-04	3.945e-04	-3.404	-3.404	0.000	(0)
CaHCO3+	2.344e-04	1.812e-04	-3.630	-3.742	-0.112	(0)
CaCl+	1.099e-04	8.492e-05	-3.959	-4.071	-0.112	(0)
CaCO3	6.781e-06	6.781e-06	-5.169	-5.169	0.000	(0)
CaCl2	3.083e-06	3.083e-06	-5.511	-5.511	0.000	(0)
CaB(OH)4+	3.230e-08	2.496e-08	-7.491	-7.603	-0.112	(0)
CaOH+	3.282e-10	2.536e-10	-9.484	-9.596	-0.112	(0)
Cl(-1)	2.048e-02					
Cl-	1.992e-02	1.517e-02	-1.701	-1.819	-0.118	(0)
NaCl	2.386e-04	2.386e-04	-3.622	-3.622	0.000	(0)
MgCl+	1.995e-04	1.542e-04	-3.700	-3.812	-0.112	(0)
CaCl+	1.099e-04	8.492e-05	-3.959	-4.071	-0.112	(0)
KCl	1.391e-05	1.391e-05	-4.857	-4.857	0.000	(0)
CaCl2	3.083e-06	3.083e-06	-5.511	-5.511	0.000	(0)
LiCl	3.240e-07	3.240e-07	-6.489	-6.489	0.000	(0)
HCl	1.242e-08	1.242e-08	-7.906	-7.906	0.000	(0)
Cl(1)	9.342e-20					
HClO	9.027e-20	9.027e-20	-19.044	-19.044	0.000	(0)
ClO-	3.149e-21	2.434e-21	-20.502	-20.614	-0.112	(0)
Cl(3)	1.371e-33					
ClO2-	1.369e-33	1.058e-33	-32.864	-32.975	-0.112	(0)
HClO2	1.565e-36	1.565e-36	-35.806	-35.806	0.000	(0)
Cl(5)	3.416e-37					
ClO3-	3.416e-37	2.622e-37	-36.466	-36.581	-0.115	(0)
Cl(7)	0.000e+00					
ClO4-	0.000e+00	0.000e+00	-43.644	-43.759	-0.115	(0)
H(0)	1.404e-20					
H2	7.020e-21	7.115e-21	-20.154	-20.148	0.006	(0)
K	1.968e-03					
K+	1.940e-03	1.478e-03	-2.712	-2.830	-0.118	(0)
KCl	1.391e-05	1.391e-05	-4.857	-4.857	0.000	(0)
KSO4-	1.375e-05	1.062e-05	-4.862	-4.974	-0.112	(0)
KHSO4	3.437e-09	3.437e-09	-8.464	-8.464	0.000	(0)
KOH	5.670e-12	5.670e-12	-11.246	-11.246	0.000	(0)
Li	8.381e-05					
Li+	8.345e-05	6.609e-05	-4.079	-4.180	-0.101	(0)
LiCl	3.240e-07	3.240e-07	-6.489	-6.489	0.000	(0)
LiSO4-	4.297e-08	3.321e-08	-7.367	-7.479	-0.112	(0)
LiOH	1.675e-12	1.675e-12	-11.776	-11.776	0.000	(0)
Mg	7.635e-03					
MgSO4	5.604e-03	5.604e-03	-2.252	-2.252	0.000	(0)
Mg+2	1.722e-03	7.271e-04	-2.764	-3.138	-0.374	(0)
MgCl+	1.995e-04	1.542e-04	-3.700	-3.812	-0.112	(0)
MgHCO3+	1.088e-04	8.408e-05	-3.963	-4.075	-0.112	(0)
MgCO3	4.310e-07	4.310e-07	-6.366	-6.366	0.000	(0)
MgB(OH)4+	1.722e-08	1.331e-08	-7.764	-7.876	-0.112	(0)
Mg4(OH)4+4	3.583e-27	7.441e-29	-26.446	-28.128	-1.683	(0)
Na	1.645e-02					
Na+	1.620e-02	1.252e-02	-1.791	-1.902	-0.112	(0)
NaCl	2.386e-04	2.386e-04	-3.622	-3.622	0.000	(0)
NaSO4-	9.132e-06	7.058e-06	-5.039	-5.151	-0.112	(0)
NaHSiO3	8.532e-07	8.532e-07	-6.069	-6.069	0.000	(0)
NaHCO3	3.340e-07	3.340e-07	-6.476	-6.476	0.000	(0)
NaOH	8.373e-08	8.373e-08	-7.077	-7.077	0.000	(0)
NaB(OH)4	5.405e-09	5.405e-09	-8.267	-8.267	0.000	(0)
NaCO3-	1.613e-12	1.247e-12	-11.792	-11.904	-0.112	(0)
O(0)	6.739e-15					
O2	3.369e-15	3.415e-15	-14.472	-14.467	0.006	(0)
S(6)	6.266e-03					
MgSO4	5.604e-03	5.604e-03	-2.252	-2.252	0.000	(0)
CaSO4	3.945e-04	3.945e-04	-3.404	-3.404	0.000	(0)
SO4-2	2.417e-04	8.533e-05	-3.617	-4.069	-0.452	(0)
KSO4-	1.375e-05	1.062e-05	-4.862	-4.974	-0.112	(0)
NaSO4-	9.132e-06	7.058e-06	-5.039	-5.151	-0.112	(0)
HSO4-	3.286e-06	2.540e-06	-5.483	-5.595	-0.112	(0)
LiSO4-	4.297e-08	3.321e-08	-7.367	-7.479	-0.112	(0)
KHSO4	3.437e-09	3.437e-09	-8.464	-8.464	0.000	(0)
H2SO4	8.132e-18	8.132e-18	-17.090	-17.090	0.000	(0)
Si	2.734e-03					
SiO2	2.728e-03	2.728e-03	-2.564	-2.564	0.000	(0)
HSiO3-	5.680e-06	4.390e-06	-5.246	-5.358	-0.112	(0)
NaHSiO3	8.532e-07	8.532e-07	-6.069	-6.069	0.000	(0)
H6(H2SiO4)4-2	8.052e-12	2.843e-12	-11.094	-11.546	-0.452	(0)
H2SiO4-2	1.037e-13	3.660e-14	-12.984	-13.437	-0.452	(0)
H4(H2SiO4)4-4	9.264e-21	1.425e-22	-20.033	-21.846	-1.813	(0)

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

Phase	SI**	log IAP	log K(473 K, 194 atm)	
Afwillite	-16.01	22.50	38.50	Ca3Si2O4(OH)6
Akermanite	-3.19	22.15	25.35	Ca2MgSi2O7
Anhydrite	0.43	-6.86	-7.29	CaSO4
Antarcticite	-10.26	-6.43	3.83	CaCl2·6H2O

Anthophyllite	10.26	41.51	31.25	Mg7Si8O22 (OH) 2
Antigorite	92.93	338.13	245.21	Mg48Si34O85 (OH) 62
Aphthitalite	-14.64	-18.53	-3.89	NaK3 (SO4) 2
Aragonite	0.29	-0.15	-0.44	CaCO3
Arcanite	-7.82	-9.73	-1.90	K2SO4
Artinite	-2.63	8.36	11.00	Mg2CO3 (OH) 2:3H2O
B	-59.90	7.42	67.32	B
B(g)	-114.64	7.42	122.05	B
B2O3	-10.49	-6.87	3.63	B2O3
Bassanite	-0.24	-6.86	-6.62	CaSO4:0.5H2O
Bischofite	-10.91	-6.78	4.13	MgCl2:6H2O
Bloedite	-12.43	-15.08	-2.65	Na2Mg (SO4) 2:4H2O
Borax	-22.96	-5.55	17.42	Na2 (B4O5 (OH) 4) :8H2O
Boric acid	-4.47	-3.43	1.03	B (OH) 3
Brucite	-0.37	8.86	9.23	Mg (OH) 2
Burkeite	-26.40	-16.91	9.49	Na6CO3 (SO4) 2
C	-32.17	5.11	37.28	C
C(g)	-103.39	5.11	108.50	C
Ca	-69.62	16.44	86.06	Ca
Ca(g)	-83.45	16.44	99.90	Ca
Ca2Cl2 (OH) 2:H2O	-23.38	2.78	26.16	Ca2Cl2 (OH) 2:H2O
Ca4Cl2 (OH) 6:13H2O	-46.29	21.19	67.49	Ca4Cl2 (OH) 6:13H2O
Calcite	0.44	-0.15	-0.59	CaCO3
Carnallite	-15.43	-11.43	4.01	KMgCl3:6H2O
CaSO4:0.5H2O (beta)	-0.26	-6.86	-6.60	CaSO4:0.5H2O
Chalcedony	-0.29	-2.56	-2.28	SiO2
Chloromagnesite	-16.76	-6.78	9.99	MgCl2
Chrysotile	5.25	21.45	16.21	Mg3Si2O5 (OH) 4
Cl2 (g)	-21.36	-22.87	-1.51	Cl2
CO2 (g)	0.19	-1.98	-2.17	CO2
Coesite	-0.65	-2.56	-1.92	SiO2
Colemanite	-23.79	-2.19	21.60	Ca2B6O11:5H2O
Cristobalite (alpha)	-0.42	-2.56	-2.14	SiO2
Cristobalite (beta)	-0.63	-2.56	-1.94	SiO2
Dicalcium silicate	-6.49	15.86	22.34	Ca2SiO4
Diopside	1.83	12.94	11.12	CaMgSi2O6
Dolomite	2.13	-0.65	-2.78	CaMg (CO3) 2
Dolomite-dis	1.39	-0.65	-2.03	CaMg (CO3) 2
Dolomite-ord	2.14	-0.65	-2.79	CaMg (CO3) 2
Enstatite	0.86	6.30	5.44	MgSiO3
Epsomite	-4.94	-7.21	-2.27	MgSO4:7H2O
Forsterite	1.11	15.16	14.05	Mg2SiO4
Foshagite	-11.60	29.15	40.74	Ca4Si3O9 (OH) 2:0.5H2O
Gaylussite	-12.26	-1.32	10.94	CaNa2 (CO3) 2:5H2O
Glauberite	-9.26	-14.73	-5.47	Na2Ca (SO4) 2
Gypsum	-0.63	-6.86	-6.23	CaSO4:2H2O
Gyrolite	-5.27	10.73	15.99	Ca2Si3O7 (OH) 2:1.5H2O
H2 (g)	-17.34	-20.15	-2.81	H2
H2O (g)	1.20	-0.00	-1.20	H2O
Hallite	-4.96	-3.72	1.24	NaCl
Hatrurite	-19.34	25.07	44.40	Ca3SiO5
HCl (g)	-8.71	-7.82	0.89	HCl
Hexahydrate	-5.22	-7.21	-1.99	MgSO4:6H2O
Hillebrandite	-7.24	15.85	23.09	Ca2SiO3 (OH) 2:0.17H2O
Huntite	1.83	-1.64	-3.47	CaMg3 (CO3) 4
Hydroboracite	-22.94	-2.54	20.41	MgCaB6O11:6H2O
Hydromagnesite	-2.43	6.87	9.30	Mg5 (CO3) 4 (OH) 2:4H2O
Hydrophilite	-11.24	-6.43	4.82	CaCl2
Ice	-0.89	-0.00	0.89	H2O
K	-38.66	6.79	45.45	K
K(g)	-43.61	6.79	50.40	K
K2CO3:1.5H2O	-16.33	-3.02	13.31	K2CO3:1.5H2O
K2O	-50.09	6.34	56.43	K2O
K3H (SO4) 2	-19.01	-22.63	-3.62	K3H (SO4) 2
K8H4 (CO3) 6:3H2O	-58.38	-30.80	27.58	K8H4 (CO3) 6:3H2O
Kainite	-11.41	-11.86	-0.44	KMgClSO4:3H2O
Kalicinite	-6.47	-6.19	0.28	KHCO3
Kieserite	-6.90	-7.21	-0.31	MgSO4:H2O
KMgCl3	-22.36	-11.43	10.94	KMgCl3
KMgCl3:2H2O	-19.33	-11.43	7.90	KMgCl3:2H2O
KNaCO3:6H2O	-12.09	-2.09	9.99	KNaCO3:6H2O
Lansfordite	-5.12	-0.50	4.62	MgCO3:5H2O
Larnite	-7.15	15.86	23.01	Ca2SiO4
Leonite	-12.65	-16.94	-4.29	K2Mg (SO4) 2:4H2O
Li	-40.28	5.44	45.72	Li
Li (g)	-52.25	5.44	57.69	Li
Lime	-10.73	9.21	19.94	CaO
Magnesite	0.73	-0.50	-1.23	MgCO3
Mercallite	-11.46	-12.90	-1.44	KHSO4
Merwinite	-7.95	31.36	39.31	MgCa3 (SiO4) 2
Mg	-57.76	16.09	73.85	Mg
Mg(g)	-68.07	16.09	84.16	Mg
Mg1.25SO4 (OH) 0.5:0.5H2O	-2.37	-4.99	-2.62	Mg1.25SO4 (OH) 0.5:0.5H2O
Mg1.5SO4 (OH)	-2.28	-2.78	-0.50	Mg1.5SO4 (OH)
MgCl2:2H2O	-12.22	-6.78	5.44	MgCl2:2H2O
MgCl2:4H2O	-10.11	-6.78	3.33	MgCl2:4H2O
MgCl2:H2O	-13.69	-6.78	6.91	MgCl2:H2O
MgOHCl	-6.46	1.04	7.51	MgOHCl
MgSO4	-4.52	-7.21	-2.69	MgSO4
Mirabilite	-14.41	-7.88	6.53	Na2SO4:10H2O
Misenite	-76.05	-87.12	-11.08	K8H6 (SO4) 7
Monohydrocalcite	-1.47	-0.15	1.32	CaCO3:H2O
Monticellite	-0.79	15.51	16.29	CaMgSiO4
Na	-35.05	7.71	42.76	Na
Na(g)	-41.70	7.71	49.41	Na
Na2CO3	-9.44	-1.16	8.28	Na2CO3
Na2CO3:7H2O	-15.43	-1.17	14.26	Na2CO3:7H2O
Na2O	-36.87	8.19	45.07	Na2O
Na2SiO3	-11.09	5.63	16.72	Na2SiO3
Na3H (SO4) 2	-18.95	-19.85	-0.89	Na3H (SO4) 2
Na4Ca (SO4) 3:2H2O	-16.62	-22.61	-5.98	Na4Ca (SO4) 3:2H2O
Na4SiO4	-35.87	13.83	49.69	Na4SiO4
Na6Si2O7	-51.65	19.46	71.10	Na6Si2O7
Nahcolite	-5.86	-5.26	0.60	NaHCO3
Natron	-14.87	-1.17	13.70	Na2CO3:10H2O
Natrosillite	-10.95	3.07	14.02	Na2Si2O5
Nesquehonite	-4.80	-0.50	4.30	MgCO3:3H2O
O2 (g)	-11.60	-14.47	-2.87	O2

Okenite	-4.89	4.08	8.97	CaSi2O4(OH)2:H2O
Oxychloride-Mg	-15.62	9.90	25.52	Mg2Cl(OH)3:4H2O
Pentahydrate	-5.60	-7.21	-1.61	MgSO4:5H2O
Periclase	-2.79	8.86	11.65	MgO
Picromerite	-12.23	-16.94	-4.71	K2Mg(SO4)2:6H2O
Pirssonite	-12.55	-1.31	11.23	Na2Ca(CO3)2:2H2O
Polyhalite	-16.25	-30.65	-14.40	K2MgCa2(SO4)4:2H2O
Portlandite	-5.01	9.21	14.22	Ca(OH)2
Pseudowollastonite	-1.54	6.65	8.19	CaSiO3
Quartz	-0.11	-2.56	-2.45	SiO2
Rankinite	-8.42	22.50	30.93	Ca3Si2O7
Sepiolite	2.31	20.06	17.75	Mg4Si6O15(OH)2:6H2O
Si	-79.53	11.90	91.43	Si
Si(g)	-121.52	11.90	133.42	Si
SiO2(am)	-0.73	-2.56	-1.83	SiO2
Starkeyite	-6.03	-7.21	-1.18	MgSO4:4H2O
Sylvite	-5.88	-4.65	1.23	KCl
Syngenite	-8.94	-16.59	-7.64	K2Ca(SO4)2:H2O
Tachyhydrite	-36.60	-19.99	16.61	Mg2CaCl6:12H2O
Talc	6.92	16.33	9.41	Mg3Si4O10(OH)2
Thenardite	-6.14	-7.87	-1.73	Na2SO4
Thermonatrite	-10.25	-1.16	9.08	Na2CO3:H2O
Tobermorite-11A	-13.11	30.66	43.77	Ca5Si6H11O22.5
Tobermorite-14A	-16.21	30.66	46.87	Ca5Si6H21O27.5
Tobermorite-9A	-13.48	30.66	44.14	Ca5Si6H6O20
Tremolite	11.75	42.21	30.46	Ca2Mg5Si8O22(OH)2
Tridymite	-0.44	-2.56	-2.13	SiO2
Trona-K	-19.78	-8.28	11.50	K2NaH(CO3)2:2H2O
Wollastonite	-1.49	6.65	8.14	CaSiO3
Xonotlite	-19.03	39.87	58.91	Ca6Si6O17(OH)2

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

Beginning of batch-reaction calculations.

TIME STEP 10 HOURS (0.001 YEAR)

Reaction step 7.

Using solution 1. P-3
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

Time step: 3e+06 seconds (Incremented time: 3.33333e+06 seconds)

Rate name	Delta Moles	Total Moles	Reactant	Coefficient
Quartz	-6.932e-01	1.802e+01	SiO2	1
Anorthite	-4.103e-01	2.275e+01	CaAl2(SiO4)2	1
Albite	-6.997e-02	2.494e+01	NaAlSi3O8	1
K-Feldspar	-2.818e-06	8.079e+00	KAlSi3O8	1
Diopside	4.103e-01	8.113e+00	CaMgSi2O6	1
Enstatite	-4.801e-01	2.854e+01	MgSiO3	1
Kaolinite	2.686e-01	3.226e+00	Al2Si2O5(OH)4	1
Montmor-Na	2.115e-01	2.631e+00	Na.33Mg.33Al1.67Si4O10(OH)2	1
Dolomite	1.703e-05	6.034e-01	CaMg(CO3)2	1
Siderite	-0.000e+00	0.000e+00	FeCO3	1

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

Phase	SI	log IAP	log K(T, P)	Moles in assemblage		
				Initial	Final	Delta
CO2(g)	-0.75	-2.92	-2.17	0.000e+00	0	0.000e+00

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

Elements	Molality	Moles
Al	6.962e-03	6.824e-03
B	3.758e-04	3.683e-04
C	4.681e-03	4.588e-03
Ca	3.994e-06	3.915e-06
Cl	2.090e-02	2.048e-02
K	2.550e-03	2.499e-03
Li	8.552e-05	8.381e-05
Mg	3.437e-05	3.369e-05
Na	5.182e-02	5.079e-02
S	6.393e-03	6.266e-03
Si	5.076e-04	4.975e-04

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

pH	=	7.713	Charge balance
pe	=	-1.106	Adjusted to redox equilibrium
Density (g/cm ³)	=	0.88050	
Volume (L)	=	1.11690	
Activity of water	=	0.998	
Ionic strength (mol/kgw)	=	5.294e-02	
Mass of water (kg)	=	9.801e-01	
Total alkalinity (eq/kg)	=	3.188e-02	
Total CO2 (mol/kg)	=	4.681e-03	
Temperature (°C)	=	200.00	
Pressure (atm)	=	194.00	
Electrical balance (eq)	=	9.655e-03	
Percent error, 100*(Cat- An)/(Cat+ An)	=	10.40	
Iterations	=	260	
Total H	=	1.088466e+02	
Total O	=	5.447473e+01	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm ³ /mol
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OH-	4.047e-04	2.934e-04	-3.393	-3.533	-0.140	(0)
H+	2.453e-08	1.938e-08	-7.610	-7.713	-0.102	0.00
H2O	5.553e+01	9.984e-01	1.744	-0.001	0.000	20.53
Al	6.962e-03					
AlO2-	6.327e-03	4.634e-03	-2.199	-2.334	-0.135	(0)
NaAlO2	6.250e-04	6.250e-04	-3.204	-3.204	0.000	(0)
HA1O2	9.778e-06	9.778e-06	-5.010	-5.010	0.000	(0)
Al (OH) 2+	1.587e-10	1.162e-10	-9.799	-9.935	-0.135	(0)
AlOH+2	1.813e-15	5.328e-16	-14.741	-15.273	-0.532	(0)
Al+3	1.193e-21	1.365e-22	-20.923	-21.865	-0.942	(0)
AlSO4+	2.991e-22	2.190e-22	-21.524	-21.659	-0.135	(0)
Al (SO4) 2-	3.642e-23	2.667e-23	-22.439	-22.574	-0.135	(0)
Al2 (OH) 2+4	1.274e-34	1.238e-36	-33.895	-35.907	-2.013	(0)
Al3 (OH) 4+5	0.000e+00	0.000e+00	-45.392	-48.450	-3.058	(0)
Al13O4 (OH) 24+7	0.000e+00	0.000e+00	-128.950	-134.946	-5.997	(0)
B (-5)	0.000e+00					
BH4-	0.000e+00	0.000e+00	-86.208	-86.343	-0.135	(0)
B (3)	3.758e-04					
B (OH) 3	3.392e-04	3.392e-04	-3.470	-3.470	0.000	(0)
BO2-	3.583e-05	2.624e-05	-4.446	-4.581	-0.135	(0)
NaB (OH) 4	7.520e-07	7.520e-07	-6.124	-6.124	0.000	(0)
CaB (OH) 4+	4.094e-10	2.998e-10	-9.388	-9.523	-0.135	(0)
MgB (OH) 4+	2.805e-10	2.054e-10	-9.552	-9.687	-0.135	(0)
B2O (OH) 5-	1.674e-18	1.226e-18	-17.776	-17.911	-0.135	(0)
C (-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-87.722	-87.722	0.000	(0)
C (-3)	0.000e+00					
C2H6	0.000e+00	0.000e+00	-57.402	-57.402	0.000	(0)
C (-4)	2.914e-40					
CH4	2.914e-40	2.914e-40	-39.535	-39.535	0.000	(0)
C (2)	8.933e-19					
CO	8.933e-19	8.933e-19	-18.049	-18.049	0.000	(0)
C (4)	4.681e-03					
HCO3-	3.480e-03	2.549e-03	-2.458	-2.594	-0.135	(0)
CO2	1.179e-03	1.193e-03	-2.929	-2.923	0.005	53.80
CO3-2	1.512e-05	4.443e-06	-4.820	-5.352	-0.532	(0)
NaHCO3	5.689e-06	5.689e-06	-5.245	-5.245	0.000	(0)
CaCO3	5.144e-07	5.144e-07	-6.289	-6.289	0.000	(0)
CaHCO3+	3.637e-07	2.663e-07	-6.439	-6.575	-0.135	(0)
MgHCO3+	2.169e-07	1.589e-07	-6.664	-6.799	-0.135	(0)
(CO2) 2	2.119e-07	2.145e-07	-6.674	-6.669	0.005	107.59
MgCO3	4.202e-08	4.202e-08	-7.377	-7.377	0.000	(0)
NaCO3-	1.497e-09	1.096e-09	-8.825	-8.960	-0.135	(0)
Ca	3.994e-06					
CaSO4	1.830e-06	1.830e-06	-5.738	-5.738	0.000	(0)
Ca+2	1.257e-06	4.095e-07	-5.901	-6.388	-0.487	(0)
CaCO3	5.144e-07	5.144e-07	-6.289	-6.289	0.000	(0)
CaHCO3+	3.637e-07	2.663e-07	-6.439	-6.575	-0.135	(0)
CaCl+	2.795e-08	2.047e-08	-7.554	-7.689	-0.135	(0)
CaCl2	7.098e-10	7.098e-10	-9.149	-9.149	0.000	(0)
CaB (OH) 4+	4.094e-10	2.998e-10	-9.388	-9.523	-0.135	(0)
CaOH+	4.507e-12	3.301e-12	-11.346	-11.481	-0.135	(0)
Cl (-1)	2.090e-02					
Cl-	2.022e-02	1.450e-02	-1.694	-1.839	-0.145	(0)
NaCl	6.662e-04	6.662e-04	-3.176	-3.176	0.000	(0)
KCl	1.447e-05	1.447e-05	-4.839	-4.839	0.000	(0)
LiCl	2.999e-07	2.999e-07	-6.523	-6.523	0.000	(0)
MgCl+	6.523e-08	4.777e-08	-7.186	-7.321	-0.135	(0)
CaCl+	2.795e-08	2.047e-08	-7.554	-7.689	-0.135	(0)
CaCl2	7.098e-10	7.098e-10	-9.149	-9.149	0.000	(0)
HCl	2.299e-10	2.299e-10	-9.638	-9.638	0.000	(0)
Cl (1)	7.923e-28					
ClO-	5.191e-28	3.802e-28	-27.285	-27.420	-0.135	(0)
HClO	2.732e-28	2.732e-28	-27.564	-27.564	0.000	(0)
Cl (3)	0.000e+00					
ClO2-	0.000e+00	0.000e+00	-46.433	-46.568	-0.135	(0)
HClO2	0.000e+00	0.000e+00	-51.111	-51.111	0.000	(0)
Cl (5)	0.000e+00					
ClO3-	0.000e+00	0.000e+00	-56.821	-56.961	-0.140	(0)
Cl (7)	0.000e+00					
ClO4-	0.000e+00	0.000e+00	-70.785	-70.925	-0.140	(0)
H (0)	8.511e-14					
H2	4.255e-14	4.350e-14	-13.371	-13.362	0.010	(0)
K	2.550e-03					
K+	2.245e-03	1.610e-03	-2.649	-2.793	-0.145	(0)
KSO4-	2.904e-04	2.126e-04	-3.537	-3.672	-0.135	(0)
KCl	1.447e-05	1.447e-05	-4.839	-4.839	0.000	(0)
KHSO4	1.333e-09	1.333e-09	-8.875	-8.875	0.000	(0)
KOH	3.185e-10	3.185e-10	-9.497	-9.497	0.000	(0)
Li	8.552e-05					
Li+	8.441e-05	6.404e-05	-4.074	-4.194	-0.120	(0)
LiSO4-	8.076e-07	5.914e-07	-6.093	-6.228	-0.135	(0)
LiCl	2.999e-07	2.999e-07	-6.523	-6.523	0.000	(0)
LiOH	8.371e-11	8.371e-11	-10.077	-10.077	0.000	(0)
Mg	3.437e-05					
MgSO4	3.340e-05	3.340e-05	-4.476	-4.476	0.000	(0)
Mg+2	6.465e-07	2.358e-07	-6.189	-6.628	-0.438	(0)
MgHCO3+	2.169e-07	1.589e-07	-6.664	-6.799	-0.135	(0)
MgCl+	6.523e-08	4.777e-08	-7.186	-7.321	-0.135	(0)
MgCO3	4.202e-08	4.202e-08	-7.377	-7.377	0.000	(0)
MgB (OH) 4+	2.805e-10	2.054e-10	-9.552	-9.687	-0.135	(0)
Mg4 (OH) 4+4	5.995e-34	5.824e-36	-33.222	-35.235	-2.013	(0)
Na	5.182e-02					
Na+	4.997e-02	3.659e-02	-1.301	-1.437	-0.135	(0)
NaCl	6.662e-04	6.662e-04	-3.176	-3.176	0.000	(0)
NaAlO2	6.250e-04	6.250e-04	-3.204	-3.204	0.000	(0)
NaSO4-	5.178e-04	3.792e-04	-3.286	-3.421	-0.135	(0)
NaHSiO3	2.063e-05	2.063e-05	-4.686	-4.686	0.000	(0)
NaOH	1.262e-05	1.262e-05	-4.899	-4.899	0.000	(0)
NaHCO3	5.689e-06	5.689e-06	-5.245	-5.245	0.000	(0)
NaB (OH) 4	7.520e-07	7.520e-07	-6.124	-6.124	0.000	(0)
NaCO3-	1.497e-09	1.096e-09	-8.825	-8.960	-0.135	(0)
O (0)	1.786e-28					
O2	8.931e-29	9.129e-29	-28.049	-28.040	0.010	(0)
S (-2)	2.385e-34					
HS-	2.097e-34	1.520e-34	-33.678	-33.818	-0.140	(0)
S-2	1.442e-35	4.392e-36	-34.841	-35.357	-0.516	(0)

H2S	1.437e-35	1.437e-35	-34.843	-34.843	0.000	(0)
S2-2	0.000e+00	0.000e+00	-62.418	-62.967	-0.549	(0)
S3-2	0.000e+00	0.000e+00	-88.812	-89.361	-0.549	(0)
S4-2	0.000e+00	0.000e+00	-115.352	-115.901	-0.549	(0)
S5-2	0.000e+00	0.000e+00	-142.032	-142.580	-0.549	(0)
S (2)	1.919e-39					
S203-2	9.596e-40	2.713e-40	-39.018	-39.567	-0.549	(0)
HS203-	0.000e+00	0.000e+00	-46.130	-46.265	-0.135	(0)
S (3)	0.000e+00					
S204-2	0.000e+00	0.000e+00	-44.649	-45.165	-0.516	(0)
S (4)	5.952e-17					
HS03-	5.418e-17	3.968e-17	-16.266	-16.401	-0.135	(0)
SO3-2	5.330e-18	1.566e-18	-17.273	-17.805	-0.532	(0)
SO2	9.997e-21	9.997e-21	-20.000	-20.000	0.000	(0)
H2SO3	9.608e-25	9.608e-25	-24.017	-24.017	0.000	(0)
S206-2	2.446e-33	6.914e-34	-32.612	-33.160	-0.549	(0)
S306-2	0.000e+00	0.000e+00	-61.151	-61.700	-0.549	(0)
S406-2	0.000e+00	0.000e+00	-77.272	-77.821	-0.549	(0)
S506-2	0.000e+00	0.000e+00	-116.286	-116.834	-0.549	(0)
S (5)	2.840e-38					
S205-2	1.420e-38	4.015e-39	-37.848	-38.396	-0.549	(0)
S (6)	6.393e-03					
SO4-2	5.548e-03	1.568e-03	-2.256	-2.805	-0.549	(0)
NaSO4-	5.178e-04	3.792e-04	-3.286	-3.421	-0.135	(0)
KSO4-	2.904e-04	2.126e-04	-3.537	-3.672	-0.135	(0)
MgSO4	3.340e-05	3.340e-05	-4.476	-4.476	0.000	(0)
CaSO4	1.830e-06	1.830e-06	-5.738	-5.738	0.000	(0)
HSO4-	1.235e-06	9.045e-07	-5.908	-6.044	-0.135	(0)
LiSO4-	8.076e-07	5.914e-07	-6.093	-6.228	-0.135	(0)
KHSO4	1.333e-09	1.333e-09	-8.875	-8.875	0.000	(0)
H2SO4	5.613e-20	5.613e-20	-19.251	-19.251	0.000	(0)
AlSO4+	2.991e-22	2.190e-22	-21.524	-21.659	-0.135	(0)
Al (SO4) 2-	3.642e-23	2.667e-23	-22.439	-22.574	-0.135	(0)
S (7)	0.000e+00					
S208-2	0.000e+00	0.000e+00	-42.838	-43.387	-0.549	(0)
S (8)	2.899e-32					
HS05-	2.899e-32	2.123e-32	-31.538	-31.673	-0.135	(0)
Si	5.076e-04					
SiO2	4.374e-04	4.374e-04	-3.359	-3.359	0.000	(0)
HSiO3-	4.959e-05	3.631e-05	-4.305	-4.440	-0.135	(0)
NaHSiO3	2.063e-05	2.063e-05	-4.686	-4.686	0.000	(0)
H2SiO4-2	5.523e-11	1.561e-11	-10.258	-10.806	-0.549	(0)
H6 (H2SiO4) 4-2	1.765e-11	4.989e-12	-10.753	-11.302	-0.549	(0)
H4 (H2SiO4) 4-4	1.060e-16	6.658e-19	-15.975	-18.177	-2.202	(0)

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

Phase	SI**	log IAP	log K (473 K, 194 atm)	
Afwillite	-18.11	20.39	38.50	Ca3Si2O4 (OH) 6
Akermanite	-5.19	20.15	25.35	Ca2MgSi2O7
Al	-64.53	22.30	86.83	Al
Al (g)	-93.96	22.30	116.26	Al
Al2 (SO4) 3	-41.26	-52.14	-10.89	Al2 (SO4) 3
Al2 (SO4) 3:6H2O	-35.18	-52.15	-16.97	Al2 (SO4) 3:6H2O
Albite	-0.01	-2.53	-2.52	NaAlSi3O8
Albite_high	-0.61	-2.53	-1.92	NaAlSi3O8
Albite_low	-0.01	-2.53	-2.52	NaAlSi3O8
Alum-K	-23.07	-30.28	-7.21	KAl (SO4) 2:12H2O
Alunite	-8.00	-27.73	-19.72	KAl3 (OH) 6 (SO4) 2
Amesite-14A	12.00	33.56	21.55	Mg4Al4Si2O10 (OH) 8
Analcime	0.45	0.39	-0.06	Na.96Al.96Si2.04O6:H2O
Analcime-dehy	-3.17	0.39	3.56	Na.96Al.96Si2.04O6
Andalusite	-0.13	-0.81	-0.68	Al2SiO5
Anhydrite	-1.90	-9.19	-7.29	CaSO4
Anorthite	-0.03	4.86	4.89	CaAl2 (SiO4) 2
Antarcticite	-13.90	-10.07	3.83	CaCl2:6H2O
Anthophyllite	3.45	34.71	31.25	Mg7Si8O22 (OH) 2
Antigorite	62.83	308.03	245.21	Mg48Si34O85 (OH) 62
Aphthitalite	-11.54	-15.43	-3.89	NaK3 (SO4) 2
Aragonite	-0.83	-1.27	-0.44	CaCO3
Arcanite	-6.49	-8.39	-1.90	K2SO4
Artinite	-3.71	7.29	11.00	Mg2CO3 (OH) 2:3H2O
B	-49.76	17.56	67.32	B
B (g)	-104.49	17.56	122.05	B
B2O3	-10.56	-6.94	3.63	B2O3
Bassanite	-2.57	-9.19	-6.62	CaSO4:0.5H2O
Beidellite-Ca	0.06	-7.87	-7.93	Ca.165Al2.33Si3.67O10 (OH) 2
Beidellite-H	-1.01	-9.36	-8.35	H.33Al2.33Si3.67O10 (OH) 2
Beidellite-K	-0.30	-7.74	-7.44	K.33Al2.33Si3.67O10 (OH) 2
Beidellite-Mg	0.23	-7.91	-8.15	Mg.165Al2.33Si3.67O10 (OH) 2
Beidellite-Na	0.07	-7.29	-7.37	Na.33Al2.33Si3.67O10 (OH) 2
Bischofite	-14.44	-10.31	4.13	MgCl2:6H2O
Bloedite	-12.46	-15.11	-2.65	Na2Mg (SO4) 2:4H2O
Boehmite	1.42	1.27	-0.15	AlO2H
Borax	-18.75	-1.33	17.42	Na2 (B4O5 (OH) 4) :8H2O
Boric_acid	-4.50	-3.47	1.03	B (OH) 3
Brucite	-0.43	8.80	9.23	Mg (OH) 2
Burkeite	-18.60	-9.11	9.49	Na6CO3 (SO4) 2
C	-19.55	17.73	37.28	C
C (g)	-90.77	17.73	108.50	C
Ca	-63.01	23.06	86.06	Ca
Ca (g)	-76.84	23.06	99.90	Ca
Ca-Al Pyroxene	-2.87	8.22	11.09	CaAl2SiO6
Ca2Al2O5:8H2O	-38.38	20.61	58.99	Ca2Al2O5:8H2O
Ca2Cl2 (OH) 2:H2O	-27.19	-1.03	26.16	Ca2Cl2 (OH) 2:H2O
Ca3Al2O6	-29.45	29.66	59.11	Ca3Al2O6
Ca4Al2O7:13H2O	-67.68	38.68	106.37	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-63.85	38.68	102.53	Ca4Al2O7:19H2O
Ca4Cl2 (OH) 6:13H2O	-50.45	17.03	67.49	Ca4Cl2 (OH) 6:13H2O
CaAl2O4	-6.08	11.58	17.67	CaAl2O4
CaAl2O4:10H2O	-25.80	11.57	37.37	CaAl2O4:10H2O
CaAl4O7	-7.35	14.13	21.48	CaAl4O7
Calcite	-0.68	-1.27	-0.59	CaCO3
Carnallite	-18.95	-14.94	4.01	KMgCl3:6H2O
CaSO4:0.5H2O (beta)	-2.60	-9.19	-6.60	CaSO4:0.5H2O
Celadonite	1.20	1.55	0.35	KMgAlSi4O10 (OH) 2
CH4 (g)	-36.79	-39.54	-2.75	CH4

Chalcedony	-1.08	-3.36	-2.28	SiO2
Chloromagnesite	-20.29	-10.31	9.99	MgCl2
Chrysotile	3.46	19.67	16.21	Mg3Si2O5(OH)4
Cl2(g)	-31.62	-33.12	-1.51	Cl2
Clinocllore-14A	10.84	36.45	25.61	Mg5Al2Si3O10(OH)8
Clinocllore-7A	8.27	36.45	28.18	Mg5Al2Si3O10(OH)8
Clinozoisite	1.24	11.81	10.57	Ca2Al3Si3O12(OH)
CO(g)	-15.25	-18.05	-2.80	CO
CO2(g)	-0.75	-2.92	-2.17	CO2
Coesite	-1.44	-3.36	-1.92	SiO2
Colemanite	-24.34	-2.74	21.60	Ca2B6O11:5H2O
Cordierite_anhyd	-1.40	5.89	7.29	Mg2Al4Si5O18
Cordierite_hydr	-0.15	5.89	6.03	Mg2Al4Si5O18:H2O
Corundum	4.01	2.54	-1.47	Al2O3
Cristobalite(alpha)	-1.22	-3.36	-2.14	SiO2
Cristobalite(beta)	-1.42	-3.36	-1.94	SiO2
Dawsonite	-2.20	-2.76	-0.56	NaAlCO3(OH)2
Diaspore	1.61	1.27	-0.33	Al2O3
Dicalcium_silicate	-7.63	14.71	22.34	Ca2SiO4
Diopside	0.00	11.12	11.12	CaMgSi2O6
Dolomite	0.00	-2.78	-2.78	CaMg(CO3)2
Dolomite-dis	-0.74	-2.78	-2.03	CaMg(CO3)2
Dolomite-ord	0.01	-2.78	-2.79	CaMg(CO3)2
Enstatite	-0.00	5.44	5.44	MgSiO3
Epsomite	-7.16	-9.44	-2.27	MgSO4:7H2O
Ettringite	-41.92	2.06	43.98	Ca6Al2(SO4)3(OH)12:26H2O
Eucryptite	-2.26	1.43	3.70	LiAlSiO4
Forsterite	0.19	14.24	14.05	Mg2SiO4
Foshagite	-14.68	26.07	40.74	Ca4Si3O9(OH)2:0.5H2O
Gaylussite	-9.97	0.97	10.94	CaNa2(CO3)2:5H2O
Gehlenite	-5.78	17.26	23.04	Ca2Al2SiO7
Gibbsite	0.97	1.27	0.30	Al(OH)3
Gismondine	-31.24	9.72	40.96	Ca2Al4Si4O16:9H2O
Glauberite	-9.40	-14.87	-5.47	Na2Ca(SO4)2
Grossular	-1.60	19.58	21.17	Ca3Al2(SiO4)3
Gypsum	-2.97	-9.19	-6.23	CaSO4:2H2O
Gyrolite	-8.00	7.99	15.99	Ca2Si3O7(OH)2:1.5H2O
H2(g)	-10.55	-13.36	-2.81	H2
H2O(g)	1.20	-0.00	-1.20	H2O
H2S(g)	-33.25	-41.53	-8.28	H2S
Halite	-4.51	-3.28	1.24	NaCl
Hatruite	-20.65	23.75	44.40	Ca3SiO5
HCl(g)	-10.44	-9.55	0.89	HCl
Hexahydrite	-7.44	-9.44	-1.99	MgSO4:6H2O
Hillebrandite	-8.38	14.71	23.09	Ca2SiO3(OH)2:0.17H2O
Huntite	-2.32	-5.79	-3.47	CaMg3(CO3)4
Hydroboracite	-23.39	-2.98	20.41	MgCaB6O11:6H2O
Hydromagnesite	-6.54	2.76	9.30	Mg5(CO3)4(OH)2:4H2O
Hydrophillite	-14.88	-10.07	4.82	CaCl2
Ice	-0.89	-0.00	0.89	H2O
Illite	1.30	-3.69	-4.98	K0.6Mg0.25Al1.8Al0.5Si3.5O10(OH)2
Jadeite	-0.74	0.83	1.57	NaAl(SiO3)2
K	-33.52	11.93	45.45	K
K(g)	-38.47	11.93	50.40	K
K-Feldspar	-0.00	-3.89	-3.89	KAlSi3O8
K2CO3:1.5H2O	-13.78	-0.47	13.31	K2CO3:1.5H2O
K2O	-46.59	9.84	56.43	K2O
K3H(SO4)2	-18.08	-21.70	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-50.06	-22.48	27.58	K8H4(CO3)6:3H2O
Kainite	-13.62	-14.07	-0.44	KMgClSO4:3H2O
KAl(SO4)2	-20.74	-30.27	-9.53	KAl(SO4)2
Kalinite	-5.67	-5.39	0.28	KHCO3
Kalsilite	-0.11	2.83	2.94	KAlSiO4
Kaolinite	0.59	-4.18	-4.77	Al2Si2O5(OH)4
Katoite	-48.76	29.65	78.41	Ca3Al2H12O12
Kieserite	-9.12	-9.43	-0.31	MgSO4:H2O
KMgCl3	-25.87	-14.94	10.94	KMgCl3
KMgCl3:2H2O	-22.84	-14.94	7.90	KMgCl3:2H2O
KNaCO3:6H2O	-9.11	0.89	9.99	KNaCO3:6H2O
Kyanite	-0.14	-0.81	-0.67	Al2SiO5
Lansfordite	-6.13	-1.51	4.62	MgCO3:5H2O
Larnite	-8.30	14.71	23.01	Ca2SiO4
Laumontite	-0.70	-1.86	-1.16	CaAl2Si4O12:4H2O
Lawsonite	0.33	4.86	4.53	CaAl2Si2O7(OH)2:H2O
Leonite	-13.54	-17.83	-4.29	K2Mg(SO4)2:4H2O
Li	-35.19	10.53	45.72	Li
Li(g)	-47.16	10.53	57.69	Li
Lime	-10.91	9.04	19.94	CaO
Magnesite	-0.28	-1.51	-1.23	MgCO3
Margarite	2.86	7.41	4.55	CaAl4Si2O10(OH)2
Maximum_Microcline	0.02	-3.89	-3.91	KAlSi3O8
Mayenite	-104.29	126.25	230.54	Ca12Al14O33
Mercallite	-11.87	-13.31	-1.44	KHSO4
Merwinite	-10.12	29.19	39.31	MgCa3(SiO4)2
Mesolite	2.65	2.60	-0.05	Na.676Ca.657Al1.99Si3.01O10:2.647H2O
Mg	-51.04	22.82	73.85	Mg
Mg(g)	-61.34	22.82	84.16	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-4.61	-7.23	-2.62	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-4.54	-5.03	-0.50	Mg1.5SO4(OH)
MgCl2:2H2O	-15.75	-10.31	5.44	MgCl2:2H2O
MgCl2:4H2O	-13.64	-10.31	3.33	MgCl2:4H2O
MgCl2:H2O	-17.22	-10.31	6.91	MgCl2:H2O
MgOHCl	-8.26	-0.75	7.51	MgOHCl
MgSO4	-6.74	-9.43	-2.69	MgSO4
Mirabilite	-12.22	-5.68	6.53	Na2SO4:10H2O
Misenite	-77.18	-88.25	-11.08	K8H6(SO4)7
Monohydrocalcite	-2.59	-1.27	1.32	CaCO3:H2O
Monticellite	-1.82	14.48	16.29	CaMgSiO4
Montmor-Ca	0.01	-6.92	-6.93	Ca.165Mg.33Al1.67Si4O10(OH)2
Montmor-K	-0.24	-6.79	-6.55	K.33Mg.33Al1.67Si4O10(OH)2
Montmor-Mg	0.22	-6.96	-7.18	Mg.495Al1.67Si4O10(OH)2
Montmor-Na	0.07	-6.34	-6.41	Na.33Mg.33Al1.67Si4O10(OH)2
Mordenite	-3.66	-10.92	-7.26	Ca.2895Na.361Al.94Si5.06O12:3.468H2O
Mordenite-dehy	-11.90	-10.92	0.98	Ca.2895Na.361Al.94Si5.06O12
Muscovite	3.60	-1.34	-4.95	KAl3Si3O10(OH)2
Na	-29.48	13.29	42.76	Na
Na(g)	-36.12	13.29	49.41	Na
Na2CO3	-6.03	2.25	8.28	Na2CO3

Na2CO3:7H2O	-12.02	2.24	14.26	Na2CO3:7H2O
Na2O	-32.52	12.55	45.07	Na2O
Na2SiO3	-7.53	9.19	16.72	Na2SiO3
Na3H(SO4)2	-16.74	-17.63	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-14.57	-20.55	-5.98	Na4Ca(SO4)3:2H2O
Na4SiO4	-27.95	21.74	49.69	Na4SiO4
Na6Si2O7	-40.17	30.94	71.10	Na6Si2O7
Nahcolite	-4.63	-4.03	0.60	NaHCO3
Natrolite	0.52	5.02	4.50	Na2Al2Si3O10:2H2O
Natron	-11.46	2.24	13.70	Na2CO3:10H2O
Natrosilite	-8.19	5.83	14.02	Na2Si2O5
Nepheline	-0.07	4.19	4.26	NaAlSiO4
Nesquehonite	-5.81	-1.51	4.30	MgCO3:3H2O
O2(g)	-25.17	-28.04	-2.87	O2
Okenite	-6.65	2.32	8.97	CaSi2O4(OH)2:2H2O
Oxychloride-Mg	-17.48	8.04	25.52	Mg2Cl(OH)3:4H2O
Paragonite	2.92	0.01	-2.91	NaAl3Si3O10(OH)2
Pargasite	2.54	43.20	40.66	NaCa2Al3Mg4Si6O22(OH)2
Pentahydrate	-7.83	-9.44	-1.61	MgSO4:5H2O
Periclase	-2.86	8.80	11.65	MgO
Petalite	-1.50	-8.65	-7.14	LiAlSi4O10
Phlogopite	7.01	22.50	15.50	KAlMg3Si3O10(OH)2
Picromerite	-13.12	-17.83	-4.71	K2Mg(SO4)2:6H2O
Pirssonite	-10.26	0.98	11.23	Na2Ca(CO3)2:2H2O
Polyhalite	-21.81	-36.21	-14.40	K2MgCa2(SO4)4:2H2O
Portlandite	-5.18	9.04	14.22	Ca(OH)2
Prehnite	0.42	10.54	10.12	CaAl2Si3O10(OH)2
Pseudowollastonite	-2.51	5.68	8.19	CaSiO3
Pyrophyllite	-1.68	-10.89	-9.21	Al2Si4O10(OH)2
Quartz	-0.91	-3.36	-2.45	SiO2
Rankinite	-10.53	20.39	30.93	Ca3Si2O7
S	-27.16	-55.55	-28.39	S
S2(g)	-59.97	-71.41	-11.44	S2
Sanidine high	-0.46	-3.89	-3.43	KAlSi3O8
Saponite-Ca	5.21	15.97	10.76	Ca.165Mg3Al.33Si3.67O10(OH)2
Saponite-H	4.15	14.48	10.34	H.33Mg3Al.33Si3.67O10(OH)2
Saponite-K	4.86	16.11	11.24	K.33Mg3Al.33Si3.67O10(OH)2
Saponite-Mg	5.38	15.93	10.55	Mg3.165Al.33Si3.67O10(OH)2
Saponite-Na	5.23	16.55	11.33	Na.33Mg3Al.33Si3.67O10(OH)2
Scolecite	1.30	1.50	0.20	CaAl2Si3O10:3H2O
Sepiolite	-2.72	15.03	17.75	Mg4Si6O15(OH)2:6H2O
Si	-66.75	24.68	91.43	Si
Si(g)	-108.74	24.68	133.42	Si
Sillimanite	-0.29	-0.81	-0.52	Al2SiO5
SiO2(am)	-1.53	-3.36	-1.83	SiO2
SO2(g)	-19.04	-20.00	-0.96	SO2
Spinel	0.24	11.34	11.10	Al2MgO4
Spodumene	-1.84	-1.93	-0.09	LiAlSi2O6
Starkeyite	-8.26	-9.43	-1.18	MgSO4:4H2O
Stilbite	-1.24	-10.05	-8.81	Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O
Sylvite	-5.87	-4.63	1.23	KCl
Synogenite	-9.94	-17.58	-7.64	K2Ca(SO4)2:2H2O
Tachyhydrite	-47.30	-30.68	16.61	Mg2CaCl6:12H2O
Talc	3.54	12.95	9.41	Mg3Si4O10(OH)2
Thenardite	-3.95	-5.68	-1.73	Na2SO4
Thermonatrite	-6.84	2.25	9.08	Na2CO3:H2O
Tobermorite-11A	-18.74	25.03	43.77	Ca5Si6H11O22.5
Tobermorite-14A	-21.84	25.02	46.87	Ca5Si6H21O27.5
Tobermorite-9A	-19.11	25.03	44.14	Ca5Si6H6O20
Tremolite	4.73	35.19	30.46	Ca2Mg5Si8O22(OH)2
Tridymite	-1.23	-3.36	-2.13	SiO2
Trona-K	-16.00	-4.50	11.50	K2NaH(CO3)2:2H2O
Wairakite	-1.48	-1.86	-0.37	CaAl2Si4O10(OH)4
Wollastonite	-2.46	5.68	8.14	CaSiO3
Xonotlite	-24.84	34.07	58.91	Ca6Si6O17(OH)2
Zoisite	1.21	11.81	10.60	Ca2Al3(SiO4)3OH

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

TIME STEP 1 YEAR

Reaction step 11.

Using solution 1. P-3
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

Time step: 3e+10 seconds (Incremented time: 3.33333e+10 seconds)

Rate name	Delta Moles	Total Moles	Reactant	Coefficient
Quartz	-0.000e+00	0.000e+00	SiO2	1
Anorthite	4.957e-09	1.133e+00	CaAl2(SiO4)2	1
Albite	-2.239e-10	2.579e+01	NaAlSi3O8	1
K-Feldspar	-1.043e-11	8.079e+00	KAlSi3O8	1
Diopside	-4.887e-09	2.973e+01	CaMgSi2O6	1
Enstatite	4.957e-09	7.792e+00	MgSiO3	1
Kaolinite	-4.863e-09	2.660e+01	Al2Si2O5(OH)4	1
Montmor-Na	-0.000e+00	0.000e+00	Na.33Mg.33Al1.67Si4O10(OH)2	1
Dolomite	-6.936e-11	6.050e-01	CaMg(CO3)2	1
Siderite	-0.000e+00	0.000e+00	FeCO3	1

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

Phase	SI	log IAP	log K(T, P)	Moles in assemblage		
				Initial	Final	Delta
CO2(g)	-1.37	-3.54	-2.17	0.000e+00	0	0.000e+00

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

Elements	Molality	Moles
Al	1.548e-01	2.872e-02
B	1.986e-03	3.683e-04

C	7.782e-03	1.443e-03
Ca	1.119e-06	2.075e-07
Cl	1.104e-01	2.048e-02
K	1.806e-02	3.349e-03
Li	4.519e-04	8.381e-05
Mg	5.386e-06	9.989e-07
Na	3.794e-01	7.037e-02
S	3.379e-02	6.266e-03
Si	3.746e-04	6.948e-05

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

pH	=	8.537	Charge balance
pe	=	-2.488	Adjusted to redox equilibrium
Density (g/cm ³)	=	0.90074	
Volume (L)	=	0.21134	
Activity of water	=	0.989	
Ionic strength (mol/kgw)	=	3.319e-01	
Mass of water (kg)	=	1.855e-01	
Total alkalinity (eq/kg)	=	6.324e-01	
Total CO2 (mol/kg)	=	7.782e-03	
Temperature (°C)	=	200.00	
Pressure (atm)	=	194.00	
Electrical balance (eq)	=	9.655e-03	
Percent error, 100*(Cat- An)/(Cat+ An)	=	8.50	
Iterations	=	125	
Total H	=	2.059863e+01	
Total O	=	1.038660e+01	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm ³ /mol
OH-	3.449e-03	1.940e-03	-2.462	-2.712	-0.250	(0)
H+	4.044e-09	2.903e-09	-8.393	-8.537	-0.144	0.00
H2O	5.553e+01	9.890e-01	1.744	-0.005	0.000	20.53
Al	1.548e-01					
AlO2-	1.109e-01	6.457e-02	-0.955	-1.190	-0.235	(0)
NaAlO2	4.393e-02	4.393e-02	-1.357	-1.357	0.000	(0)
HALO2	2.041e-05	2.041e-05	-4.690	-4.690	0.000	(0)
Al(OH)2+	6.243e-11	3.635e-11	-10.205	-10.439	-0.235	(0)
AlOH+2	2.158e-16	2.521e-17	-15.666	-16.598	-0.932	(0)
Al+3	2.570e-23	9.768e-25	-22.590	-24.010	-1.420	(0)
AlSO4+	4.480e-24	2.609e-24	-23.349	-23.584	-0.235	(0)
Al(SO4)2-	9.076e-25	5.284e-25	-24.042	-24.277	-0.235	(0)
Al2(OH)2+4	7.071e-36	2.771e-39	-35.150	-38.557	-3.407	(0)
Al3(OH)4+5	0.000e+00	0.000e+00	-46.521	-51.604	-5.084	(0)
Al13O4(OH)24+7	0.000e+00	0.000e+00	-126.590	-136.569	-9.979	(0)
B(-5)	0.000e+00					
BH4-	0.000e+00	0.000e+00	-80.337	-80.572	-0.235	(0)
B(3)	1.986e-03					
B(OH)3	1.009e-03	1.009e-03	-2.996	-2.996	0.000	(0)
BO2-	9.028e-04	5.257e-04	-3.044	-3.279	-0.235	(0)
NaB(OH)4	7.457e-05	7.457e-05	-4.127	-4.127	0.000	(0)
CaB(OH)4+	9.400e-10	5.473e-10	-9.027	-9.262	-0.235	(0)
MgB(OH)4+	6.453e-10	3.757e-10	-9.190	-9.425	-0.235	(0)
B2O(OH)5-	1.243e-16	7.235e-17	-15.906	-16.141	-0.235	(0)
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-82.238	-82.238	0.000	(0)
C(-3)	0.000e+00					
C2H6	0.000e+00	0.000e+00	-50.803	-50.803	0.000	(0)
C(-4)	2.098e-36					
CH4	2.098e-36	2.098e-36	-35.678	-35.678	0.000	(0)
C(2)	2.869e-18					
CO	2.869e-18	2.869e-18	-17.542	-17.542	0.000	(0)
C(4)	7.782e-03					
HCO3-	7.056e-03	4.109e-03	-2.151	-2.386	-0.235	(0)
CO3-2	4.090e-04	4.779e-05	-3.388	-4.321	-0.932	(0)
CO2	2.695e-04	2.909e-04	-3.569	-3.536	0.033	53.80
NaHCO3	4.626e-05	4.626e-05	-4.335	-4.335	0.000	(0)
CaCO3	5.139e-07	5.139e-07	-6.289	-6.289	0.000	(0)
NaCO3-	1.021e-07	5.948e-08	-6.991	-7.226	-0.235	(0)
CaHCO3+	6.847e-08	3.987e-08	-7.164	-7.399	-0.235	(0)
MgCO3	4.207e-08	4.207e-08	-7.376	-7.376	0.000	(0)
MgHCO3+	4.092e-08	2.383e-08	-7.388	-7.623	-0.235	(0)
(CO2)2	1.181e-08	1.275e-08	-7.928	-7.895	0.033	107.59
Ca	1.119e-06					
CaCO3	5.139e-07	5.139e-07	-6.289	-6.289	0.000	(0)
CaSO4	2.827e-07	2.827e-07	-6.549	-6.549	0.000	(0)
Ca+2	2.401e-07	3.803e-08	-6.620	-7.420	-0.800	(0)
CaHCO3+	6.847e-08	3.987e-08	-7.164	-7.399	-0.235	(0)
CaCl+	1.192e-08	6.939e-09	-7.924	-8.159	-0.235	(0)
CaB(OH)4+	9.400e-10	5.473e-10	-9.027	-9.262	-0.235	(0)
CaCl2	8.787e-10	8.787e-10	-9.056	-9.056	0.000	(0)
CaOH+	3.480e-12	2.026e-12	-11.458	-11.693	-0.235	(0)
Cl(-1)	1.104e-01					
Cl-	9.791e-02	5.293e-02	-1.009	-1.276	-0.267	(0)
NaCl	1.227e-02	1.227e-02	-1.911	-1.911	0.000	(0)
KCl	2.623e-04	2.623e-04	-3.581	-3.581	0.000	(0)
LiCl	4.871e-06	4.871e-06	-5.312	-5.312	0.000	(0)
MgCl+	2.787e-08	1.623e-08	-7.555	-7.790	-0.235	(0)
CaCl+	1.192e-08	6.939e-09	-7.924	-8.159	-0.235	(0)
CaCl2	8.787e-10	8.787e-10	-9.056	-9.056	0.000	(0)
HCl	1.258e-10	1.258e-10	-9.900	-9.900	0.000	(0)
Cl(1)	1.924e-28					
ClO-	1.810e-28	1.054e-28	-27.742	-27.977	-0.235	(0)
HClO	1.135e-29	1.135e-29	-28.945	-28.945	0.000	(0)
Cl(3)	0.000e+00					
ClO2-	0.000e+00	0.000e+00	-48.010	-48.245	-0.235	(0)
HClO2	0.000e+00	0.000e+00	-53.612	-53.612	0.000	(0)
Cl(5)	0.000e+00					
ClO3-	0.000e+00	0.000e+00	-59.507	-59.757	-0.250	(0)
Cl(7)	0.000e+00					
ClO4-	0.000e+00	0.000e+00	-74.591	-74.841	-0.250	(0)
H(0)	1.010e-12					
H2	5.049e-13	5.675e-13	-12.297	-12.246	0.051	(0)
K	1.806e-02					

K+	1.478e-02	7.990e-03	-1.830	-2.097	-0.267	(0)
KS04-	3.017e-03	1.756e-03	-2.520	-2.755	-0.235	(0)
KCl	2.623e-04	2.623e-04	-3.581	-3.581	0.000	(0)
KOH	1.045e-08	1.045e-08	-7.981	-7.981	0.000	(0)
KHSO4	1.650e-09	1.650e-09	-8.783	-8.783	0.000	(0)
Li	4.519e-04					
Li+	4.395e-04	2.848e-04	-3.357	-3.545	-0.188	(0)
LiSO4-	7.518e-06	4.377e-06	-5.124	-5.359	-0.235	(0)
LiCl	4.871e-06	4.871e-06	-5.312	-5.312	0.000	(0)
LiOH	2.462e-09	2.462e-09	-8.609	-8.609	0.000	(0)
Mg	5.386e-06					
MgSO4	5.171e-06	5.171e-06	-5.286	-5.286	0.000	(0)
Mg+2	1.032e-07	2.194e-08	-6.986	-7.659	-0.673	(0)
MgCO3	4.207e-08	4.207e-08	-7.376	-7.376	0.000	(0)
MgHCO3+	4.092e-08	2.383e-08	-7.388	-7.623	-0.235	(0)
MgCl+	2.787e-08	1.623e-08	-7.555	-7.790	-0.235	(0)
MgB (OH) 4+	6.453e-10	3.757e-10	-9.190	-9.425	-0.235	(0)
Mg4 (OH) 4+4	2.129e-33	8.341e-37	-32.672	-36.079	-3.407	(0)
Na	3.794e-01					
Na+	3.170e-01	1.846e-01	-0.499	-0.734	-0.235	(0)
NaAlO2	4.393e-02	4.393e-02	-1.357	-1.357	0.000	(0)
NaCl	1.227e-02	1.227e-02	-1.911	-1.911	0.000	(0)
NaSO4-	5.466e-03	3.183e-03	-2.262	-2.497	-0.235	(0)
NaOH	4.210e-04	4.210e-04	-3.376	-3.376	0.000	(0)
NaHSiO3	1.676e-04	1.676e-04	-3.776	-3.776	0.000	(0)
NaB (OH) 4	7.457e-05	7.457e-05	-4.127	-4.127	0.000	(0)
NaHCO3	4.626e-05	4.626e-05	-4.335	-4.335	0.000	(0)
NaCO3-	1.021e-07	5.948e-08	-6.991	-7.226	-0.235	(0)
O (0)	9.364e-31					
O2	4.682e-31	5.263e-31	-30.330	-30.279	0.051	(0)
S (-2)	3.726e-30					
HS-	2.028e-30	1.140e-30	-29.693	-29.943	-0.250	(0)
S-2	1.683e-30	2.199e-31	-29.774	-30.658	-0.884	(0)
H2S	1.615e-32	1.615e-32	-31.792	-31.792	0.000	(0)
S2-2	0.000e+00	0.000e+00	-55.346	-56.332	-0.986	(0)
S3-2	0.000e+00	0.000e+00	-79.804	-80.791	-0.986	(0)
S4-2	0.000e+00	0.000e+00	-104.409	-105.396	-0.986	(0)
S5-2	0.000e+00	0.000e+00	-129.153	-130.140	-0.986	(0)
S (2)	9.927e-36					
S2O3-2	4.963e-36	5.122e-37	-35.304	-36.291	-0.986	(0)
HS2O3-	0.000e+00	0.000e+00	-43.579	-43.814	-0.235	(0)
S (3)	0.000e+00					
S2O4-2	0.000e+00	0.000e+00	-42.125	-43.009	-0.884	(0)
S (4)	5.175e-16					
SO3-2	2.937e-16	3.432e-17	-15.532	-16.464	-0.932	(0)
HSO3-	2.238e-16	1.303e-16	-15.650	-15.885	-0.235	(0)
SO2	4.965e-21	4.965e-21	-20.304	-20.304	0.000	(0)
H2SO3	4.727e-25	4.727e-25	-24.325	-24.325	0.000	(0)
S2O6-2	5.537e-33	5.713e-34	-32.257	-33.243	-0.986	(0)
S3O6-2	0.000e+00	0.000e+00	-58.861	-59.847	-0.986	(0)
S4O6-2	0.000e+00	0.000e+00	-73.046	-74.033	-0.986	(0)
S5O6-2	0.000e+00	0.000e+00	-110.125	-111.111	-0.986	(0)
S (5)	8.469e-37					
S2O5-2	4.235e-37	4.370e-38	-36.373	-37.360	-0.986	(0)
S (6)	3.379e-02					
SO4-2	2.529e-02	2.610e-03	-1.597	-2.583	-0.986	(0)
NaSO4-	5.466e-03	3.183e-03	-2.262	-2.497	-0.235	(0)
KS04-	3.017e-03	1.756e-03	-2.520	-2.755	-0.235	(0)
LiSO4-	7.518e-06	4.377e-06	-5.124	-5.359	-0.235	(0)
MgSO4	5.171e-06	5.171e-06	-5.286	-5.286	0.000	(0)
HSO4-	3.873e-07	2.255e-07	-6.412	-6.647	-0.235	(0)
CaSO4	2.827e-07	2.827e-07	-6.549	-6.549	0.000	(0)
KHSO4	1.650e-09	1.650e-09	-8.783	-8.783	0.000	(0)
H2SO4	2.097e-21	2.097e-21	-20.678	-20.678	0.000	(0)
AlSO4+	4.480e-24	2.609e-24	-23.349	-23.584	-0.235	(0)
Al (SO4) 2-	9.076e-25	5.284e-25	-24.042	-24.277	-0.235	(0)
S (7)	0.000e+00					
S2O8-2	0.000e+00	0.000e+00	-44.723	-45.709	-0.986	(0)
S (8)	6.901e-34					
HSO5-	6.901e-34	4.018e-34	-33.161	-33.396	-0.235	(0)
Si	3.746e-04					
NaHSiO3	1.676e-04	1.676e-04	-3.776	-3.776	0.000	(0)
SiO2	1.066e-04	1.066e-04	-3.972	-3.972	0.000	(0)
HSiO3-	1.004e-04	5.848e-05	-3.998	-4.233	-0.235	(0)
H2SiO4-2	1.611e-09	1.663e-10	-8.793	-9.779	-0.986	(0)
H6 (H2SiO4) 4-2	7.031e-12	7.256e-13	-11.153	-12.139	-0.986	(0)
H4 (H2SiO4) 4-4	4.238e-14	4.314e-18	-13.373	-17.365	-3.992	(0)

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

Phase	SI**	log IAP	log K (473 K, 194 atm)
Afwillite	-17.52	20.99	38.50
Akermanite	-4.58	20.76	25.35
Al	-62.53	24.30	86.83
Al (g)	-91.96	24.30	116.26
Al2 (SO4) 3	-44.88	-55.77	-10.89
Al2 (SO4) 3:6H2O	-38.83	-55.80	-16.97
Albite	0.00	-2.52	-2.52
Albite_high	-0.61	-2.52	-1.92
Albite_low	-0.00	-2.52	-2.52
Alum-K	-24.12	-31.33	-7.21
Alunite	-8.38	-28.10	-19.72
Amesite-14A	14.50	36.05	21.55
Analcime	0.97	0.91	-0.06
Analcime-dehy	-2.65	0.92	3.56
Andalusite	-0.10	-0.78	-0.68
Anhydrite	-2.71	-10.00	-7.29
Anorthite	0.00	4.89	4.89
Antarcticite	-13.83	-10.00	3.83
Anthophyllite	2.84	34.09	31.25
Anthigorite	71.29	316.50	245.21
Aphthitalite	-9.31	-12.19	-3.89
Aragonite	-0.83	-1.27	-0.44
Arcanite	-4.87	-6.78	-1.90
Artinite	-3.11	7.88	11.00
B	-47.60	19.72	67.32
B (g)	-102.33	19.72	122.05
CaSi2O4 (OH) 6			
Ca2MgSi2O7			
Al			
Al2 (SO4) 3			
Al2 (SO4) 3:6H2O			
NaAlSi3O8			
NaAlSi3O8			
NaAlSi3O8			
KAl (SO4) 2:12H2O			
KAl3 (OH) 6 (SO4) 2			
Mg4Al4Si2O10 (OH) 8			
Na.96Al.96Si2.04O6:H2O			
Na.96Al.96Si2.04O6			
Al2SiO5			
CaSO4			
CaAl2 (SiO4) 2			
CaCl2:6H2O			
Mg7Si8O22 (OH) 2			
Mg48Si34O85 (OH) 62			
NaK3 (SO4) 2			
CaCO3			
K2SO4			
Mg2CO3 (OH) 2:3H2O			
B			

B2O3	-9.60	-5.98	3.63	B2O3
Bassanite	-3.38	-10.01	-6.62	CaSO4:0.5H2O
Beidellite-Ca	-1.34	-9.28	-7.93	Ca.165Al2.33Si3.67O10 (OH) 2
Beidellite-H	-2.52	-10.87	-8.35	H.33Al2.33Si3.67O10 (OH) 2
Beidellite-K	-1.30	-8.75	-7.44	K.33Al2.33Si3.67O10 (OH) 2
Beidellite-Mg	-1.17	-9.32	-8.15	Mg.165Al2.33Si3.67O10 (OH) 2
Beidellite-Na	-0.93	-8.30	-7.37	Na.33Al2.33Si3.67O10 (OH) 2
Bischofite	-14.37	-10.24	4.13	MgCl2:6H2O
Bloedite	-11.66	-14.31	-2.65	Na2Mg (SO4) 2:4H2O
Boehmite	1.74	1.59	-0.15	AlO2H
Borax	-13.82	3.60	17.42	Na2 (B4O5 (OH) 4) :8H2O
Boric_acid	-4.03	-3.00	1.03	B (OH) 3
Brucite	0.18	9.41	9.23	Mg (OH) 2
Burkeite	-12.91	-3.42	9.49	Na6CO3 (SO4) 2
C	-17.92	19.36	37.28	C
C (g)	-89.14	19.36	108.50	C
Ca	-61.27	24.79	86.06	Ca
Ca (g)	-75.11	24.79	99.90	Ca
Ca-Al Pyroxene	-2.22	8.86	11.09	CaAl2SiO6
Ca2Al2O5:8H2O	-36.54	22.45	58.99	Ca2Al2O5:8H2O
Ca2Cl2 (OH) 2:H2O	-26.49	-0.33	26.16	Ca2Cl2 (OH) 2:H2O
Ca3Al2O6	-26.97	32.14	59.11	Ca3Al2O6
Ca4Al2O7:13H2O	-64.64	41.72	106.37	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-60.83	41.69	102.53	Ca4Al2O7:19H2O
Ca4Cl2 (OH) 6:13H2O	-48.59	18.90	67.49	Ca4Cl2 (OH) 6:13H2O
CaAl2O4	-4.83	12.84	17.67	CaAl2O4
CaAl2O4:10H2O	-24.58	12.79	37.37	CaAl2O4:10H2O
CaAl4O7	-5.45	16.02	21.48	CaAl4O7
Calcite	-0.68	-1.27	-0.59	CaCO3
Carnallite	-17.62	-13.61	4.01	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-3.41	-10.01	-6.60	CaSO4:0.5H2O
Celadonite	1.20	1.55	0.35	KMgAlSi4O10 (OH) 2
CH4 (g)	-32.93	-35.68	-2.75	CH4
Chalcedony	-1.69	-3.97	-2.28	SiO2
Chloromagnesite	-20.20	-10.21	9.99	MgCl2
Chrysotile	4.07	20.28	16.21	Mg3Si2O5 (OH) 4
Cl2 (g)	-33.25	-34.76	-1.51	Cl2
Clinocllore-14A	12.70	38.30	25.61	Mg5Al2Si3O10 (OH) 8
Clinocllore-7A	10.12	38.30	28.18	Mg5Al2Si3O10 (OH) 8
Clinozoisite	1.59	12.16	10.57	Ca2Al3Si3O12 (OH)
CO (g)	-14.75	-17.54	-2.80	CO
CO2 (g)	-1.37	-3.54	-2.17	CO2
Coesite	-2.06	-3.97	-1.92	SiO2
Colemanite	-20.26	1.34	21.60	Ca2B6O11:5H2O
Cordierite_anhyd	-1.96	5.33	7.29	Mg2Al4Si5O18
Cordierite_hydr	-0.70	5.33	6.03	Mg2Al4Si5O18:H2O
Corundum	4.65	3.19	-1.47	Al2O3
Cristobalite(alpha)	-1.83	-3.97	-2.14	SiO2
Cristobalite(beta)	-2.03	-3.97	-1.94	SiO2
Dawsonite	-0.97	-1.53	-0.56	NaAlCO3 (OH) 2
Diaspore	1.93	1.59	-0.33	AlHO2
Dicalcium_silicate	-7.02	15.33	22.34	Ca2SiO4
Diopside	-0.00	11.12	11.12	CaMgSi2O6
Dolomite	-0.00	-2.78	-2.78	CaMg (CO3) 2
Dolomite-dis	-0.74	-2.78	-2.03	CaMg (CO3) 2
Dolomite-ord	0.01	-2.78	-2.79	CaMg (CO3) 2
Enstatite	-0.00	5.44	5.44	MgSiO3
Epsomite	-8.00	-10.28	-2.27	MgSO4:7H2O
Etringite	-42.00	1.97	43.98	Ca6Al2 (SO4) 3 (OH) 12:26H2O
Eucryptite	-1.09	2.61	3.70	LiAlSiO4
Forsterite	0.80	14.85	14.05	Mg2SiO4
Foshagite	-14.07	26.67	40.74	Ca4Si3O9 (OH) 2:0.5H2O
Gaylussite	-7.55	3.39	10.94	CaNa2 (CO3) 2:5H2O
Gehlenite	-4.52	18.51	23.04	Ca2Al2SiO7
Gibbsite	1.29	1.59	0.30	Al (OH) 3
Gismondine	-31.22	9.74	40.96	Ca2Al4Si4O16:9H2O
Glauberite	-8.59	-14.05	-5.47	Na2Ca (SO4) 2
Grossular	-0.96	20.22	21.17	Ca3Al2 (SiO4) 3
Gypsum	-3.78	-10.01	-6.23	CaSO4:2H2O
Gyrolite	-8.62	7.37	15.99	Ca2Si3O7 (OH) 2:1.5H2O
H2 (g)	-9.44	-12.25	-2.81	H2
H2O (g)	1.19	-0.00	-1.20	H2O
H2S (g)	-30.20	-38.48	-8.28	H2S
Halite	-3.25	-2.01	1.24	NaCl
Hatrurite	-19.43	24.98	44.40	Ca3SiO5
HCl (g)	-10.70	-9.81	0.89	HCl
Hexahydrate	-8.28	-10.27	-1.99	MgSO4:6H2O
Hillebrandite	-7.77	15.32	23.09	Ca2SiO3 (OH) 2:0.17H2O
Huntite	-2.32	-5.79	-3.47	CaMg3 (CO3) 4
Hydroboracite	-19.31	1.10	20.41	MgCaB6O11:6H2O
Hydromagnesite	-5.94	3.35	9.30	Mg5 (CO3) 4 (OH) 2:4H2O
Hydrophilite	-14.79	-9.97	4.82	CaCl2
Ice	-0.90	-0.00	0.89	H2O
Illite	0.95	-4.03	-4.98	K0.6Mg0.25Al1.8Al0.5Si3.5O10 (OH) 2
Jadeite	-0.12	1.45	1.57	NaAl (SiO3) 2
K	-31.44	14.01	45.45	K
K (g)	-36.39	14.01	50.40	K
K-Feldspar	0.00	-3.89	-3.89	KAlSi3O8
K2CO3:1.5H2O	-11.36	1.95	13.31	K2CO3:1.5H2O
K2O	-43.56	12.87	56.43	K2O
K3H (SO4) 2	-16.37	-20.00	-3.62	K3H (SO4) 2
K8H4 (CO3) 6:3H2O	-41.61	-14.04	27.58	K8H4 (CO3) 6:3H2O
Kainite	-13.19	-13.63	-0.44	KMgClSO4:3H2O
KAl (SO4) 2	-21.74	-31.27	-9.53	KAl (SO4) 2
Kalicinite	-4.77	-4.48	0.28	KHCO3
Kalsilite	1.12	4.06	2.94	KAlSiO4
Kaolinite	0.00	-4.77	-4.77	Al2Si2O5 (OH) 4
Katoite	-46.30	32.11	78.41	Ca3Al2H12O12
Kieserite	-9.94	-10.25	-0.31	MgSO4:H2O
KMgCl3	-24.52	-13.59	10.94	KMgCl3
KMgCl3:2H2O	-21.50	-13.59	7.90	KMgCl3:2H2O
KNaCO3:6H2O	-6.70	3.29	9.99	KNaCO3:6H2O
Kyanite	-0.11	-0.78	-0.67	Al2SiO5
Lansfordite	-6.15	-1.53	4.62	MgCO3:5H2O
Larnite	-7.68	15.33	23.01	Ca2SiO4
Laumontite	-1.91	-3.07	-1.16	CaAl2Si4O12:4H2O
Lawsonite	0.36	4.88	4.53	CaAl2Si2O7 (OH) 2:H2O
Leonite	-12.75	-17.04	-4.29	K2Mg (SO4) 2:4H2O

Li	-33.16	12.56	45.72	Li
Li (g)	-45.13	12.56	57.69	Li
Lime	-10.29	9.65	19.94	CaO
Magnesite	-0.28	-1.51	-1.23	MgCO3
Margarite	3.53	8.08	4.55	CaAl4Si2O10(OH)2
Maximum Microcline	0.02	-3.89	-3.91	KAlSi3O8
Mayenite	-92.43	138.11	230.54	Ca12Al14O33
Mercallite	-11.78	-13.22	-1.44	KHSO4
Merwinite	-8.90	30.41	39.31	MgCa3(SiO4)2
Mesolite	2.87	2.82	-0.05	Na.676Ca.657Al1.99Si3.01O10:2.647H2O
Mg	-49.30	24.55	73.85	Mg
Mg (g)	-59.61	24.55	84.16	Mg
Mg1.25SO4 (OH) 0.5:0.5H2O	-5.27	-7.89	-2.62	Mg1.25SO4 (OH) 0.5:0.5H2O
Mg1.5SO4 (OH)	-5.04	-5.54	-0.50	Mg1.5SO4 (OH)
MgCl2:2H2O	-15.66	-10.22	5.44	MgCl2:2H2O
MgCl2:4H2O	-13.56	-10.23	3.33	MgCl2:4H2O
MgCl2:H2O	-17.13	-10.22	6.91	MgCl2:H2O
MgOHC1	-7.91	-0.40	7.51	MgOHC1
MgSO4	-7.55	-10.24	-2.69	MgSO4
Mirabilite	-10.63	-4.10	6.53	Na2SO4:10H2O
Misenite	-75.01	-86.09	-11.08	K8H6(SO4)7
Monohydrocalcite	-2.60	-1.27	1.32	CaCO3:H2O
Monticellite	-1.21	15.09	16.29	CaMgSiO4
Montmor-Ca	-1.61	-8.54	-6.93	Ca.165Mg.33Al1.67Si4O10(OH)2
Montmor-K	-1.45	-8.00	-6.55	K.33Mg.33Al1.67Si4O10(OH)2
Montmor-Mg	-1.40	-8.57	-7.18	Mg.495Al1.67Si4O10(OH)2
Montmor-Na	-1.14	-7.55	-6.41	Na.33Mg.33Al1.67Si4O10(OH)2
Mordenite	-5.75	-13.01	-7.26	Ca.2895Na.361Al.94Si5.06O12:3.468H2O
Mordenite-dehy	-13.97	-12.99	0.98	Ca.2895Na.361Al.94Si5.06O12
Muscovite	4.24	-0.70	-4.95	KAl3Si3O10(OH)2
Na	-27.39	15.37	42.76	Na
Na (g)	-34.04	15.37	49.41	Na
Na2CO3	-3.60	4.68	8.28	Na2CO3
Na2CO3:7H2O	-9.61	4.65	14.26	Na2CO3:7H2O
Na2O	-29.47	15.60	45.07	Na2O
Na2SiO3	-5.09	11.63	16.72	Na2SiO3
Na3H(SO4)2	-15.01	-15.91	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-12.13	-18.11	-5.98	Na4Ca(SO4)3:2H2O
Na4SiO4	-22.46	27.23	49.69	Na4SiO4
Na6Si2O7	-32.24	38.86	71.10	Na6Si2O7
Nahcolite	-3.72	-3.12	0.60	NaHCO3
Natrolite	2.37	6.86	4.50	Na2Al2Si3O10:2H2O
Natron	-9.06	4.64	13.70	Na2CO3:10H2O
Natrosilite	-6.36	7.66	14.02	Na2Si2O5
Nepheline	1.16	5.42	4.26	NaAlSiO4
Nesquehonite	-5.82	-1.52	4.30	MgCO3:3H2O
O2 (g)	-27.41	-30.28	-2.87	O2
Okenite	-7.28	1.70	8.97	CaSi2O4(OH)2:2H2O
Oxychloride-Mg	-16.54	8.98	25.52	Mg2Cl(OH)3:4H2O
Paragonite	3.57	0.66	-2.91	NaAl3Si3O10(OH)2
Pargasite	5.02	45.68	40.66	NaCa2Al3Mg4Si6O22(OH)2
Pentahydrate	-8.66	-10.27	-1.61	MgSO4:5H2O
Periclase	-2.24	9.41	11.65	MgO
Petalite	-2.16	-9.31	-7.14	LiAlSi4O10
Phlogopite	8.84	24.34	15.50	KAlMg3Si3O10(OH)2
Picromerite	-12.34	-17.05	-4.71	K2Mg(SO4)2:6H2O
Pirssonite	-7.83	3.40	11.23	Na2Ca(CO3)2:2H2O
Polyhalite	-22.64	-37.04	-14.40	K2MgCa2(SO4)4:2H2O
Portlandite	-4.58	9.64	14.22	Ca(OH)2
Prehnite	0.44	10.56	10.12	Ca2Al2Si3O10(OH)2
Pseudowollastonite	-2.51	5.68	8.19	CaSiO3
Pyrophyllite	-3.49	-12.71	-9.21	Al2Si4O10(OH)2
Quartz	-1.52	-3.97	-2.45	SiO2
Rankinite	-9.92	21.00	30.93	Ca3Si2O7
S	-25.23	-53.61	-28.39	S
S2 (g)	-56.10	-67.54	-11.44	S2
Sanidine_high	-0.46	-3.89	-3.43	KAlSi3O8
Saponite-Ca	5.00	15.77	10.76	Ca.165Mg3Al.33Si3.67O10(OH)2
Saponite-H	3.84	14.17	10.34	H.33Mg3Al.33Si3.67O10(OH)2
Saponite-K	5.06	16.30	11.24	K.33Mg3Al.33Si3.67O10(OH)2
Saponite-Mg	5.17	15.73	10.55	Mg3.165Al.33Si3.67O10(OH)2
Saponite-Na	5.42	16.75	11.33	Na.33Mg3Al.33Si3.67O10(OH)2
Scolecite	0.71	0.91	0.20	CaAl2Si3O10:3H2O
Sepiolite	-3.98	13.77	17.75	Mg4Si6O15(OH)2:6H2O
Si	-65.13	26.31	91.43	Si
Si (g)	-107.12	26.31	133.42	Si
Sillimanite	-0.26	-0.78	-0.52	Al2SiO5
SiO2 (am)	-2.14	-3.97	-1.83	SiO2
SO2 (g)	-19.34	-20.30	-0.96	SO2
Spinel	1.50	12.60	11.10	Al2MgO4
Spodumene	-1.27	-1.36	-0.09	LiAlSi2O6
Starkeyite	-9.08	-10.26	-1.18	MgSO4:4H2O
Stilbite	-3.91	-12.72	-8.81	Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O
Sylvite	-4.61	-3.37	1.23	KCl
Syngenite	-9.14	-16.79	-7.64	K2Ca(SO4)2:2H2O
Tachyhydrite	-47.07	-30.45	16.61	Mg2Ca16:12H2O
Talc	2.93	12.34	9.41	Mg3Si4O10(OH)2
Thenardite	-2.32	-4.05	-1.73	Na2SO4
Thermonatrite	-4.40	4.68	9.08	Na2CO3:H2O
Tobermorite-11A	-19.38	24.39	43.77	Ca5Si6H11O22.5
Tobermorite-14A	-22.50	24.36	46.87	Ca5Si6H21O27.5
Tobermorite-9A	-19.74	24.40	44.14	Ca5Si6H6O20
Tremolite	4.11	34.57	30.46	Ca2Mg5Si8O22(OH)2
Tridymite	-1.84	-3.97	-2.13	SiO2
Trona-K	-12.67	-1.17	11.50	K2NaH(CO3)2:2H2O
Wairakite	-2.69	-3.06	-0.37	CaAl2Si4O10(OH)4
Wollastonite	-2.46	5.68	8.14	CaSiO3
Xonotlite	-24.85	34.06	58.91	Ca6Si6O17(OH)2
Zoisite	1.56	12.16	10.60	Ca2Al3(SiO4)3OH

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

End of simulation.

APPENDIX E

EQUILIBRIUM MODELING RESULT IN DIENG FIELD

Database file: D:\20181 FALL\4. Dieng PHREEQC\llnl (+actinolite).dat

Reading data base.

LLNL AQUEOUS_MODEL_PARAMETERS
NAMED_EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE D:\20181 FALL\4. Dieng PHREEQC\llnl (+actinolite).dat
SOLUTION_SPECIES
CO3-2 + 2 H+ = CO2 + H2O
log_k 16.681
delta_h -5.738 kcal
analytical_expression 464.1965 0.09344813 -26986.16 -165.75951 2248628.9
dw 1.92e-9
vm 7.29 0.92 2.07 -1.23 -1.60 # ref. 1 + McBride et al. 2015, JCD 60, 171
2CO2 = (CO2)2 # activity correction for CO2 solubility at high P, T
log_k -1.8
analytical_expression 8.68 -0.0103 -2190
vm 14.58 1.84 4.14 -2.46 -3.20
END

End of simulation.

Reading input data for simulation 2.

PHASES
CO2(g)
CO2 = CO2
log_k -1.468
delta_h -4.776 kcal
analytical_expression 10.5624 -2.3547e-2 -3972.8 0 5.8746e5 1.9194e-5
t_c 304.2 # critical T, K
p_c 72.86 # critical P, atm
omega 0.225 # acentric factor
Ankerite
CaMg0.3Fe0.7(CO3)2 + 2H+ = Ca++ + 0.3Mg++ + 0.7Fe++ + 2HCO3-
log_k 1.54
delta_h 0
analytical_expression -1.8649e+03 -2.9583e-01 1.0468e+05 6.7554e+02 -6.0514e+06
Actinolite
Ca2Mg2.5Fe2.5Si8O22(OH)2 + 14H+ = 2Ca+2 + 2.5Fe+2 + 8H2O + 2.5Mg+2 + 8SiO2
log_k 61.2367
delta_h -406.404 kJ
analytical_expression 85.291 0.046337 39465 -54.414 -3191300 0
END

End of simulation.

Reading input data for simulation 3.

SOLUTION 1 Sileri 2300p10
temp 300
pH 5.9
pe 4
redox pe
units ppm
density 1
Ca 405
Cl 6741
K 919
Mg 67
Na 3351
S(6) 288
Si 70
C(4) 366
water 1 # kg
pressure 223 atm
EQUILIBRIUM PHASES 1 Reservoir
Albite 0 22.54
Anhydrite 0 0
Ankerite 0 0
Anorthite 0 25.49
Aragonite 0 0
CO2(g) 2.348 1.2
Calcite 0 0
Dawsonite 0 0
Diopside 0 4.11
Dolomite 0 0
Enstatite 0 33.75
Fluorapatite 0 0.21
Gypsum 0 0

```

Ilmenite 0 1.74
K-Feldspar 0 13.11
Magnesite 0 0
Zircon 0 0.03
Quartz 0 42.16
Siderite 0 0
Actinolite 0 1.47
SELECTED_OUTPUT 1
file D:\20181 FALL\4. Dieng PHREEQC\equilibrium sileri.sel
reset false
solution true
ph true
pe true
temperature true
totals C(4)
gases CO2(g)
molalities K+ Na+ Ca+2 Mg+2
HCO3- SO4-2 Cl- CO3-2
saturation_indices Anhydrite Gypsum Aragonite Calcite
Dolomite Magnesite CO2(g)
USER_PUNCH
10 PUNCH description
PRINT
species false
END

```

Beginning of initial solution calculations.

Initial solution 1. Sileri 2300p10

WARNING: USER_PUNCH: Headings count does not match number of calls to PUNCH.

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

Elements	Molality	Moles
C(4)	6.074e-03	6.074e-03
Ca	1.023e-02	1.023e-02
Cl	1.925e-01	1.925e-01
K	2.380e-02	2.380e-02
Mg	2.791e-03	2.791e-03
Na	1.476e-01	1.476e-01
S(6)	3.036e-03	3.036e-03
Si	1.180e-03	1.180e-03

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

```

pH = 5.900
pe = 4.000
Density (g/cm³) = 0.74729
Volume (L) = 1.35457
Activity of water = 0.994
Ionic strength (mol/kgw) = 1.454e-01
Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = 7.750e-05
Total CO2 (mol/kg) = 6.074e-03
Temperature (°C) = 300.00
Pressure (atm) = 223.00
Electrical balance (eq) = -1.241e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.44
Iterations = 10
Total H = 1.110508e+02
Total O = 5.555211e+01

```

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

Phase	SI**	log IAP	log K(573 K, 223 atm)
Afwillite	-12.69	19.18	31.87 Ca3Si2O4(OH)6
Akermanite	-1.16	17.79	18.95 Ca2MgSi2O7
Anhydrite	1.53	-8.39	-9.92 CaSO4
Antarcticite	-9.60	-5.80	3.79 CaCl2·6H2O
Anthophyllite	5.22	25.21	19.99 Mg7Si8O22(OH)2
Antigorite	60.18	233.91	173.73 Mg48Si34O85(OH)62
Aphthitalite	-13.29	-17.18	-3.89 NaK3(SO4)2
Aragonite	-0.34	-2.38	-2.03 CaCO3
Arcanite	-5.48	-8.97	-3.49 K2SO4
Artinite	-4.70	3.17	7.86 Mg2CO3(OH)2·3H2O
Bassanite	0.82	-8.39	-9.21 CaSO4·0.5H2O
Bischofite	-11.29	-7.20	4.09 MgCl2·6H2O
Bloedite	-14.56	-17.24	-2.68 Na2Mg(SO4)2·4H2O
Brucite	-0.15	6.95	7.10 Mg(OH)2
Burkeite	-25.79	-16.31	9.49 Na6CO3(SO4)2
C	-33.46	-5.37	28.09 C
C(g)	-91.21	-5.37	85.84 C
Ca	-58.64	11.02	69.67 Ca
Ca(g)	-69.28	11.02	80.30 Ca
Ca2Cl2(OH)2·2H2O	-23.59	2.55	26.14 Ca2Cl2(OH)2·2H2O
Ca4Cl2(OH)6·13H2O	-48.16	19.21	67.38 Ca4Cl2(OH)6·13H2O
Calcite	-0.18	-2.38	-2.20 CaCO3
Carnallite	-14.36	-10.39	3.97 KMgCl3·6H2O
CaSO4·0.5H2O(beta)	0.87	-8.39	-9.26 CaSO4·0.5H2O
Chalcedony	-1.07	-2.93	-1.86 SiO2
Chloromagnesite	-11.99	-7.19	4.80 MgCl2
Chrysotile	3.37	14.99	11.62 Mg3Si2O5(OH)4
Cl2(g)	-13.14	-16.81	-3.67 Cl2
CO2(g)	-0.14	-2.21	-2.07 CO2
Coesite	-1.38	-2.93	-1.55 SiO2
Cristobalite(alpha)	-1.16	-2.93	-1.77 SiO2
Cristobalite(beta)	-1.31	-2.93	-1.62 SiO2
Dicalcium silicate	-3.83	13.77	17.59 Ca2SiO4
Diopside	1.53	9.44	7.91 CaMgSi2O6
Dolomite	-0.09	-6.15	-6.06 CaMg(CO3)2
Dolomite-dis	-0.60	-6.15	-5.55 CaMg(CO3)2
Dolomite-ord	-0.08	-6.15	-6.07 CaMg(CO3)2
Enstatite	0.45	4.02	3.57 MgSiO3
Epsomite	-7.49	-9.81	-2.31 MgSO4·7H2O

Forsterite	1.26	10.97	9.71	Mg2SiO4
Foshagite	-8.15	24.60	32.74	Ca4Si3O9(OH)2:0.5H2O
Gaylussite	-14.73	-3.81	10.91	CaNa2(CO3)2:5H2O
Glauberite	-10.36	-15.83	-5.47	Na2Ca(SO4)2
Gypsum	-0.03	-8.40	-8.37	CaSO4:2H2O
Gyrolite	-5.95	7.90	13.85	Ca2Si3O7(OH)2:1.5H2O
H2(g)	-16.26	-18.64	-2.39	H2
H2O(g)	1.85	-0.00	-1.85	H2O
Halite	-2.90	-2.42	0.48	NaCl
Hatrurite	-13.14	22.11	35.25	Ca3SiO5
HCl(g)	-5.92	-7.07	-1.15	HCl
Hexahydrite	-7.78	-9.80	-2.03	MgSO4:6H2O
Hillebrandite	-5.03	13.76	18.80	Ca2SiO3(OH)2:0.17H2O
Huntite	-2.79	-13.70	-10.90	CaMg3(CO3)4
Hydromagnesite	-8.14	-8.16	-0.02	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-6.82	-5.79	1.04	CaCl2
Ice	-1.35	-0.00	1.35	H2O
K	-32.48	5.22	37.70	K
K(g)	-35.94	5.22	41.16	K
K2CO3:1.5H2O	-16.27	-2.96	13.30	K2CO3:1.5H2O
K2O	-40.47	7.76	48.23	K2O
K3H(SO4)2	-18.21	-21.83	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-60.86	-33.30	27.56	K8H4(CO3)6:3H2O
Kainite	-12.52	-12.98	-0.46	KMgClSO4:3H2O
Kalinite	-7.13	-6.84	0.28	KHCO3
Kieserite	-9.47	-9.79	-0.32	MgSO4:H2O
KMgCl3	-16.89	-10.37	6.51	KMgCl3
KMgCl3:2H2O	-15.56	-10.38	5.19	KMgCl3:2H2O
KNaCO3:6H2O	-12.17	-2.21	9.96	KNaCO3:6H2O
Lansfordite	-8.38	-3.79	4.59	MgCO3:5H2O
Larnite	-4.31	13.77	18.07	Ca2SiO4
Leonite	-14.46	-18.77	-4.31	K2Mg(SO4)2:4H2O
Lime	-7.67	8.35	16.01	CaO
Magnesite	-0.68	-3.77	-3.09	MgCO3
Mercallite	-11.42	-12.86	-1.44	KHSO4
Merwinite	-3.83	26.13	29.96	MgCa3(SiO4)2
Mg	-49.41	9.63	59.03	Mg
Mg(g)	-57.14	9.63	66.76	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-1.44	-8.05	-6.61	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-1.20	-6.31	-5.11	Mg1.5SO4(OH)
MgCl2:2H2O	-9.01	-7.19	1.82	MgCl2:2H2O
MgCl2:4H2O	-8.09	-7.20	0.90	MgCl2:4H2O
MgCl2:H2O	-9.82	-7.19	2.64	MgCl2:H2O
MgOHCl	-4.31	-0.12	4.19	MgOHCl
MgSO4	-3.16	-9.79	-6.62	MgSO4
Mirabilite	-18.08	-7.47	10.62	Na2SO4:10H2O
Misenite	-75.04	-86.12	-11.08	K8H6(SO4)7
Monohydrocalcite	-3.15	-2.38	0.77	CaCO3:H2O
Monticellite	0.31	12.37	12.05	CaMgSiO4
Na	-29.41	5.99	35.40	Na
Na(g)	-34.20	5.99	40.19	Na
Na2CO3	-8.27	-1.43	6.85	Na2CO3
Na2CO3:7H2O	-18.69	-1.44	17.25	Na2CO3:7H2O
Na2O	-29.33	9.30	38.63	Na2O
Na2SiO3	-8.91	6.37	15.28	Na2SiO3
Na3H(SO4)2	-18.64	-19.53	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-17.28	-23.28	-5.99	Na4Ca(SO4)3:2H2O
Na4SiO4	-28.20	15.67	43.87	Na4SiO4
Na6Si2O7	-40.56	22.03	62.59	Na6Si2O7
Nahcolite	-6.16	-6.08	0.08	NaHCO3
Natron	-16.96	-1.45	15.51	Na2CO3:10H2O
Natrosillite	-9.54	3.44	12.97	Na2Si2O5
Nesquehonite	-7.09	-3.78	3.31	MgCO3:3H2O
O2(g)	-2.99	-5.35	-2.36	O2
Okenite	-6.64	2.48	9.12	CaSi2O4(OH)2:H2O
Oxychloride-Mg	-18.66	6.82	25.48	Mg2Cl(OH)3:4H2O
Pentahydrite	-8.16	-9.80	-1.64	MgSO4:5H2O
Periclase	-1.72	6.95	8.67	MgO
Picromerite	-14.04	-18.78	-4.74	K2Mg(SO4)2:6H2O
Pirssonite	-15.03	-3.81	11.22	Na2Ca(CO3)2:2H2O
Polyhalite	-21.14	-35.55	-14.41	K2MgCa2(SO4)4:2H2O
Portlandite	-3.31	8.34	11.65	Ca(OH)2
Pseudowollastonite	-0.87	5.42	6.29	CaSiO3
Quartz	-0.93	-2.93	-2.00	SiO2
Rankinite	-4.97	19.18	24.15	Ca3Si2O7
Sepiolite	-4.03	10.21	14.23	Mg4Si6O15(OH)2:6H2O
Si	-71.33	2.43	73.75	Si
Si(g)	-105.24	2.43	107.67	Si
SiO2(am)	-1.34	-2.93	-1.59	SiO2
Starkeyite	-8.60	-9.80	-1.20	MgSO4:4H2O
Sylvite	-3.81	-3.19	0.62	KCl
Syngenite	-9.72	-17.37	-7.65	K2Ca(SO4)2:H2O
Tachyhydrite	-36.73	-20.19	16.54	Mg2CaCl6:12H2O
Talc	3.44	9.13	5.69	Mg3Si4O10(OH)2
Thenardite	-3.93	-7.44	-3.51	Na2SO4
Thermonatrite	-9.64	-1.43	8.21	Na2CO3:H2O
Tobermorite-11A	-12.79	24.15	36.94	Ca5Si6H11O22.5
Tobermorite-14A	-18.09	24.14	42.23	Ca5Si6H21O27.5
Tobermorite-9A	-11.85	24.16	36.01	Ca5Si6H6O20
Tremolite	7.50	28.01	20.50	Ca2Mg5Si8O22(OH)2
Tridymite	-1.75	-2.93	-1.18	SiO2
Trona-K	-20.53	-9.04	11.49	K2NaH(CO3)2:2H2O
Wollastonite	-0.87	5.42	6.29	CaSiO3
Xonotlite	-19.76	32.51	52.27	Ca6Si6O17(OH)2

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

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Sileri 2300p10
Using pure phase assemblage 1. Reservoir

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

Phase	SI	log IAP	log K(T, P)	Moles in assemblage		
				Initial	Final	Delta
Actinolite	0.00	20.50	20.50	1.470e+00	1.470e+00	3.721e-04
Albite	0.00	-4.48	-4.48	2.254e+01	2.252e+01	-2.145e-02
Anhydrite	0.00	-9.92	-9.92	0.000e+00	2.698e-03	2.698e-03
Ankerite	-0.26	-7.18	-6.92	0.000e+00	0	0.000e+00
Anorthite	0.00	-2.68	-2.68	2.549e+01	2.550e+01	7.162e-03
Aragonite	-0.61	-2.64	-2.03	0.000e+00	0	0.000e+00
CO2(g)	1.60	-0.47	-2.07	1.200e+00	0	-1.200e+00
Calcite	-0.44	-2.64	-2.20	0.000e+00	0	0.000e+00
Dawsonite	-5.31	-7.47	-2.16	0.000e+00	0	0.000e+00
Diopside	0.00	7.91	7.91	4.110e+00	3.678e+00	-4.322e-01
Dolomite	0.00	-6.06	-6.06	0.000e+00	4.295e-01	4.295e-01
Enstatite	0.00	3.57	3.57	3.375e+01	3.375e+01	3.512e-03
Fluorapatite	0.00	-47.99	-47.99	2.100e-01	2.100e-01	-1.358e-08
Gypsum	-1.56	-9.93	-8.37	0.000e+00	0	0.000e+00
Ilmenite	0.00	0.95	0.95	1.740e+00	1.739e+00	-9.489e-04
K-Feldspar	0.00	-5.46	-5.46	1.311e+01	1.312e+01	7.092e-03
Magnesite	-0.32	-3.41	-3.09	0.000e+00	0	0.000e+00
Quartz	0.00	-2.00	-2.00	4.216e+01	4.304e+01	8.778e-01
Siderite	-0.27	-5.02	-4.74	0.000e+00	0	0.000e+00
Zircon	-0.00	-11.44	-11.44	3.000e-02	3.000e-02	-2.687e-11

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

Elements	Molality	Moles
Al	2.971e-05	2.970e-05
C	3.471e-01	3.471e-01
Ca	2.318e-03	2.318e-03
Cl	1.925e-01	1.925e-01
F	1.358e-08	1.358e-08
Fe	1.851e-05	1.851e-05
K	1.670e-02	1.670e-02
Mg	1.040e-03	1.040e-03
Na	1.690e-01	1.690e-01
P	4.073e-08	4.073e-08
S	3.380e-04	3.380e-04
Si	9.938e-03	9.938e-03
Ti	9.489e-04	9.489e-04
Zr	2.687e-11	2.687e-11

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

pH	=	5.229	Charge balance
pe	=	4.673	Adjusted to redox equilibrium
Density (g/cm ³)	=	0.73187	
Volume (L)	=	1.40388	
Activity of water	=	0.988	
Ionic strength (mol/kgw)	=	1.442e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	6.277e-04	
Total CO2 (mol/kg)	=	3.471e-01	
Temperature (°C)	=	300.00	
Pressure (atm)	=	223.00	
Electrical balance (eq)	=	-1.241e-03	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.43	
Iterations	=	15	
Total H	=	1.110501e+02	
Total O	=	5.624275e+01	

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

Phase	SI**	log IAP	log K(573 K, 223 atm)
Actinolite	0.00	20.50	20.50 Ca2Mg2.5Fe2.5Si8O22(OH)2
Afwillite	-16.86	15.00	31.87 Ca3Si2O4(OH)6
Akermanite	-4.70	14.25	18.95 Ca2MgSi2O7
Al	-65.70	1.51	67.21 Al
Al(g)	-89.12	1.51	90.62 Al
Al2(SO4)3	-28.19	-53.81	-25.62 Al2(SO4)3
Al2(SO4)3·6H2O	-26.35	-53.84	-27.48 Al2(SO4)3·6H2O
Albite	0.00	-4.48	-4.48 NaAlSi3O8
Albite_high	-0.40	-4.48	-4.09 NaAlSi3O8
Albite_low	-0.00	-4.48	-4.48 NaAlSi3O8
AlF3	-18.85	-44.96	-26.12 AlF3
Alum-K	-20.30	-32.04	-11.74 KAl(SO4)2·12H2O
Alunite	-7.17	-37.01	-29.84 KAl3(OH)6(SO4)2
Amesite-14A	4.74	8.22	3.48 Mg4Al4Si2O10(OH)8
Analcime	-0.45	-2.63	-2.18 Na.96Al.96Si2.04O6·H2O
Analcime-dehy	-3.16	-2.62	0.54 Na.96Al.96Si2.04O6
Anatase	5.45	-3.01	-8.46 TiO2
Andalusite	-0.42	-7.02	-6.60 Al2SiO5
Andradite	13.75	16.57	2.82 Ca3Fe2(SiO4)3
Anhydrite	0.00	-9.92	-9.92 CaSO4
Ankerite	-0.26	-7.18	-6.92 CaMg0.3Fe0.7(CO3)2
Annite	2.60	6.44	3.84 KFe3AlSi3O10(OH)2
Anorthite	0.00	-2.68	-2.68 CaAl2(SiO4)2
Antarcticcite	-10.26	-6.47	3.79 CaCl2·6H2O
Anthophyllite	2.98	22.97	19.99 Mg7Si8O22(OH)2
Antigorite	25.45	199.17	173.73 Mg48Si34O85(OH)62
Aphthitalite	-15.43	-19.31	-3.89 NaK3(SO4)2
Aragonite	-0.61	-2.64	-2.03 CaCO3
Arcanite	-6.65	-10.14	-3.49 K2SO4
Artinite	-5.72	2.14	7.86 Mg2CO3(OH)2·3H2O
Baddeleyite	-1.62	-9.43	-7.81 ZrO2
Bassanite	-0.71	-9.92	-9.21 CaSO4·0.5H2O
Beidellite-Ca	0.87	-12.16	-13.02 Ca.165Al2.33Si3.67O10(OH)2
Beidellite-H	0.04	-13.20	-13.24 H.33Al2.33Si3.67O10(OH)2
Beidellite-K	0.08	-12.19	-12.28 K.33Al2.33Si3.67O10(OH)2
Beidellite-Mg	1.00	-12.28	-13.28 Mg.165Al2.33Si3.67O10(OH)2
Beidellite-Na	0.37	-11.87	-12.25 Na.33Al2.33Si3.67O10(OH)2
Berlinite	-3.91	-24.36	-20.45 AlPO4
Bischofite	-11.33	-7.24	4.09 MgCl2·6H2O
Bloedite	-16.23	-18.91	-2.68 Na2Mg(SO4)2·4H2O
Boehmite	0.36	-2.51	-2.87 AlO2H

Brucite	-1.54	5.57	7.10	Mg(OH)2
Brushite	-21.97	-15.52	6.45	CaHPO4·2H2O
Burkeite	-26.79	-17.31	9.49	Na6CO3(SO4)2
C	-31.72	-3.63	28.09	C
C(g)	-89.47	-3.63	85.84	C
Ca	-60.65	9.02	69.67	Ca
Ca(g)	-71.28	9.02	80.30	Ca
Ca-Al Pyroxene	-3.22	-0.68	2.54	CaAl2SiO6
Ca2Al2O5·8H2O	-51.30	7.62	58.92	Ca2Al2O5·8H2O
Ca2Cl2(OH)2·H2O	-26.24	-0.10	26.14	Ca2Cl2(OH)2·H2O
Ca3Al2O6	-28.78	14.01	42.78	Ca3Al2O6
Ca4Al2Fe2O10	-20.05	23.90	43.95	Ca4Al2Fe2O10
Ca4Al2O7·13H2O	-85.97	20.28	106.25	Ca4Al2O7·13H2O
Ca4Al2O7·19H2O	-82.13	20.25	102.38	Ca4Al2O7·19H2O
Ca4Cl2(OH)6·13H2O	-54.87	12.51	67.38	Ca4Cl2(OH)6·13H2O
CaAl2O4	-6.49	1.32	7.81	CaAl2O4
CaAl2O4·10H2O	-36.02	1.27	37.29	CaAl2O4·10H2O
CaAl4O7	-10.39	-3.70	6.69	CaAl4O7
Calcite	-0.44	-2.64	-2.20	CaCO3
Carnallite	-14.54	-10.57	3.97	KMgCl3·6H2O
CaSO4·0.5H2O(beta)	-0.66	-9.92	-9.26	CaSO4·0.5H2O
CaZrO3	77.98	-3.09	-81.07	CaZrO3
Celadonite	0.20	-1.90	-2.10	KMgAlSi4O10(OH)2
CH4(g)	-61.66	-64.15	-2.49	CH4
Chalcedony	-0.14	-2.00	-1.86	SiO2
Chamosite-7A	1.56	0.90	-0.66	Fe2Al2SiO5(OH)4
Chloromagnesite	-12.01	-7.21	4.80	MgCl2
Chrysotile	1.08	12.70	11.62	Mg3Si2O5(OH)4
Cl2(g)	-11.78	-15.46	-3.67	Cl2
Clinochlore-14A	4.78	16.81	12.03	Mg5Al2Si3O10(OH)8
Clinochlore-7A	2.42	16.81	14.39	Mg5Al2Si3O10(OH)8
Clinoptilolite-Ca	2.14	-26.80	-28.94	Ca1.7335Al3.45Fe.017Si14.533036:10.922H2O
Clinoptilolite-dehy-Ca	-12.33	-26.74	-14.42	Ca1.7335Al3.45Fe.017Si14.533036
Clinoptilolite-dehy-K	-20.91	-27.13	-6.22	K3.467Al3.45Fe.017Si14.533036
Clinoptilolite-dehy-Na	-17.32	-23.75	-6.43	Na3.467Al3.45Fe.017Si14.533036
Clinoptilolite-hy-Ca	1.34	-26.80	-28.15	Ca1.7335Al3.45Fe.017Si14.533036:11.645H2O
Clinoptilolite-hy-K	-3.55	-27.17	-23.62	K3.467Al3.45Fe.017Si14.533036:7.499H2O
Clinoptilolite-hy-Na	-2.95	-23.81	-20.86	Na3.467Al3.45Fe.017Si14.533036:10.877H2O
Clinoptilolite-K	-6.80	-27.19	-20.39	K3.467Al3.45Fe.017Si14.533036:10.922H2O
Clinoptilolite-Na	-2.99	-23.81	-20.82	Na3.467Al3.45Fe.017Si14.533036:10.922H2O
Clinzoisite	0.03	-0.86	-0.89	Ca2Al3Si3O12(OH)
CO(g)	-18.45	-20.62	-2.17	CO
CO2(g)	1.60	-0.47	-2.07	CO2
Coesite	-0.45	-2.00	-1.55	SiO2
Cordierite_anhyd	-0.69	-8.91	-8.22	Mg2Al4Si5O18
Cordierite_hydr	0.13	-8.92	-9.05	Mg2Al4Si5O18·H2O
Corundum	4.74	-5.02	-9.76	Al2O3
Cristobalite(alpha)	-0.23	-2.00	-1.77	SiO2
Cristobalite(beta)	-0.38	-2.00	-1.62	SiO2
Cronstedtite-7A	17.01	9.47	-7.54	Fe2Fe2SiO5(OH)4
Daphnite-14A	4.99	8.79	3.80	Fe5AlAlSi3O10(OH)8
Daphnite-7A	2.74	8.79	6.05	Fe5AlAlSi3O10(OH)8
Dawsonite	-5.31	-7.47	-2.16	NaAlCO3(OH)2
Diaspore	0.47	-2.51	-2.98	AlHO2
Dicalcium_silicate	-6.91	10.68	17.59	Ca2SiO4
Diopside	0.00	7.91	7.91	CaMgSi2O6
Dolomite	0.00	-6.06	-6.06	CaMg(CO3)2
Dolomite-dis	-0.51	-6.06	-5.55	CaMg(CO3)2
Dolomite-ord	0.01	-6.06	-6.07	CaMg(CO3)2
Enstatite	0.00	3.57	3.57	MgSiO3
Epidote	8.72	3.43	-5.29	Ca2FeAl2Si3O12OH
Epidote-ord	8.68	3.43	-5.26	FeCa2Al2(OH)(SiO4)3
Epsomite	-8.41	-10.73	-2.31	MgSO4·7H2O
Etringite	-58.25	-15.92	42.33	Ca6Al2(SO4)3(OH)12·26H2O
F2(g)	-51.98	-30.98	21.00	F2
Fayalite	0.88	5.93	5.05	Fe2SiO4
Fe	-20.14	6.64	26.78	Fe
Fe(OH)2	-1.83	3.96	5.79	Fe(OH)2
Fe(OH)3	3.79	1.77	-2.03	Fe(OH)3
Fe2(SO4)3	-13.46	-45.24	-31.78	Fe2(SO4)3
FeF2	-14.05	-24.34	-10.29	FeF2
FeF3	-15.83	-40.68	-24.85	FeF3
FeO	-0.37	3.97	4.33	FeO
Ferrite-Ca	13.00	9.89	-3.10	CaFe2O4
Ferrite-Dicalcium	2.04	16.23	14.20	Ca2Fe2O5
Ferrite-Mg	13.99	9.12	-4.87	MgFe2O4
Ferrosilite	0.41	1.96	1.55	FeSiO3
FeSO4	-4.84	-12.30	-7.45	FeSO4
Fluorapatite	0.00	-47.99	-47.99	Ca5(PO4)3F
Fluorite	-9.31	-21.96	-12.65	CaF2
Forsterite	-0.57	9.14	9.71	Mg2SiO4
Foshagite	-13.39	19.35	32.74	Ca4Si3O9(OH)2·0.5H2O
Gaylussite	-14.50	-3.58	10.91	CaNa2(CO3)2·5H2O
Gehlenite	-6.18	5.66	11.84	Ca2Al2SiO7
Gibbsite	0.10	-2.52	-2.62	Al(OH)3
Gismondine	-46.28	-5.41	40.87	Ca2Al4Si4O16·9H2O
Glauberite	-12.65	-18.12	-5.47	Na2Ca(SO4)2
Goethite	6.50	1.77	-4.72	FeOOH
Greenalite	1.03	7.89	6.86	Fe3Si2O5(OH)4
Grossular	-2.55	8.00	10.55	Ca3Al2(SiO4)3
Gypsum	-1.56	-9.93	-8.37	CaSO4·2H2O
Gyrolite	-7.19	6.66	13.85	Ca2Si3O7(OH)2·1.5H2O
H2(g)	-16.26	-18.65	-2.39	H2
H2O(g)	1.85	-0.01	-1.85	H2O
H2S(g)	-56.61	-65.61	-8.99	H2S
Halite	-2.84	-2.36	0.48	NaCl
Hatrurite	-18.23	17.02	35.25	Ca3SiO5
HCl(g)	-5.24	-6.39	-1.15	HCl
Hedenbergite	-0.78	6.30	7.08	CaFe(SiO3)2
Hematite	16.44	3.55	-12.89	Fe2O3
Hercynite	1.28	-1.05	-2.34	FeAl2O4
Hexahydrate	-8.69	-10.72	-2.03	MgSO4·6H2O
Hillebrandite	-8.12	10.67	18.80	Ca2SiO3(OH)2·0.17H2O
Huntite	-1.98	-12.88	-10.90	CaMg3(CO3)4
Hydromagnesite	-8.09	-8.10	-0.02	Mg5(CO3)4(OH)2·4H2O
Hydrophilite	-7.47	-6.44	1.04	CaCl2
Hydroxylapatite	-1.00	-33.84	-32.84	Ca5(OH)(PO4)3
Ice	-1.35	-0.01	1.35	H2O

Illite	0.71	-9.56	-10.27	K0.6Mg0.25Al1.8Al0.5Si3.5O10(OH)2
Ilmenite	0.00	0.95	0.95	FeTiO3
Jadeite	-1.64	-2.48	-0.84	NaAl(SiO3)2
Jarosite	5.69	-24.15	-29.84	KFe3(SO4)2(OH)6
Jarosite-Na	-17.43	-23.18	-5.75	NaFe3(SO4)2(OH)6
K	-33.30	4.40	37.70	K
K(g)	-36.76	4.40	41.16	K
K-Feldspar	0.00	-5.46	-5.46	KAlSi3O8
K2CO3:1.5H2O	-16.18	-2.87	13.30	K2CO3:1.5H2O
K2O	-42.11	6.12	48.23	K2O
K3H(SO4)2	-19.73	-23.35	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-57.02	-29.46	27.56	K8H4(CO3)6:3H2O
Kainite	-13.58	-14.04	-0.46	KMgClSO4:3H2O
KAl(SO4)2	-14.91	-31.98	-17.06	KAl(SO4)2
Kalclinitite	-6.21	-5.93	0.28	KHCO3
Kalsilite	-1.57	-1.45	0.12	KAlSiO4
Kaolinite	-0.03	-9.04	-9.00	Al2Si2O5(OH)4
Katoite	-64.37	13.97	78.34	Ca3Al2H12O12
Kieserite	-10.38	-10.70	-0.32	MgSO4:H2O
KMgCl3	-17.05	-10.54	6.51	KMgCl3
KMgCl3:2H2O	-15.73	-10.55	5.19	KMgCl3:2H2O
KNaCO3:6H2O	-11.88	-1.92	9.96	KNaCO3:6H2O
Kyanite	-0.51	-7.02	-6.51	Al2SiO5
Lansfordite	-8.03	-3.44	4.59	MgCO3:5H2O
Larnite	-7.39	10.68	18.07	Ca2SiO4
Laumontite	-0.36	-6.71	-6.35	CaAl2Si4O12:4H2O
Lawrencite	-6.88	-8.81	-1.93	FeCl2
Lawsonite	-1.00	-2.69	-1.70	CaAl2Si2O7(OH)2:H2O
Leonite	-16.54	-20.86	-4.31	K2Mg(SO4)2:4H2O
Lime	-9.67	6.34	16.01	CaO
Magnesite	-0.32	-3.41	-3.09	MgCO3
Magnetite	17.66	7.52	-10.14	Fe3O4
Margarite	0.60	-7.71	-8.31	CaAl4Si2O10(OH)2
Maximum Microcline	0.00	-5.46	-5.46	KAlSi3O8
Mayenite	-108.84	40.96	149.80	Ca12Al14O33
Melanterite	-8.81	-12.33	-3.52	FeSO4:7H2O
Mercallite	-11.77	-13.21	-1.44	KHSO4
Merwinite	-9.37	20.59	29.96	MgCa3(SiO4)2
Mesolite	0.51	-4.14	-4.65	Na.676Ca.657Al1.99Si3.01O10:2.647H2O
Mg	-50.78	8.25	59.03	Mg
Mg(g)	-58.52	8.25	66.76	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-2.69	-9.30	-6.61	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-2.80	-7.91	-5.11	Mg1.5SO4(OH)
MgCl2:2H2O	-9.03	-7.22	1.82	MgCl2:2H2O
MgCl2:4H2O	-8.12	-7.23	0.90	MgCl2:4H2O
MgCl2:H2O	-9.85	-7.21	2.64	MgCl2:H2O
MgOHC1	-5.01	-0.82	4.19	MgOHC1
MgSO4	-4.07	-10.69	-6.62	MgSO4
Minnesotaitite	2.44	3.89	1.45	Fe3Si4O10(OH)2
Mirabilite	-18.86	-8.25	10.62	Na2SO4:10H2O
Misenerite	-78.31	-89.38	-11.08	K8H6(SO4)7
Molybite	-11.50	-17.39	-5.89	FeCl3
Monohydrocalcite	-3.41	-2.65	0.77	CaCO3:H2O
Monticellite	-2.14	9.91	12.05	CaMgSiO4
Montmor-Ca	1.27	-9.32	-10.60	Ca.165Mg.33Al1.67Si4O10(OH)2
Montmor-K	0.65	-9.36	-10.01	K.33Mg.33Al1.67Si4O10(OH)2
Montmor-Mg	1.42	-9.45	-10.88	Mg.495Al1.67Si4O10(OH)2
Montmor-Na	0.82	-9.04	-9.86	Na.33Mg.33Al1.67Si4O10(OH)2
Mordenite	-1.06	-9.22	-8.16	Ca.2895Na.361Al.94Si5.06O12:3.468H2O
Mordenite-dehy	-6.89	-9.20	-2.31	Ca.2895Na.361Al.94Si5.06O12
Muscovite	1.30	-10.49	-11.78	KAl3Si3O10(OH)2
Na	-30.03	5.37	35.40	Na
Na(g)	-34.81	5.37	40.18	Na
Na2CO3	-7.76	-0.92	6.85	Na2CO3
Na2CO3:7H2O	-18.20	-0.95	17.25	Na2CO3:7H2O
Na2O	-30.56	8.07	38.63	Na2O
Na2SiO3	-9.22	6.06	15.28	Na2SiO3
Na3H(SO4)2	-19.54	-20.43	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-20.33	-26.32	-5.99	Na4Ca(SO4)3:2H2O
Na4SiO4	-29.73	14.13	43.87	Na4SiO4
Na6Si2O7	-42.39	20.20	62.59	Na6Si2O7
NaFeO2	-0.74	5.81	6.55	NaFeO2
Nahcolite	-5.03	-4.95	0.08	NaHCO3
Natrolite	-2.72	-2.97	-0.25	Na2Al2Si3O10:2H2O
Natron	-16.48	-0.97	15.51	Na2CO3:10H2O
Natrosilite	-8.91	4.06	12.97	Na2Si2O5
Nepheline	-1.52	-0.48	1.04	NaAlSiO4
Nesquehonite	-6.74	-3.43	3.31	MgCO3:3H2O
Nontronite-Ca	16.27	-3.59	-19.86	Ca.165Fe2Al.33Si3.67H2O12
Nontronite-H	15.55	-4.63	-20.18	H.33Fe2Al.33Si3.67H2O12
Nontronite-K	15.49	-3.62	-19.12	K.33Fe2Al.33Si3.67H2O12
Nontronite-Mg	16.40	-3.71	-20.11	Mg.165Fe2Al.33Si3.67H2O12
Nontronite-Na	15.78	-3.30	-19.08	Na.33Fe2Al.33Si3.67H2O12
O2(g)	-2.99	-5.35	-2.36	O2
Okenite	-6.79	2.33	9.12	CaSi2O4(OH)2:H2O
Oxychloride-Mg	-20.76	4.73	25.48	Mg2Cl(OH)3:4H2O
P	-69.93	-15.15	54.78	P
Paragonite	0.69	-9.51	-10.20	NaAl3Si3O10(OH)2
Parasite	-0.96	19.45	20.41	NaCa2Al3Mg4Si6O22(OH)2
Pentahydrate	-9.08	-10.72	-1.64	MgSO4:5H2O
Periclase	-3.10	5.57	8.67	MgO
Phlogopite	2.96	11.25	8.29	KAlMg3Si3O10(OH)2
Picromerite	-16.13	-20.87	-4.74	K2Mg(SO4)2:6H2O
Pirssonite	-14.79	-3.57	11.22	Na2Ca(CO3)2:2H2O
Polyhalite	-26.28	-40.69	-14.41	K2MgCa2(SO4)4:2H2O
Portlandite	-5.31	6.34	11.65	Ca(OH)2
Prehnite	-0.46	1.65	2.11	Ca2Al2Si3O10(OH)2
Pseudowollastonite	-1.95	4.34	6.29	CaSiO3
Pyrite	-95.25	-114.90	-19.65	FeS2
Pyrophyllite	-0.06	-13.04	-12.98	Al2Si4O10(OH)2
Pyrrhotite	-55.07	-61.63	-6.56	FeS
Quartz	0.00	-2.00	-2.00	SiO2
Rankinite	-1.13	15.02	24.15	Ca3Si2O7
Ripidolite-14A	5.01	13.60	8.59	Mg3Fe2Al2Si3O10(OH)8
Ripidolite-7A	2.68	13.60	10.92	Mg3Fe2Al2Si3O10(OH)8
Rutile	6.53	-3.01	-9.55	TiO2
S	-44.36	-68.28	-23.92	S
S2(g)	-91.91	-106.53	-14.62	S2

Sanidine-high	-0.26	-5.46	-5.20	KAlSi3O8
Saponite-Ca	3.86	9.58	5.72	Ca _{1.165} Mg ₃ Al _{1.33} Si _{3.67} O ₁₀ (OH) ₂
Saponite-H	3.03	8.53	5.50	H _{0.33} Mg ₃ Al _{1.33} Si _{3.67} O ₁₀ (OH) ₂
Saponite-K	3.07	9.54	6.47	K _{0.33} Mg ₃ Al _{1.33} Si _{3.67} O ₁₀ (OH) ₂
Saponite-Mg	3.97	9.45	5.48	Mg _{3.165} Al _{1.33} Si _{3.67} O ₁₀ (OH) ₂
Saponite-Na	3.37	9.86	6.49	Na _{0.33} Mg ₃ Al _{1.33} Si _{3.67} O ₁₀ (OH) ₂
Scolecite	0.74	-4.70	-5.44	CaAl ₂ Si ₃ O ₁₀ :3H ₂ O
Sellaite	-8.87	-22.73	-13.86	MgF ₂
Sepiolite	-4.00	10.23	14.23	Mg ₄ Si ₆ O ₁₅ (OH) ₂ :6H ₂ O
Si	-70.40	3.35	73.75	Si
Si(g)	-104.31	3.35	107.67	Si
Siderite	-0.27	-5.02	-4.74	FeCO ₃
SiF ₄ (g)	-35.23	-58.61	-23.38	SiF ₄
Sillimanite	-0.53	-7.02	-6.50	Al ₂ SiO ₅
SiO ₂ (am)	-0.41	-2.00	-1.59	SiO ₂
Smectite-high-Fe-Mg	3.22	-0.23	-3.45	Ca _{0.025} Na ₁ K _{0.2} Fe _{0.5} Fe _{0.2} Mg _{1.15} Al _{1.25} Si _{3.5} H ₂ O ₁₂
Smectite-low-Fe-Mg	2.40	-2.86	-5.26	Ca _{0.02} Na _{0.15} K _{0.2} Fe _{0.29} Fe _{0.16} Mg _{0.9} Al _{1.25} Si _{3.75} H ₂ O ₁₂
SO ₂ (g)	-19.78	-20.74	-0.96	SO ₂
Spinel	-1.59	0.55	2.14	Al ₂ MgO ₄
Starkeyite	-9.51	-10.71	-1.20	MgSO ₄ :4H ₂ O
Stilbite	0.38	-12.14	-12.52	Ca _{1.019} Na _{0.136} K _{0.06} Al _{2.18} Si _{6.82} O ₁₈ :7.33H ₂ O
Strengite	-1.15	-20.08	-18.93	FePO ₄ :2H ₂ O
Sylvite	-3.95	-3.33	0.62	KCl
Syngenite	-12.42	-20.07	-7.65	K ₂ Ca(SO ₄) ₂ :2H ₂ O
Tachyhydrite	-37.45	-20.91	16.54	Mg ₂ CaCl ₆ :12H ₂ O
Talc	3.01	8.70	5.69	Mg ₃ Si ₄ O ₁₀ (OH) ₂
Thenardite	-4.69	-8.19	-3.51	Na ₂ SO ₄
Thermonatrite	-9.13	-0.92	8.21	Na ₂ CO ₃ :H ₂ O
Ti	-147.06	2.34	149.40	Ti
Ti(g)	-222.11	2.34	224.45	Ti
Ti ₂ O ₃	-46.53	-3.35	43.19	Ti ₂ O ₃
Ti ₃ O ₅	-41.32	-6.36	34.96	Ti ₃ O ₅
TiC	-183.25	-1.29	181.96	TiC
TiCl ₂	-84.20	-13.11	71.09	TiCl ₂
TiCl ₃	-60.33	-20.84	39.48	TiCl ₃
TiCl ₄ (g)	-56.82	-28.57	28.25	TiCl ₄
TiF ₄ (am)	-47.38	-59.62	-12.24	TiF ₄
TiO(alpha)	-61.56	-0.34	61.23	TiO
TiO(g)	-146.01	-0.34	145.67	TiO
Titanite	-718.31	1.33	719.63	CaTiSiO ₅
Tobermorite-11A	-17.28	19.66	36.94	Ca ₅ Si ₆ H ₁₁ O _{22.5}
Tobermorite-14A	-22.59	19.64	42.23	Ca ₅ Si ₆ H ₂₁ O _{27.5}
Tobermorite-9A	-16.33	19.68	36.01	Ca ₅ Si ₆ H ₆ O ₂₀
Tremolite	4.01	24.51	20.50	Ca ₂ Mg ₅ Si ₈ O ₂₂ (OH) ₂
Tridymite	-0.82	-2.00	-1.18	SiO ₂
Troilite	-55.00	-61.63	-6.64	FeS
Trona-K	-19.32	-7.83	11.49	K ₂ NaH(CO ₃) ₂ :2H ₂ O
Vivianite	-26.71	-31.83	-5.12	Fe ₃ (PO ₄) ₂ :8H ₂ O
Wairakite	0.13	-6.70	-6.83	CaAl ₂ Si ₄ O ₁₀ (OH) ₄
Whitlockite	-1.65	-24.67	-23.02	Ca ₃ (PO ₄) ₂
Wollastonite	-1.95	4.34	6.29	CaSiO ₃
Wustite	0.09	3.52	3.44	Fe _{0.947} O
Xonotlite	-26.24	26.03	52.27	Ca ₆ Si ₆ O ₁₇ (OH) ₂
Zircon	-0.00	-11.44	-11.44	ZrSiO ₄
Zoisite	0.03	-0.86	-0.88	Ca ₂ Al ₃ (SiO ₄) ₃ OH
Zr	-88.86	-4.08	84.78	Zr
Zr(g)	-280.97	-3.94	277.03	Zr
ZrC	-214.61	-7.57	207.04	ZrC
ZrCl	-142.54	-11.67	130.87	ZrCl
ZrCl ₂	-115.66	-19.39	96.27	ZrCl ₂
ZrCl ₃	-89.55	-27.12	62.42	ZrCl ₃
ZrCl ₄	-62.83	-34.85	27.98	ZrCl ₄
ZrF ₄ (beta)	-38.14	-65.90	-27.76	ZrF ₄
ZrF ₄ (g)	-208.85	-65.90	142.95	ZrF ₄
ZrH ₂	-199.44	-1.27	198.17	ZrH ₂

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

End of simulation.

APPENDIX F

KINETIC MODELING RESULT IN DIENG FIELD FOR 1 HOUR AND 5 HOURS TIME STEP

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\llnl.dat

Reading data base.

```

LLNL AQUEOUS_MODEL_PARAMETERS
NAMED_EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

```

Reading input data for simulation 1.

```

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\llnl.dat
SOLUTION_SPECIES
CO3-2 + 2 H+ = CO2 + H2O
log_k 16.681
delta_h -5.738 kcal
analytical_expression 464.1965 0.09344813 -26986.16 -165.75951 2248628.9
dw 1.92e-9
vm 7.29 0.92 2.07 -1.23 -1.60 # ref. 1 + McBride et al. 2015, JCED 60, 171
2CO2 = (CO2)2 # activity correction for CO2 solubility at high P, T
log_k -1.8
analytical_expression 8.68 -0.0103 -2190
vm 14.58 1.84 4.14 -2.46 -3.20
END

```

End of simulation.

Reading input data for simulation 2.

```

PHASES
CO2(g)
CO2 = CO2
log_k -1.468
delta_h -4.776 kcal
analytical_expression 10.5624 -2.3547e-2 -3972.8 0 5.8746e5 1.9194e-5
t_c 304.2 # critical T, K
p_c 72.86 # critical P, atm
omega 0.225 # acentric factor
Ankerite
CaMg0.3Fe0.7(CO3)2 + 2H+ = Ca+2 + 0.7Fe+2 + 2HCO3- + 0.3Mg+2
log_k 1.54
analytical_expression -1864.9 -0.29583 104680 675.54 -6051400 0
Actinolite
Ca2Mg2.5Fe2.5Si8O22(OH)2 + 14H+ = 2Ca+2 + 2.5Fe+2 + 8H2O + 2.5Mg+2 + 8SiO2
log_k 61.2367
delta_h -406.404 kJ
analytical_expression 85.291 0.046337 39465 -54.414 -3191300 0
END

```

End of simulation.

Reading input data for simulation 3.

```

SOLUTION 1 Sileri 2300p10
temp 300
pH 5.9
pe 4
redox pe
units ppm
density 1
C(4) 366
Ca 405
Cl 6741
K 919
Mg 67
Na 3351
S(6) 288
Si 70
water 1 # kg
pressure 223 atm
EQUILIBRIUM_PHASES 1 Reservoir
CO2(g) 2.348 1.2
RATES
Quartz
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_qtz = SI("Quartz")

```

```

30 if (M <= 0 and si_qtz < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_qtz > 0) then SA = 1e-05 #nucleation
60 k_acid = 0
70 k_neut = 10^(-13.40)*EXP(-90.90e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_qtz))
190 moles = r * TIME
200 SAVE moles
end
Anorthite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_anort = SI("Anorthite")
30 if (M <= 0 and si_anort < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_anort > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-3.5)*EXP(-16.60e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.411)
70 k_neut = 10^(-9.82)*EXP(-31.50e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_anort))
190 moles = r * TIME
200 SAVE moles
end
Albite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_alb = SI("Albite")
30 if (M <= 0 and si_alb < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_alb > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-10.16)*EXP(-65.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.457)
70 k_neut = 10^(-12.56)*EXP(-69.80e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-15.60)*EXP(-71.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.572)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_alb))
190 moles = r * TIME
200 SAVE moles
end
K-Feldspar
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_kfeld = SI("K-Feldspar")
30 if (M <= 0 and si_kfeld < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_kfeld > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-10.06)*EXP(-51.70e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.500)
70 k_neut = 10^(-12.41)*EXP(-38.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-21.20)*EXP(-94.10e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.823)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_kfeld))
190 moles = r * TIME
200 SAVE moles
end
Diopside
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_diopsi = SI("Diopside")
30 if (M <= 0 and si_diopsi < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_diopsi > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-6.36)*EXP(-96.10e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.710)
70 k_neut = 10^(-11.11)*EXP(-40.60e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_diopsi))
190 moles = r * TIME
200 SAVE moles
end
Enstatite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_enst = SI("Enstatite")
30 if (M <= 0 and si_enst < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_enst > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-9.02)*EXP(-80.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.600)
70 k_neut = 10^(-12.72)*EXP(-80.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_enst))
190 moles = r * TIME
200 SAVE moles
end
Ilmenite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_ilmen = SI("Ilmenite")
30 if (M <= 0 and si_ilmen < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_ilmen > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-8.35)*EXP(-37.90e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.421)
70 k_neut = 10^(-11.16)*EXP(-37.90e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_ilmen))
190 moles = r * TIME
200 SAVE moles
end
Magnetite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_magnet = SI("Magnetite")
30 if (M <= 0 and si_magnet < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_magnet > 0) then SA = 1e-05 #nucleation

```

```

60 k_acid = 10^(-8.59)*EXP(-18.60e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.279)
70 k_neut = 10^(-10.78)*EXP(-18.60e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_magnet))
190 moles = r * TIME
200 SAVE moles
end
Actinolite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_actino = SI("Actinolite")
30 if (M <= 0 and si_actino < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_actino > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-11.15)*EXP(-22.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.000)
70 k_neut = 10^(-12.28)*EXP(-22.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-11.78)*EXP(-22.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(~1.000)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_actino))
190 moles = r * TIME
200 SAVE moles
end
Calcite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_calc = SI("Calcite")
30 if (M <= 0 and si_calc < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_calc > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-0.30)*EXP(-14.40e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.000)
70 k_neut = 10^(-5.81)*EXP(-23.50e+03/8.314*(1.0/TK-1.0/298.15))
80 k_carb = 10^(-3.48)*EXP(-35.40e+03/8.314*(1.0/TK-1.0/298.15))*PR_P("CO2(g)")^(1.000)
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_calc))
190 moles = r * TIME
200 SAVE moles
end
Illite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_ill = SI("Illite")
30 if (M <= 0 and si_ill < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_ill > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-10.12)*EXP(-58.00e+03/8.314*(1.0/TK-1.0/373.15))*ACT("H+")^(0.550)
70 k_neut = 10^(-12.26)*EXP(-54.00e+03/8.314*(1.0/TK-1.0/373.15))
80 k_base = 10^(-10.60)*EXP(-77.00e+03/8.314*(1.0/TK-1.0/373.15))*ACT("OH-")^(~0.350)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_ill))
190 moles = r * TIME
200 SAVE moles
end
Dolomite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_dolo = SI("Dolomite")
30 if (M <= 0 and si_dolo < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_dolo > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-3.76)*EXP(-56.70e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.500)
70 k_neut = 10^(-8.60)*EXP(-95.30e+03/8.314*(1.0/TK-1.0/298.15))
80 k_carb = 10^(-5.37)*EXP(-45.70e+03/8.314*(1.0/TK-1.0/298.15))*PR_P("CO2(g)")^(0.500)
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_dolo))
190 moles = r * TIME
200 SAVE moles
end
Magnesite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_magnes = SI("Magnesite")
30 if (M <= 0 and si_magnes < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_magnes > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-6.38)*EXP(-14.40e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.000)
70 k_neut = 10^(-9.34)*EXP(-23.50e+03/8.314*(1.0/TK-1.0/298.15))
80 k_carb = 10^(-5.22)*EXP(-62.80e+03/8.314*(1.0/TK-1.0/298.15))*PR_P("CO2(g)")^(1.000)
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_magnes))
190 moles = r * TIME
200 SAVE moles
end
Anhydrite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_anhyd = SI("Anhydrite")
30 if (M <= 0 and si_anhyd < 0) then goto 200
40 SA = PARM(1)*M
50 if (M = 0 and si_anhyd > 0) then SA = 1e-05 #nucleation
60 k_acid = 0
70 k_neut = 10^(-2.79)*EXP(-0.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_anhyd))
190 moles = r * TIME
200 SAVE moles
end
KINETICS 1
Quartz
formula SiO2 1
m 42.16
m0 42.16
parms 0.944 #2.944
tol 1e-09
Anorthite
formula CaAl2(SiO4)2 1
m 25.49

```

```

m0      25.49
parms   5.548
tol      1e-09
Albite
  formula NaAlSi3O8 1
  m        22.54
  m0       22.54
  parms    5.26
  tol      1e-09
K-Feldspar
  formula KAlSi3O8 1
  m        13.11
  m0       13.11
  parms    86.282
  tol      1e-09
Diopside
  formula CaMgSi2O6 1
  m         4.11
  m0        4.11
  parms    3.974
  tol      1e-09
Enstatite
  formula MgSiO3 1
  m         33.75
  m0        33.75
  parms   933.627
  tol      1e-09
Ilmenite
  formula FeTiO3 1
  m         1.74
  m0        1.74
  parms   31.101
  tol      1e-09
Actinolite
  formula Ca2Mg2.5Fe2.5Si8O22(OH)2 1
  m         1.47
  m0        1.47
  parms   392.45
  tol      1e-09
Calcite
  formula CaCO3 1
  m         0
  m0        0
  parms   15.014
  tol      1e-09
Dolomite
  formula CaMg(CO3)2 1
  m         0
  m0        0
  parms   17.149
  tol      1e-09
Magnesite
  formula MgCO3 1
  m         0
  m0        0
  parms    1.096
  tol      1e-09
steps    36000 in 10 steps # seconds
step divide 1
runge kutta 3
bad_step_max 500
cvsolve true
cvsolve_steps 100
cvsolve_order 5
KNOBS
convergence_tolerance 1e-10
INCREMENTAL_REACTIONS True
USER_GRAPH 1
  -headings
    Time Quartz Anorthite Albite K-Feldspar Diopside Enstatite Magnetite Actinolite Dolomite
  -axis_titles
    "Log10 Time" "kin" ""
  -initial_solutions
    false
  -connect_simulations
    true
  -plot_concentration_vs
    x
  -start
    10 GRAPH X log10(total_time)
    20 GRAPH Y kin("Quartz"), kin("Anorthite"), kin("Albite"), kin("K-Feldspar"), kin("Diopside"), kin("Enstatite"),
    kin("Magnetite"), kin("Actinolite"), kin("Dolomite")
  -end
  -active
    true
SELECTED_OUTPUT 1
  file
    D:\20182 SPRING\Thesis PHREEQC\3. Dieng\kin dieng_10hours.sel
  reset
    false
  time
    true
  step
    true
  ph
    true
  pe
    true
  totals
    C(4)
  molalities
    K+ Na+ Ca+2 Mg+2
    HCO3- SO4-2 Cl- CO3-2
  kinetic_reactants
    Quartz Anorthite Albite K-Feldspar
    Diopside Enstatite Magnetite Actinolite
    Dolomite
END
-----
Beginning of initial solution calculations.
-----
Initial solution 1.      Sileri 2300p10
-----Solution composition-----
Elements      Molality      Moles
C(4)          6.074e-03    6.074e-03
Ca            1.023e-02    1.023e-02
Cl            1.925e-01    1.925e-01
K             2.380e-02    2.380e-02
Mg            2.791e-03    2.791e-03

```

Na	1.476e-01	1.476e-01				
S(6)	3.036e-03	3.036e-03				
Si	1.180e-03	1.180e-03				
-----Description of solution-----						
	pH	=	5.900			
	pe	=	4.000			
	Density (g/cm ³)	=	0.74729			
	Volume (L)	=	1.35457			
	Activity of water	=	0.994			
	Ionic strength (mol/kgw)	=	1.454e-01			
	Mass of water (kg)	=	1.000e+00			
	Total alkalinity (eq/kg)	=	7.750e-05			
	Total CO2 (mol/kg)	=	6.074e-03			
	Temperature (°C)	=	300.00			
	Pressure (atm)	=	223.00			
	Electrical balance (eq)	=	-1.241e-03			
	Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.44			
	Iterations	=	11			
	Total H	=	1.110508e+02			
	Total O	=	5.555211e+01			
-----Distribution of species-----						
Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm ³ /mol
OH-	9.275e-06	4.597e-06	-5.033	-5.338	-0.305	(0)
H+	1.986e-06	1.259e-06	-5.702	-5.900	-0.198	0.00
H2O	5.553e+01	9.943e-01	1.744	-0.002	0.000	24.39
C(4)	6.074e-03					
CO2	5.961e-03	6.164e-03	-2.225	-2.210	0.015	145.38
CaHCO3+	7.386e-05	3.783e-05	-4.132	-4.422	-0.291	(0)
HCO3-	2.920e-05	1.496e-05	-4.535	-4.825	-0.291	(0)
(CO2)2	3.317e-06	3.430e-06	-5.479	-5.465	0.015	290.77
MgHCO3+	2.751e-06	1.409e-06	-5.560	-5.851	-0.291	(0)
CaCO3	4.905e-07	4.905e-07	-6.309	-6.309	0.000	(0)
NaHCO3	5.410e-09	5.410e-09	-8.267	-8.267	0.000	(0)
MgCO3	1.800e-09	1.800e-09	-8.745	-8.745	0.000	(0)
CO3-2	5.462e-10	4.238e-11	-9.263	-10.373	-1.110	(0)
NaCO3-	1.539e-15	7.885e-16	-14.813	-15.103	-0.291	(0)
Ca	1.023e-02					
CaCl+	3.630e-03	1.859e-03	-2.440	-2.731	-0.291	(0)
Ca+2	3.377e-03	3.545e-04	-2.471	-3.450	-0.979	(0)
CaCl2	2.554e-03	2.554e-03	-2.593	-2.593	0.000	(0)
CaSO4	5.949e-04	5.949e-04	-3.226	-3.226	0.000	(0)
CaHCO3+	7.386e-05	3.783e-05	-4.132	-4.422	-0.291	(0)
CaCO3	4.905e-07	4.905e-07	-6.309	-6.309	0.000	(0)
CaOH+	8.664e-11	4.438e-11	-10.062	-10.353	-0.291	(0)
Cl(-1)	1.925e-01					
Cl-	1.418e-01	6.776e-02	-0.848	-1.169	-0.321	(0)
NaCl	3.783e-02	3.783e-02	-1.422	-1.422	0.000	(0)
CaCl+	3.630e-03	1.859e-03	-2.440	-2.731	-0.291	(0)
KCl	3.451e-03	3.451e-03	-2.462	-2.462	0.000	(0)
CaCl2	2.554e-03	2.554e-03	-2.593	-2.593	0.000	(0)
MgCl+	7.157e-04	3.666e-04	-3.145	-3.436	-0.291	(0)
HCl	2.450e-06	2.450e-06	-5.611	-5.611	0.000	(0)
Cl(1)	9.046e-14					
HClO	8.683e-14	8.683e-14	-13.061	-13.061	0.000	(0)
ClO-	3.631e-15	1.860e-15	-14.440	-14.731	-0.291	(0)
Cl(3)	3.097e-22					
ClO2-	3.094e-22	1.585e-22	-21.510	-21.800	-0.291	(0)
HClO2	2.949e-25	2.949e-25	-24.530	-24.530	0.000	(0)
Cl(5)	4.816e-22					
ClO3-	4.816e-22	2.387e-22	-21.317	-21.622	-0.305	(0)
Cl(7)	3.169e-25					
ClO4-	3.169e-25	1.571e-25	-24.499	-24.804	-0.305	(0)
H(0)	4.188e-19					
H2	2.094e-19	2.273e-19	-18.679	-18.643	0.036	(0)
K	2.380e-02					
K+	2.009e-02	9.604e-03	-1.697	-2.018	-0.321	(0)
KCl	3.451e-03	3.451e-03	-2.462	-2.462	0.000	(0)
KSO4-	2.507e-04	1.284e-04	-3.601	-3.891	-0.291	(0)
KHSO4	1.383e-06	1.383e-06	-5.859	-5.859	0.000	(0)
KOH	2.951e-11	2.951e-11	-10.530	-10.530	0.000	(0)
Mg	2.791e-03					
MgSO4	1.973e-03	1.973e-03	-2.705	-2.705	0.000	(0)
MgCl+	7.157e-04	3.666e-04	-3.145	-3.436	-0.291	(0)
Mg+2	9.938e-05	1.418e-05	-4.003	-4.848	-0.846	(0)
MgHCO3+	2.751e-06	1.409e-06	-5.560	-5.851	-0.291	(0)
MgCO3	1.800e-09	1.800e-09	-8.745	-8.745	0.000	(0)
Mg4(OH)4+4	5.289e-32	4.437e-36	-31.277	-35.353	-4.076	(0)
Na	1.476e-01					
Na+	1.097e-01	5.620e-02	-0.960	-1.250	-0.291	(0)
NaCl	3.783e-02	3.783e-02	-1.422	-1.422	0.000	(0)
NaSO4-	8.325e-06	4.264e-06	-5.080	-5.370	-0.291	(0)
NaOH	6.307e-06	6.307e-06	-5.200	-5.200	0.000	(0)
NaHSiO3	9.401e-07	9.401e-07	-6.027	-6.027	0.000	(0)
NaHCO3	5.410e-09	5.410e-09	-8.267	-8.267	0.000	(0)
NaCO3-	1.539e-15	7.885e-16	-14.813	-15.103	-0.291	(0)
O(0)	8.149e-06					
O2	4.075e-06	4.423e-06	-5.390	-5.354	0.036	(0)
S(6)	3.036e-03					
MgSO4	1.973e-03	1.973e-03	-2.705	-2.705	0.000	(0)
CaSO4	5.949e-04	5.949e-04	-3.226	-3.226	0.000	(0)
KSO4-	2.507e-04	1.284e-04	-3.601	-3.891	-0.291	(0)
SO4-2	1.668e-04	1.148e-05	-3.778	-4.940	-1.162	(0)
HSO4-	4.081e-05	2.091e-05	-4.389	-4.680	-0.291	(0)
NaSO4-	8.325e-06	4.264e-06	-5.080	-5.370	-0.291	(0)
KHSO4	1.383e-06	1.383e-06	-5.859	-5.859	0.000	(0)
H2SO4	1.735e-18	1.735e-18	-17.761	-17.761	0.000	(0)
Si	1.180e-03					
SiO2	1.178e-03	1.178e-03	-2.929	-2.929	0.000	(0)
NaHSiO3	9.401e-07	9.401e-07	-6.027	-6.027	0.000	(0)
HSiO3-	8.017e-07	4.106e-07	-6.096	-6.387	-0.291	(0)
H6(H2SiO4)4-2	9.701e-13	6.678e-14	-12.013	-13.175	-1.162	(0)
H2SiO4-2	1.473e-13	1.014e-14	-12.832	-13.994	-1.162	(0)

H4 (H2SiO4) 4-4	9.406e-20	2.112e-24	-19.027	-23.675	-4.649	(0)
-----Saturation indices-----						
Phase	SI**	log IAP	log K (573 K, 223 atm)			
Afwillite	-12.69	19.18	31.87	Ca3Si2O4 (OH) 6		
Akermanite	-1.16	17.79	18.95	Ca2MgSi2O7		
Anhydrite	1.53	-8.39	-9.92	CaSO4		
Antarcticite	-9.60	-5.80	3.79	CaCl2:6H2O		
Anthophyllite	5.22	25.21	19.99	Mg7Si8O22 (OH) 2		
Antigorite	60.18	233.91	173.73	Mg48Si34O85 (OH) 62		
Aphthitalite	-13.29	-17.18	-3.89	NaK3 (SO4) 2		
Aragonite	-0.34	-2.38	-2.03	CaCO3		
Arcanite	-5.48	-8.97	-3.49	K2SO4		
Artinite	-4.70	3.17	7.86	Mg2CO3 (OH) 2:3H2O		
Bassanite	0.82	-8.39	-9.21	CaSO4:0.5H2O		
Bischofite	-11.29	-7.20	4.09	MgCl2:6H2O		
Bloedite	-14.56	-17.24	-2.68	Na2Mg (SO4) 2:4H2O		
Brucite	-0.15	6.95	7.10	Mg (OH) 2		
Burkeite	-25.79	-16.31	9.49	Na6CO3 (SO4) 2		
C	-33.46	-5.37	28.09	C		
C (g)	-91.21	-5.37	85.84	C		
Ca	-58.64	11.02	69.67	Ca		
Ca (g)	-69.28	11.02	80.30	Ca		
Ca2Cl2 (OH) 2:H2O	-23.59	2.55	26.14	Ca2Cl2 (OH) 2:H2O		
Ca4Cl2 (OH) 6:13H2O	-48.16	19.21	67.38	Ca4Cl2 (OH) 6:13H2O		
Calcite	-0.18	-2.38	-2.20	CaCO3		
Carnallite	-14.36	-10.39	3.97	KMgCl3:6H2O		
CaSO4:0.5H2O (beta)	0.87	-8.39	-9.26	CaSO4:0.5H2O		
Chalcedony	-1.07	-2.93	-1.86	SiO2		
Chloromagnesite	-11.99	-7.19	4.80	MgCl2		
Chrysotile	3.37	14.99	11.62	Mg3Si2O5 (OH) 4		
Cl2 (g)	-13.14	-16.81	-3.67	Cl2		
CO2 (g)	-0.14	-2.21	-2.07	CO2		
Coesite	-1.38	-2.93	-1.55	SiO2		
Cristobalite (alpha)	-1.16	-2.93	-1.77	SiO2		
Cristobalite (beta)	-1.31	-2.93	-1.62	SiO2		
Dicalcium silicate	-3.83	13.77	17.59	Ca2SiO4		
Diopside	1.53	9.44	7.91	CaMgSi2O6		
Dolomite	-0.09	-6.15	-6.06	CaMg (CO3) 2		
Dolomite-dis	-0.60	-6.15	-5.55	CaMg (CO3) 2		
Dolomite-ord	-0.08	-6.15	-6.07	CaMg (CO3) 2		
Enstatite	0.45	4.02	3.57	MgSiO3		
Epsomite	-7.49	-9.81	-2.31	MgSO4:7H2O		
Forsterite	1.26	10.97	9.71	Mg2SiO4		
Foshagite	-8.15	24.60	32.74	Ca4Si3O9 (OH) 2:0.5H2O		
Gaylussite	-14.73	-3.81	10.91	CaNa2 (CO3) 2:5H2O		
Glauberite	-10.36	-15.83	-5.47	Na2Ca (SO4) 2		
Gypsum	-0.03	-8.40	-8.37	CaSO4:2H2O		
Gyrolite	-5.95	7.90	13.85	Ca2Si3O7 (OH) 2:1.5H2O		
H2 (g)	-16.26	-18.64	-2.39	H2		
H2O (g)	1.85	-0.00	-1.85	H2O		
Halite	-2.90	-2.42	0.48	NaCl		
Hatruite	-13.14	22.11	35.25	Ca3SiO5		
HCl (g)	-5.92	-7.07	-1.15	HCl		
Hexahydrite	-7.78	-9.80	-2.03	MgSO4:6H2O		
Hillebrandite	-5.03	13.76	18.80	Ca2SiO3 (OH) 2:0.17H2O		
Huntite	-2.79	-13.70	-10.90	CaMg3 (CO3) 4		
Hydromagnesite	-8.14	-8.16	-0.02	Mg5 (CO3) 4 (OH) 2:4H2O		
Hydrophilite	-6.82	-5.79	1.04	CaCl2		
Ice	-1.35	-0.00	1.35	H2O		
K	-32.48	5.22	37.70	K		
K (g)	-35.94	5.22	41.16	K		
K2CO3:1.5H2O	-16.27	-2.96	13.30	K2CO3:1.5H2O		
K2O	-40.47	7.76	48.23	K2O		
K3H (SO4) 2	-18.21	-21.83	-3.62	K3H (SO4) 2		
K8H4 (CO3) 6:3H2O	-60.86	-33.30	27.56	K8H4 (CO3) 6:3H2O		
Kainite	-12.52	-12.98	-0.46	KMgCl3SO4:3H2O		
Kalicanite	-7.13	-6.84	0.28	KHCO3		
Kieserite	-9.47	-9.79	-0.32	MgSO4:H2O		
KMgCl3	-16.89	-10.37	6.51	KMgCl3		
KMgCl3:2H2O	-15.56	-10.38	5.19	KMgCl3:2H2O		
KNaCO3:6H2O	-12.17	-2.21	9.96	KNaCO3:6H2O		
Lansfordite	-8.38	-3.79	4.59	MgCO3:5H2O		
Larnite	-4.31	13.77	18.07	Ca2SiO4		
Leonite	-14.46	-18.77	-4.31	K2Mg (SO4) 2:4H2O		
Lime	-7.67	8.35	16.01	CaO		
Magnesite	-0.68	-3.77	-3.09	MgCO3		
Mercurite	-11.42	-12.86	-1.44	KHSO4		
Merwinite	-3.83	26.13	29.96	MgCa3 (SiO4) 2		
Mg	-49.41	9.63	59.03	Mg		
Mg (g)	-57.14	9.63	66.76	Mg		
Mg1.25SO4 (OH) 0.5:0.5H2O	-1.44	-8.05	-6.61	Mg1.25SO4 (OH) 0.5:0.5H2O		
Mg1.5SO4 (OH)	-1.20	-6.31	-5.11	Mg1.5SO4 (OH)		
MgCl2:2H2O	-9.01	-7.19	1.82	MgCl2:2H2O		
MgCl2:4H2O	-8.09	-7.20	0.90	MgCl2:4H2O		
MgCl2:H2O	-9.82	-7.19	2.64	MgCl2:H2O		
MgOHCl	-4.31	-0.12	4.19	MgOHCl		
MgSO4	-3.16	-9.79	-6.62	MgSO4		
Mirabilite	-18.08	-7.47	10.62	Na2SO4:10H2O		
Misenite	-75.04	-86.12	-11.08	K8H6 (SO4) 7		
Monohydrocalcite	-3.15	-2.38	0.77	CaCO3:H2O		
Monticellite	0.31	12.37	12.05	CaMgSiO4		
Na	-29.41	5.99	35.40	Na		
Na (g)	-34.20	5.99	40.18	Na		
Na2CO3	-8.27	-1.43	6.85	Na2CO3		
Na2CO3:7H2O	-18.69	-1.44	17.25	Na2CO3:7H2O		
Na2O	-29.33	9.30	38.63	Na2O		
Na2SiO3	-8.91	6.37	15.28	Na2SiO3		
Na3H (SO4) 2	-18.64	-19.53	-0.89	Na3H (SO4) 2		
Na4Ca (SO4) 3:2H2O	-17.28	-23.28	-5.99	Na4Ca (SO4) 3:2H2O		
Na4SiO4	-28.20	15.67	43.87	Na4SiO4		
Na6Si2O7	-40.56	22.03	62.59	Na6Si2O7		
Nahcolite	-6.16	-6.08	0.08	NaHCO3		
Natron	-16.96	-1.45	15.51	Na2CO3:10H2O		
Natrosilite	-9.54	3.44	12.97	Na2Si2O5		
Nesquehonite	-7.09	-3.78	3.31	MgCO3:3H2O		

O2(g)	-2.99	-5.35	-2.36	O2
Okenite	-6.64	2.48	9.12	CaSi2O4(OH)2:2H2O
Oxychloride-Mg	-18.66	6.82	25.48	Mg2Cl(OH)3:4H2O
Pentahydrate	-8.16	-9.80	-1.64	MgSO4:5H2O
Periclase	-1.72	6.95	8.67	MgO
Picromerite	-14.04	-18.78	-4.74	K2Mg(SO4)2:6H2O
Pirssonite	-15.03	-3.81	11.22	Na2Ca(CO3)2:2H2O
Polyhalite	-21.14	-35.55	-14.41	K2MgCa2(SO4)4:2H2O
Portlandite	-3.31	8.34	11.65	Ca(OH)2
Pseudowollastonite	-0.87	5.42	6.29	CaSiO3
Quartz	-0.93	-2.93	-2.00	SiO2
Rankinite	-4.97	19.18	24.15	Ca3Si2O7
Sepiolite	-4.03	10.21	14.23	Mg4Si6O15(OH)2:6H2O
Si	-71.33	2.43	73.75	Si
Si(g)	-105.24	2.43	107.67	Si
SiO2(am)	-1.34	-2.93	-1.59	SiO2
Starkeyite	-8.60	-9.80	-1.20	MgSO4:4H2O
Sylvite	-3.81	-3.19	0.62	KCl
Syngenite	-9.72	-17.37	-7.65	K2Ca(SO4)2:2H2O
Tachyhydrite	-36.73	-20.19	16.54	Mg2CaCl6:12H2O
Talc	3.44	9.13	5.69	Mg3Si4O10(OH)2
Thenardite	-3.93	-7.44	-3.51	Na2SO4
Thermonatrite	-9.64	-1.43	8.21	Na2CO3:H2O
Tobermorite-11A	-12.79	24.15	36.94	Ca5Si6H11O22.5
Tobermorite-14A	-18.09	24.14	42.23	Ca5Si6H21O27.5
Tobermorite-9A	-11.85	24.16	36.01	Ca5Si6H6O20
Tremolite	7.50	28.01	20.50	Ca2Mg5Si8O22(OH)2
Tridymite	-1.75	-2.93	-1.18	SiO2
Trona-K	-20.53	-9.04	11.49	K2NaH(CO3)2:2H2O
Wollastonite	-0.87	5.42	6.29	CaSiO3
Xonotlite	-19.76	32.51	52.27	Ca6Si6O17(OH)2

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

Beginning of batch-reaction calculations.

TIME STEP 1 HOUR

Reaction step 1.

WARNING: CNode incomplete at cnode_steps 100. Cell: 0 Time: 7.107562e-03 Cnode calls: 1, continuing...

WARNING: CNode incomplete at cnode_steps 100. Cell: 0 Time: 2.690524e-02 Cnode calls: 2, continuing...

WARNING: CNode incomplete at cnode_steps 100. Cell: 0 Time: 7.090715e-02 Cnode calls: 3, continuing...

WARNING: CNode incomplete at cnode_steps 100. Cell: 0 Time: 1.490150e-01 Cnode calls: 4, continuing...

WARNING: CNode incomplete at cnode_steps 100. Cell: 0 Time: 2.750991e-01 Cnode calls: 5, continuing...

WARNING: CNode incomplete at cnode_steps 100. Cell: 0 Time: 5.278129e+01 Cnode calls: 6, continuing...

WARNING: CNode incomplete at cnode_steps 100. Cell: 0 Time: 1.419644e+03 Cnode calls: 7, continuing...

WARNING: No data for rate Magnetite in KINETICS keyword.
Using solution 1. Siler 2300p10
Using pure phase assemblage 1. Reservoir
Using kinetics 1.

Kinetics 1.

Time step: 3600 seconds (Incremented time: 3600 seconds)

Rate name	Delta Moles	Total Moles	Reactant	Coefficient	
Quartz	3.660e-01	4.253e+01	SiO2	1	
Anorthite	-1.803e-02	2.547e+01	CaAl2(SiO4)2	1	
Albite	2.448e-02	2.256e+01	NaAlSi3O8	1	
K-Feldspar	1.156e-02	1.312e+01	KAlSi3O8	1	
Diopside	-2.252e-01	3.885e+00	CaMgSi2O6	1	
Enstatite	-1.488e-02	3.374e+01	MgSiO3	1	
Ilmenite	-2.684e-03	1.737e+00	FeTiO3	1	
Actinolite	1.022e-03	1.471e+00	Ca2Mg2.5Fe2.5Si8O22(OH)2	1	1
Calcite	-0.000e+00	0.000e+00	CaCO3	1	
Dolomite	2.302e-01	2.302e-01	CaMg(CO3)2	1	
Magnesite	-0.000e+00	0.000e+00	MgCO3	1	

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

Phase	SI	log IAP	log K(T, P)	Moles in assemblage		
				Initial	Final	Delta
CO2(g)	1.91	-0.16	-2.07	1.200e+00	0	-1.200e+00

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

Elements	Molality	Moles
Al	7.733e-06	7.732e-06
C	7.458e-01	7.457e-01
Ca	2.122e-02	2.121e-02
Cl	1.925e-01	1.925e-01
Fe	1.301e-04	1.301e-04
K	1.223e-02	1.223e-02
Mg	1.012e-02	1.012e-02
Na	1.231e-01	1.231e-01
S	3.036e-03	3.036e-03
Si	2.015e-02	2.015e-02
Ti	2.684e-03	2.684e-03

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

pH = 4.575 Charge balance
pe = 5.327 Adjusted to redox equilibrium
Density (g/cm³) = 0.71554
Volume (L) = 1.46149

Activity of water = 0.983
 Ionic strength (mol/kgw) = 1.437e-01
 Mass of water (kg) = 9.999e-01
 Total alkalinity (eq/kg) = 9.368e-04
 Total CO2 (mol/kg) = 7.458e-01
 Temperature (°C) = 300.00
 Pressure (atm) = 223.00
 Electrical balance (eq) = -1.241e-03
 Percent error, 100*(Cat-|An|)/(|Cat+|+|An|) = -0.46
 Iterations = 13895
 Total H = 1.110488e+02
 Total O = 5.707417e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm ³ /mol
H+	4.191e-05	2.660e-05	-4.378	-4.575	-0.197	0.00
OH-	4.325e-07	2.150e-07	-6.364	-6.668	-0.304	(0)
H2O	5.553e+01	9.825e-01	1.744	-0.008	0.000	24.38
Al	7.733e-06					
HAlO2	4.556e-06	4.556e-06	-5.341	-5.341	0.000	(0)
NaAlO2	1.738e-06	1.738e-06	-5.760	-5.760	0.000	(0)
AlO2-	1.422e-06	7.304e-07	-5.847	-6.136	-0.289	(0)
Al(OH)2+	1.688e-08	8.666e-09	-7.773	-8.062	-0.289	(0)
AlOH+2	5.473e-11	4.286e-12	-10.262	-11.368	-1.106	(0)
Al+3	2.598e-15	4.346e-17	-14.585	-16.362	-1.776	(0)
AlSO4+	1.445e-19	7.423e-20	-18.840	-19.129	-0.289	(0)
Al(SO4)2-	1.872e-23	9.616e-24	-22.728	-23.017	-0.289	(0)
Al2(OH)2+4	7.647e-28	6.621e-32	-27.117	-31.179	-4.063	(0)
Al3(OH)4+5	4.000e-39	0.000e+00	-38.398	-44.496	-6.098	(0)
Al13O4(OH)24+7	0.000e+00	0.000e+00	-151.893	-163.846	-11.953	(0)
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-118.438	-118.438	0.000	(0)
C(-3)	0.000e+00					
C2H6	0.000e+00	0.000e+00	-102.610	-102.610	0.000	(0)
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-63.844	-63.844	0.000	(0)
C(2)	4.864e-21					
CO	4.864e-21	4.864e-21	-20.313	-20.313	0.000	(0)
C(4)	7.458e-01					
CO2	6.627e-01	6.850e-01	-0.179	-0.164	0.014	145.38
(CO2)2	4.098e-02	4.236e-02	-1.387	-1.373	0.014	290.77
CaHCO3+	8.422e-04	4.325e-04	-3.075	-3.364	-0.289	(0)
HCO3-	1.514e-04	7.773e-05	-3.820	-4.109	-0.289	(0)
MgHCO3+	1.331e-04	6.833e-05	-3.876	-4.165	-0.289	(0)
CaCO3	2.654e-07	2.654e-07	-6.576	-6.576	0.000	(0)
FeHCO3+	1.976e-07	1.015e-07	-6.704	-6.994	-0.289	(0)
NaHCO3	2.375e-08	2.375e-08	-7.624	-7.624	0.000	(0)
MgCO3	4.131e-09	4.131e-09	-8.384	-8.384	0.000	(0)
CO3-2	1.331e-10	1.042e-11	-9.876	-10.982	-1.106	(0)
FeCO3	1.831e-11	1.831e-11	-10.737	-10.737	0.000	(0)
FeCO3+	2.181e-12	1.120e-12	-11.661	-11.951	-0.289	(0)
NaCO3-	3.190e-16	1.638e-16	-15.496	-15.786	-0.289	(0)
Ca	2.122e-02					
CaCl+	7.640e-03	3.923e-03	-2.117	-2.406	-0.289	(0)
Ca+2	7.375e-03	7.799e-04	-2.132	-3.108	-0.976	(0)
CaCl2	5.168e-03	5.168e-03	-2.287	-2.287	0.000	(0)
CaHCO3+	8.422e-04	4.325e-04	-3.075	-3.364	-0.289	(0)
CaSO4	1.902e-04	1.902e-04	-3.721	-3.721	0.000	(0)
CaCO3	2.654e-07	2.654e-07	-6.576	-6.576	0.000	(0)
CaOH+	8.890e-12	4.565e-12	-11.051	-11.341	-0.289	(0)
Cl(-1)	1.925e-01					
Cl-	1.355e-01	6.499e-02	-0.868	-1.187	-0.319	(0)
NaCl	3.065e-02	3.065e-02	-1.514	-1.514	0.000	(0)
CaCl+	7.640e-03	3.923e-03	-2.117	-2.406	-0.289	(0)
MgCl+	6.389e-03	3.281e-03	-2.195	-2.484	-0.289	(0)
CaCl2	5.168e-03	5.168e-03	-2.287	-2.287	0.000	(0)
KCl	1.732e-03	1.732e-03	-2.761	-2.761	0.000	(0)
FeCl+	8.408e-05	4.318e-05	-4.075	-4.365	-0.289	(0)
HCl	4.965e-05	4.965e-05	-4.304	-4.304	0.000	(0)
FeCl4-2	2.008e-05	1.396e-06	-4.697	-5.855	-1.158	(0)
FeCl2	2.147e-06	2.147e-06	-5.668	-5.668	0.000	(0)
FeCl+2	6.051e-08	4.738e-09	-7.218	-8.324	-1.106	(0)
FeCl2+	4.758e-13	2.443e-13	-12.323	-12.612	-0.289	(0)
FeCl4-	2.416e-18	1.241e-18	-17.617	-17.906	-0.289	(0)
Cl(1)	1.759e-12					
HClO	1.755e-12	1.755e-12	-11.756	-11.756	0.000	(0)
ClO-	3.465e-15	1.779e-15	-14.460	-14.750	-0.289	(0)
Cl(3)	3.004e-22					
ClO2-	2.944e-22	1.512e-22	-21.531	-21.820	-0.289	(0)
HClO2	5.946e-24	5.946e-24	-23.226	-23.226	0.000	(0)
Cl(5)	4.571e-22					
ClO3-	4.571e-22	2.272e-22	-21.340	-21.644	-0.304	(0)
Cl(7)	2.999e-25					
ClO4-	2.999e-25	1.491e-25	-24.523	-24.827	-0.304	(0)
Fe(2)	1.300e-04					
FeCl+	8.408e-05	4.318e-05	-4.075	-4.365	-0.289	(0)
Fe+2	2.352e-05	2.487e-06	-4.629	-5.604	-0.976	(0)
FeCl4-2	2.008e-05	1.396e-06	-4.697	-5.855	-1.158	(0)
FeCl2	2.147e-06	2.147e-06	-5.668	-5.668	0.000	(0)
FeHCO3+	1.976e-07	1.015e-07	-6.704	-6.994	-0.289	(0)
FeSO4	6.579e-10	6.579e-10	-9.182	-9.182	0.000	(0)
FeOH+	6.348e-11	3.260e-11	-10.197	-10.487	-0.289	(0)
FeCO3	1.831e-11	1.831e-11	-10.737	-10.737	0.000	(0)
Fe(OH)2	1.073e-17	1.073e-17	-16.969	-16.969	0.000	(0)
Fe(OH)3-	3.447e-23	1.770e-23	-22.463	-22.752	-0.289	(0)
Fe(OH)4-2	1.055e-32	7.336e-34	-31.977	-33.135	-1.158	(0)
Fe(3)	7.321e-08					
FeCl+2	6.051e-08	4.738e-09	-7.218	-8.324	-1.106	(0)
FeSO4+	8.112e-09	4.166e-09	-8.091	-8.380	-0.289	(0)
Fe(OH)2+	3.066e-09	1.574e-09	-8.513	-8.803	-0.289	(0)
FeOH+2	1.465e-09	1.147e-10	-8.834	-9.940	-1.106	(0)
Fe(OH)3	3.051e-11	3.051e-11	-10.515	-10.515	0.000	(0)
Fe+3	2.563e-11	4.288e-13	-10.591	-12.368	-1.776	(0)
FeCO3+	2.181e-12	1.120e-12	-11.661	-11.951	-0.289	(0)
FeCl2+	4.758e-13	2.443e-13	-12.323	-12.612	-0.289	(0)

	Fe2 (OH) 2+4	4.092e-15	3.543e-19	-14.388	-18.451	-4.063	(0)
	Fe (OH) 4-	6.185e-16	3.176e-16	-15.209	-15.498	-0.289	(0)
	FeCl4-	2.416e-18	1.241e-18	-17.617	-17.906	-0.289	(0)
	Fe3 (OH) 4+5	1.461e-19	1.165e-25	-18.835	-24.934	-6.098	(0)
	Fe (SO4) 2-	3.804e-21	1.953e-21	-20.420	-20.709	-0.289	(0)
H (0)		4.153e-19					
H2		2.077e-19	2.252e-19	-18.683	-18.647	0.035	(0)
K		1.223e-02					
K+		1.048e-02	5.025e-03	-1.980	-2.299	-0.319	(0)
KCl		1.732e-03	1.732e-03	-2.761	-2.761	0.000	(0)
KSO4-		1.901e-05	9.761e-06	-4.721	-5.010	-0.289	(0)
KHSO4		2.222e-06	2.222e-06	-5.653	-5.653	0.000	(0)
KOH		7.220e-13	7.220e-13	-12.141	-12.141	0.000	(0)
Mg		1.012e-02					
MgCl+		6.389e-03	3.281e-03	-2.195	-2.484	-0.289	(0)
MgSO4		2.675e-03	2.675e-03	-2.573	-2.573	0.000	(0)
Mg+2		9.221e-04	1.323e-04	-3.035	-3.878	-0.843	(0)
MgHCO3+		1.331e-04	6.833e-05	-3.876	-4.165	-0.289	(0)
MgCO3		4.131e-09	4.131e-09	-8.384	-8.384	0.000	(0)
Mg4 (OH) 4+4		1.857e-33	1.608e-37	-32.731	-36.794	-4.063	(0)
Na		1.231e-01					
Na+		9.244e-02	4.747e-02	-1.034	-1.324	-0.289	(0)
NaCl		3.065e-02	3.065e-02	-1.514	-1.514	0.000	(0)
NaAlO2		1.738e-06	1.738e-06	-5.760	-5.760	0.000	(0)
NaSO4-		1.019e-06	5.234e-07	-5.992	-6.281	-0.289	(0)
NaHSiO3		6.354e-07	6.354e-07	-6.197	-6.197	0.000	(0)
NaOH		2.491e-07	2.491e-07	-6.604	-6.604	0.000	(0)
NaHCO3		2.375e-08	2.375e-08	-7.624	-7.624	0.000	(0)
NaCO3-		3.190e-16	1.638e-16	-15.496	-15.786	-0.289	(0)
O (0)		8.113e-06					
O2		4.057e-06	4.400e-06	-5.392	-5.357	0.035	(0)
S (-2)		0.000e+00					
H2S		0.000e+00	0.000e+00	-56.726	-56.726	0.000	(0)
HS-		0.000e+00	0.000e+00	-59.384	-59.688	-0.304	(0)
S-2		0.000e+00	0.000e+00	-61.623	-62.682	-1.059	(0)
S2-2		0.000e+00	0.000e+00	-106.792	-107.950	-1.158	(0)
S3-2		0.000e+00	0.000e+00	-149.105	-150.263	-1.158	(0)
S4-2		0.000e+00	0.000e+00	-191.525	-192.682	-1.158	(0)
S5-2		0.000e+00	0.000e+00	-234.067	-235.225	-1.158	(0)
S (2)		0.000e+00					
S2O3-2		0.000e+00	0.000e+00	-63.313	-64.471	-1.158	(0)
HS2O3-		0.000e+00	0.000e+00	-67.743	-68.032	-0.289	(0)
S (3)		0.000e+00					
S2O4-2		0.000e+00	0.000e+00	-59.916	-60.975	-1.059	(0)
S (4)		4.496e-20					
SO2		3.979e-20	3.979e-20	-19.400	-19.400	0.000	(0)
HSO3-		5.167e-21	2.653e-21	-20.287	-20.576	-0.289	(0)
SO3-2		2.291e-26	1.794e-27	-25.640	-26.746	-1.106	(0)
H2SO3		2.074e-27	2.074e-27	-26.683	-26.683	0.000	(0)
S2O6-2		2.205e-34	1.534e-35	-33.657	-34.814	-1.158	(0)
S3O6-2		0.000e+00	0.000e+00	-78.027	-79.184	-1.158	(0)
S4O6-2		0.000e+00	0.000e+00	-110.790	-111.947	-1.158	(0)
S5O6-2		0.000e+00	0.000e+00	-165.106	-166.264	-1.158	(0)
S (5)		0.000e+00					
S2O5-2		0.000e+00	0.000e+00	-46.122	-47.279	-1.158	(0)
S (6)		3.036e-03					
MgSO4		2.675e-03	2.675e-03	-2.573	-2.573	0.000	(0)
CaSO4		1.902e-04	1.902e-04	-3.721	-3.721	0.000	(0)
HSO4-		1.250e-04	6.419e-05	-3.903	-4.193	-0.289	(0)
SO4-2		2.400e-05	1.669e-06	-4.620	-5.778	-1.158	(0)
KSO4-		1.901e-05	9.761e-06	-4.721	-5.010	-0.289	(0)
KHSO4		2.222e-06	2.222e-06	-5.653	-5.653	0.000	(0)
NaSO4-		1.019e-06	5.234e-07	-5.992	-6.281	-0.289	(0)
FeSO4+		8.112e-09	4.166e-09	-8.091	-8.380	-0.289	(0)
FeSO4		6.579e-10	6.579e-10	-9.182	-9.182	0.000	(0)
H2SO4		1.125e-16	1.125e-16	-15.949	-15.949	0.000	(0)
AlSO4+		1.445e-19	7.423e-20	-18.840	-19.129	-0.289	(0)
Fe (SO4) 2-		3.804e-21	1.953e-21	-20.420	-20.709	-0.289	(0)
Al (SO4) 2-		1.872e-23	9.616e-24	-22.728	-23.017	-0.289	(0)
S (7)		2.757e-25					
S2O8-2		1.379e-25	9.588e-27	-24.861	-26.018	-1.158	(0)
S (8)		1.089e-16					
HSO5-		1.089e-16	5.593e-17	-15.963	-16.252	-0.289	(0)
Si		2.015e-02					
SiO2		2.015e-02	2.015e-02	-1.696	-1.696	0.000	(0)
HSiO3-		6.397e-07	3.285e-07	-6.194	-6.483	-0.289	(0)
NaHSiO3		6.354e-07	6.354e-07	-6.197	-6.197	0.000	(0)
H6 (H2SiO4) 4-2		1.674e-10	1.164e-11	-9.776	-10.934	-1.158	(0)
H2SiO4-2		5.457e-15	3.795e-16	-14.263	-15.421	-1.158	(0)
H4 (H2SiO4) 4-4		3.526e-20	8.247e-25	-19.453	-24.084	-4.631	(0)
Ti		2.684e-03					
Ti (OH) 4		2.684e-03	2.684e-03	-2.571	-2.571	0.000	(0)

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

Phase	SI**	log IAP	log K (573 K, 223 atm)
Actinolite	-0.00	20.50	20.50
Afwillite	-17.18	14.69	31.87
Akermanite	-5.00	13.94	18.95
Al	-65.84	1.37	67.21
Al (g)	-89.25	1.37	90.62
Al2 (SO4) 3	-24.44	-50.06	-25.62
Al2 (SO4) 3:6H2O	-22.62	-50.10	-27.48
Albite	-0.00	-4.49	-4.48
Albite_high	-0.40	-4.49	-4.09
Albite_low	-0.01	-4.49	-4.48
Alum-K	-18.57	-30.31	-11.74
Alunite	-5.69	-35.54	-29.84
Amesite-14A	3.56	7.04	3.48
Analcime	-0.71	-2.89	-2.18
Analcime-dehy	-3.42	-2.88	0.54
Anatase	5.90	-2.56	-8.46
Andalusite	-0.39	-6.99	-6.60
Andradite	12.89	15.71	2.82
Anhydrite	1.04	-8.89	-9.92
Ankerite	-0.35	-7.26	-6.92
Annite	1.30	5.14	3.84
Ca2Mg2.5Fe2.5Si8O22 (OH) 2			
Ca3Si2O4 (OH) 6			
Ca2MgSi2O7			
Al			
Al2 (SO4) 3			
Al2 (SO4) 3:6H2O			
NaAlSi3O8			
NaAlSi3O8			
NaAlSi3O8			
KAl (SO4) 2:12H2O			
KAl3 (OH) 6 (SO4) 2			
Mg4Al4Si2O10 (OH) 8			
Na.96Al.96Si2.04O6:H2O			
Na.96Al.96Si2.04O6			
TiO2			
Al2SiO5			
Ca3Fe2 (SiO4) 3			
CaSO4			
CaMg0.3Fe0.7 (CO3) 2			
KFe3AlSi3O10 (OH) 2			

Anorthite	0.03	-2.65	-2.68	CaAl ₂ (SiO ₄) ₂
Antarcticite	-9.32	-5.53	3.79	CaCl ₂ ·6H ₂ O
Anthophyllite	3.29	23.28	19.99	Mg ₇ Si ₈ O ₂₂ (OH) ₂
Antigorite	21.06	194.79	173.73	Mg ₄ Si ₃ 4O ₈ 5(OH) ₆ 2
Aphthitalite	-15.89	-19.78	-3.89	NaK ₃ (SO ₄) ₂
Aragonite	-0.61	-2.64	-2.03	CaCO ₃
Arcanite	-6.88	-10.38	-3.49	K ₂ SO ₄
Artinite	-6.04	1.82	7.86	Mg ₂ CO ₃ (OH) ₂ ·3H ₂ O
Bassanite	0.33	-8.89	-9.21	CaSO ₄ ·0.5H ₂ O
Beidellite-Ca	1.62	-11.41	-13.02	Ca _{1.165} Al _{2.338} Si _{3.670} O ₁₀ (OH) ₂
Beidellite-H	0.84	-12.40	-13.24	H _{3.33} Al _{2.338} Si _{3.670} O ₁₀ (OH) ₂
Beidellite-K	0.63	-11.65	-12.28	K _{3.33} Al _{2.338} Si _{3.670} O ₁₀ (OH) ₂
Beidellite-Mg	1.75	-11.53	-13.28	Mg _{1.165} Al _{2.338} Si _{3.670} O ₁₀ (OH) ₂
Beidellite-Na	0.92	-11.33	-12.25	Na _{3.33} Al _{2.338} Si _{3.670} O ₁₀ (OH) ₂
Bischofite	-10.39	-6.30	4.09	MgCl ₂ ·6H ₂ O
Bloedite	-15.43	-18.11	-2.68	Na ₂ Mg(SO ₄) ₂ ·4H ₂ O
Boehmite	0.22	-2.65	-2.87	Al ₂ O ₃ ·H ₂ O
Brucite	-1.85	5.26	7.10	Mg(OH) ₂
Burkeite	-28.52	-19.03	9.49	Na ₆ CO ₃ (SO ₄) ₂
C	-31.41	-3.32	28.09	C
C(g)	-89.16	-3.32	85.84	C
Ca	-60.95	8.71	69.67	Ca
Ca(g)	-71.59	8.71	80.30	Ca
Ca-Al Pyroxene	-3.49	-0.96	2.54	CaAl ₂ SiO ₆
Ca ₂ Al ₂ O ₅ ·8H ₂ O	-52.21	6.71	58.92	Ca ₂ Al ₂ O ₅ ·8H ₂ O
Ca ₂ Cl ₂ (OH) ₂ ·H ₂ O	-25.60	0.54	26.14	Ca ₂ Cl ₂ (OH) ₂ ·H ₂ O
Ca ₃ Al ₂ O ₆	-29.98	12.81	42.78	Ca ₃ Al ₂ O ₆
Ca ₄ Al ₂ Fe ₂ O ₁₀	-22.42	21.53	43.95	Ca ₄ Al ₂ Fe ₂ O ₁₀
Ca ₄ Al ₂ O ₇ ·13H ₂ O	-87.51	18.74	106.25	Ca ₄ Al ₂ O ₇ ·13H ₂ O
Ca ₄ Al ₂ O ₇ ·19H ₂ O	-83.69	18.70	102.38	Ca ₄ Al ₂ O ₇ ·19H ₂ O
Ca ₄ Cl ₂ (OH) ₆ ·13H ₂ O	-54.88	12.50	67.38	Ca ₄ Cl ₂ (OH) ₆ ·13H ₂ O
CaAl ₂ O ₄	-7.07	0.74	7.81	CaAl ₂ O ₄
CaAl ₂ O ₄ ·10H ₂ O	-36.63	0.66	37.29	CaAl ₂ O ₄ ·10H ₂ O
CaAl ₄ O ₇	-11.25	-4.56	6.69	CaAl ₄ O ₇
Calcite	-0.44	-2.64	-2.20	CaCO ₃
Carnallite	-13.76	-9.78	3.97	KMgCl ₃ ·6H ₂ O
CaSO ₄ ·0.5H ₂ O(beta)	0.37	-8.89	-9.26	CaSO ₄ ·0.5H ₂ O
Celadonite	0.20	-1.90	-2.10	KMgAlSi ₄ O ₁₀ (OH) ₂
CH ₄ (g)	-61.35	-63.84	-2.49	CH ₄
Chalcedony	0.17	-1.70	-1.86	SiO ₂
Chamosite-7A	0.73	0.07	-0.66	Fe ₂ Al ₂ Si ₂ O ₅ (OH) ₄
Chloromagnesite	-11.06	-6.25	4.80	MgCl ₂
Chrysotile	0.77	12.39	11.62	Mg ₃ Si ₂ O ₅ (OH) ₄
Cl ₂ (g)	-10.52	-14.20	-3.67	Cl ₂
Clinocllore-14A	3.88	15.91	12.03	Mg ₅ Al ₂ Si ₃ O ₁₀ (OH) ₈
Clinocllore-7A	1.52	15.91	14.39	Mg ₅ Al ₂ Si ₃ O ₁₀ (OH) ₈
Clinoptilolite-Ca	5.56	-23.38	-28.94	Ca _{1.7335} Al _{3.45} Fe _{0.178} Si _{14.5330} 36:10.922H ₂ O
Clinoptilolite-dehy-Ca	-8.88	-23.30	-14.42	Ca _{1.7335} Al _{3.45} Fe _{0.178} Si _{14.5330} 36
Clinoptilolite-dehy-K	-19.66	-25.88	-6.22	K _{3.467} Al _{3.45} Fe _{0.178} Si _{14.5330} 36
Clinoptilolite-dehy-Na	-16.07	-22.50	-6.43	Na _{3.467} Al _{3.45} Fe _{0.178} Si _{14.5330} 36
Clinoptilolite-hy-Ca	4.76	-23.38	-28.15	Ca _{1.7335} Al _{3.45} Fe _{0.178} Si _{14.5330} 36:11.645H ₂ O
Clinoptilolite-hy-K	-2.32	-25.94	-23.62	K _{3.467} Al _{3.45} Fe _{0.178} Si _{14.5330} 36:7.499H ₂ O
Clinoptilolite-hy-Na	-1.72	-22.98	-20.86	Na _{3.467} Al _{3.45} Fe _{0.178} Si _{14.5330} 36:10.877H ₂ O
Clinoptilolite-K	-5.57	-25.96	-20.39	K _{3.467} Al _{3.45} Fe _{0.178} Si _{14.5330} 36:10.922H ₂ O
Clinoptilolite-Na	-1.76	-22.58	-20.82	Na _{3.467} Al _{3.45} Fe _{0.178} Si _{14.5330} 36:10.922H ₂ O
Clinzoisite	-0.08	-0.97	-0.89	Ca ₂ Al ₃ Si ₃ O ₁₂ (OH)
CO(g)	-18.14	-20.31	-2.17	CO
CO ₂ (g)	1.91	-0.16	-2.07	CO ₂
Coesite	-0.14	-1.70	-1.55	SiO ₂
Cordierite_anhyd	-0.32	-8.54	-8.22	Mg ₂ Al ₄ Si ₅ O ₁₈
Cordierite_hydr	0.50	-8.55	-9.05	Mg ₂ Al ₄ Si ₅ O ₁₈ ·H ₂ O
Corundum	4.47	-5.30	-9.76	Al ₂ O ₃
Cristobalite(alpha)	0.07	-1.70	-1.77	SiO ₂
Cristobalite(beta)	-0.08	-1.70	-1.62	SiO ₂
Cronstedtite-7A	15.60	8.06	-7.54	Fe ₂ Fe ₂ Si ₂ O ₅ (OH) ₄
Daphnite-14A	3.48	7.28	3.80	Fe ₅ Al ₁ Al ₃ Si ₃ O ₁₀ (OH) ₈
Daphnite-7A	1.23	7.28	6.05	Fe ₅ Al ₁ Al ₃ Si ₃ O ₁₀ (OH) ₈
Dawsonite	-5.93	-8.08	-2.16	NaAlCO ₃ (OH) ₂
Diaspore	0.33	-2.65	-2.98	Al ₂ HO ₂
Dicalcium_silicate	-7.22	10.37	17.59	Ca ₂ SiO ₄
Diopside	-0.00	7.91	7.91	CaMgSi ₂ O ₆
Dolomite	0.00	-6.06	-6.06	CaMg(CO ₃) ₂
Dolomite-dis	-0.51	-6.06	-5.55	CaMg(CO ₃) ₂
Dolomite-ord	0.01	-6.06	-6.07	CaMg(CO ₃) ₂
Enstatite	0.00	3.57	3.57	MgSiO ₃
Epidote	8.32	3.03	-5.29	Ca ₂ FeAl ₂ Si ₃ O ₁₂ OH
Epidote-ord	8.29	3.03	-5.26	FeCa ₂ Al ₂ (OH)(SiO ₄) ₃
Epsomite	-7.40	-9.71	-2.31	MgSO ₄ ·7H ₂ O
Ettringite	-56.43	-14.09	42.33	Ca ₆ Al ₂ (SO ₄) ₃ (OH) ₁₂ ·26H ₂ O
Fayalite	0.33	5.38	5.05	Fe ₂ SiO ₄
Fe	-20.57	6.22	26.78	Fe
Fe(OH) ₂	-2.26	3.53	5.79	Fe(OH) ₂
Fe(OH) ₃	3.36	1.33	-2.03	Fe(OH) ₃
Fe ₂ (SO ₄) ₃	-10.29	-42.07	-31.78	Fe ₂ (SO ₄) ₃
FeO	-0.79	3.54	4.33	FeO
Ferrite-Ca	11.83	8.73	-3.10	CaFe ₂ O ₄
Ferrite-Dicalcium	0.56	14.76	14.20	Ca ₂ Fe ₂ O ₅
Ferrite-Mg	12.82	7.96	-4.87	MgFe ₂ O ₄
Ferrosilite	0.29	1.84	1.55	FeSiO ₃
FeSO ₄	-3.93	-11.38	-7.45	FeSO ₄
Forsterite	-0.88	8.83	9.71	Mg ₂ SiO ₄
Foshagite	-13.71	19.04	32.74	Ca ₄ Si ₃ O ₉ (OH) ₂ ·0.5H ₂ O
Gaylussite	-15.78	-4.86	10.91	CaNa ₂ (CO ₃) ₂ ·5H ₂ O
Gehlenite	-6.77	5.08	11.84	Ca ₂ Al ₂ SiO ₇
Gibbsite	-0.04	-2.66	-2.62	Al(OH) ₃
Gismondine	-46.24	-5.37	40.87	Ca ₂ Al ₄ Si ₄ O ₁₆ ·9H ₂ O
Glauberite	-11.84	-17.31	-5.47	Na ₂ Ca(SO ₄) ₂
Goethite	6.07	1.34	-4.72	FeOOH
Greenalite	0.35	7.21	6.86	Fe ₃ Si ₂ O ₅ (OH) ₄
Grossular	-2.83	7.72	10.55	Ca ₃ Al ₂ (SiO ₄) ₃
Gypsum	-0.53	-8.90	-8.37	CaSO ₄ ·2H ₂ O
Gyrolite	-6.89	6.96	13.85	Ca ₂ Si ₃ O ₇ (OH) ₂ ·1.5H ₂ O
H ₂ (g)	-16.26	-18.65	-2.39	H ₂
H ₂ O(g)	1.85	-0.01	-1.85	H ₂ O
H ₂ S(g)	-55.27	-64.26	-8.99	H ₂ S
Halite	-2.99	-2.51	0.48	NaCl
Hatrurite	-18.85	16.41	35.25	Ca ₃ SiO ₅
HCl(g)	-4.61	-5.76	-1.15	HCl

Hedenbergite	-0.90	6.18	7.08	CaFe (SiO ₃) ₂
Hematite	15.58	2.69	-12.89	Fe ₂ O ₃
Hercynite	0.58	-1.76	-2.34	FeAl ₂ O ₄
Hexahydrite	-7.68	-9.70	-2.03	MgSO ₄ ·6H ₂ O
Hillebrandite	-8.43	10.36	18.80	Ca ₂ SiO ₃ (OH) 2:0.17H ₂ O
Huntite	-1.98	-12.88	-10.90	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-8.41	-8.42	-0.02	Mg ₅ (CO ₃) ₄ (OH) 2:4H ₂ O
Hydrophilite	-6.52	-5.48	1.04	CaCl ₂
Ice	-1.35	-0.01	1.35	H ₂ O
Illite	0.91	-9.35	-10.27	K _{0.6} Mg _{0.25} Al _{1.8} Al _{0.5} Si _{3.5} O ₁₀ (OH) 2
Ilmenite	0.03	0.98	0.95	FeTiO ₃
Jadeite	-1.95	-2.79	-0.84	NaAl (SiO ₃) ₂
Jarosite	6.29	-23.55	-29.84	KFe ₃ (SO ₄) ₂ (OH) 6
Jarosite-Na	-16.83	-22.58	-5.75	NaFe ₃ (SO ₄) ₂ (OH) 6
K	-34.09	3.61	37.70	K
K (g)	-37.55	3.61	41.16	K
K-Feldspar	-0.00	-5.46	-5.46	KAlSi ₃ O ₈
K ₂ CO ₃ ·1.5H ₂ O	-17.45	-4.14	13.30	K ₂ CO ₃ ·1.5H ₂ O
K ₂ O	-43.69	4.54	48.23	K ₂ O
K ₃ H (SO ₄) ₂	-19.40	-23.03	-3.62	K ₃ H (SO ₄) ₂
K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O	-61.48	-33.92	27.56	K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O
Kainite	-12.70	-13.16	-0.46	KMgClSO ₄ ·3H ₂ O
KAl (SO ₄) ₂	-13.15	-30.22	-17.06	KAl (SO ₄) ₂
Kalcanite	-6.69	-6.41	0.28	KHCO ₃
Kalsilite	-2.19	-2.07	0.12	KAlSiO ₄
Kaolinite	0.30	-8.70	-9.00	Al ₂ Si ₂ O ₅ (OH) 4
Katoite	-65.58	12.76	78.34	Ca ₃ Al ₂ H ₁₂ O ₁₂
Kieserite	-9.35	-9.66	-0.32	MgSO ₄ ·H ₂ O
KMgCl ₃	-16.25	-9.74	6.51	KMgCl ₃
KMgCl ₃ ·2H ₂ O	-14.94	-9.75	5.19	KMgCl ₃ ·2H ₂ O
KNaCO ₃ ·6H ₂ O	-13.16	-3.20	9.96	KNaCO ₃ ·6H ₂ O
Kyanite	-0.48	-6.99	-6.51	Al ₂ SiO ₅
Lansfordite	-8.04	-3.45	4.59	MgCO ₃ ·5H ₂ O
Larnite	-7.70	10.37	18.07	Ca ₂ SiO ₄
Laumontite	0.28	-6.07	-6.35	CaAl ₂ Si ₄ O ₁₂ ·4H ₂ O
Lawrencite	-6.05	-7.98	-1.93	FeCl ₂
Lawsonite	-0.97	-2.67	-1.70	CaAl ₂ Si ₂ O ₇ (OH) 2:2H ₂ O
Leonite	-15.75	-20.06	-4.31	K ₂ Mg (SO ₄) ₂ ·4H ₂ O
Lime	-9.98	6.03	16.01	CaO
Magnesite	-0.32	-3.41	-3.09	MgCO ₃
Magnetite	16.37	6.23	-10.14	Fe ₃ O ₄
Margarite	0.35	-7.96	-8.31	CaAl ₄ Si ₂ O ₁₀ (OH) 2
Maximum Microcline	0.00	-5.46	-5.46	KAlSi ₃ O ₈
Mayenite	-114.46	35.34	149.80	Ca ₁₂ Al ₁₄ O ₃₃
Melanterite	-7.92	-11.44	-3.52	FeSO ₄ ·7H ₂ O
Mercallite	-11.21	-12.65	-1.44	KHSO ₄
Merwinite	-9.98	19.98	29.96	MgCa ₃ (SiO ₄) ₂
Mesolite	0.42	-4.23	-4.65	Na ₂ ·676Ca ₂ ·657Al ₁₁ ·99Si ₁₃ ·01O ₁₀ ·2.647H ₂ O
Mg	-51.09	7.94	59.03	Mg
Mg (g)	-58.82	7.94	66.76	Mg
Mg ₁ ·25SO ₄ (OH) 0.5:0.5H ₂ O	-1.73	-8.35	-6.61	Mg ₁ ·25SO ₄ (OH) 0.5:0.5H ₂ O
Mg ₁ ·5SO ₄ (OH)	-1.92	-7.03	-5.11	Mg ₁ ·5SO ₄ (OH)
MgCl ₂ ·2H ₂ O	-8.08	-6.27	1.82	MgCl ₂ ·2H ₂ O
MgCl ₂ ·4H ₂ O	-7.18	-6.28	0.90	MgCl ₂ ·4H ₂ O
MgCl ₂ ·H ₂ O	-8.90	-6.26	2.64	MgCl ₂ ·H ₂ O
MgOHCl	-4.69	-0.50	4.19	MgOHCl
MgSO ₄	-3.03	-9.66	-6.62	MgSO ₄
Minnesotaite	2.38	3.82	1.45	Fe ₃ Si ₄ O ₁₀ (OH) 2
Mirabilite	-19.12	-8.50	10.62	Na ₂ SO ₄ ·10H ₂ O
Misenite	-75.21	-86.28	-11.08	K ₈ H ₆ (SO ₄) ₇
Molysite	-10.04	-15.93	-5.89	FeCl ₃
Monohydrocalcite	-3.42	-2.65	0.77	CaCO ₃ ·H ₂ O
Monticellite	-2.45	9.60	12.05	CaMgSiO ₄
Montmor-Ca	2.12	-8.48	-10.60	Ca ₁ ·65Mg ₁ ·33Al ₁₁ ·67Si ₄ O ₁₀ (OH) 2
Montmor-K	1.28	-8.73	-10.01	K ₁ ·33Mg ₁ ·33Al ₁₁ ·67Si ₄ O ₁₀ (OH) 2
Montmor-Mg	2.27	-8.61	-10.88	Mg ₁ ·495Al ₁₁ ·67Si ₄ O ₁₀ (OH) 2
Montmor-Na	1.45	-8.40	-9.86	Na ₁ ·33Mg ₁ ·33Al ₁₁ ·67Si ₄ O ₁₀ (OH) 2
Mordenite	-0.01	-8.18	-8.16	Ca ₁ ·2895Na ₁ ·361Al ₁ ·94Si ₁₅ ·06O ₁₂ ·3.468H ₂ O
Mordenite-dehy	-5.84	-8.15	-2.31	Ca ₁ ·2895Na ₁ ·361Al ₁ ·94Si ₁₅ ·06O ₁₂
Muscovite	1.02	-10.77	-11.78	KAl ₃ Si ₃ O ₁₀ (OH) 2
Na	-30.81	4.59	35.40	Na
Na (g)	-35.60	4.59	40.18	Na
Na ₂ CO ₃	-9.03	-2.18	6.85	Na ₂ CO ₃
Na ₂ CO ₃ ·7H ₂ O	-19.48	-2.24	17.25	Na ₂ CO ₃ ·7H ₂ O
Na ₂ O	-32.14	6.50	38.63	Na ₂ O
Na ₂ SiO ₃	-10.48	4.80	15.28	Na ₂ SiO ₃
Na ₃ H (SO ₄) ₂	-19.21	-20.10	-0.89	Na ₃ H (SO ₄) ₂
Na ₄ Ca (SO ₄) ₃ ·2H ₂ O	-19.76	-25.75	-5.99	Na ₄ Ca (SO ₄) ₃ ·2H ₂ O
Na ₄ SiO ₄	-32.57	11.30	43.87	Na ₄ SiO ₄
Na ₆ Si ₂ O ₇	-46.50	16.09	62.59	Na ₆ Si ₂ O ₇
NaFeO ₂	-1.96	4.59	6.55	NaFeO ₂
Nahcolite	-5.51	-5.43	0.08	NaHCO ₃
Natrolite	-3.65	-3.90	-0.25	Na ₂ Al ₂ Si ₃ O ₁₀ ·2H ₂ O
Natron	-17.77	-2.26	15.51	Na ₂ CO ₃ ·10H ₂ O
Natrosilite	-9.87	3.10	12.97	Na ₂ Si ₂ O ₅
Nepheline	-2.14	-1.10	1.04	NaAlSi ₃ O ₈
Nesquehonite	-6.75	-3.44	3.31	MgCO ₃ ·3H ₂ O
Nontronite-Ca	16.44	-3.42	-19.86	Ca ₁ ·65Fe ₂ Al ₁ ·33Si ₃ ·67H ₂ O ₁₂
Nontronite-H	15.77	-4.41	-20.18	H ₁ ·33Fe ₂ Al ₁ ·33Si ₃ ·67H ₂ O ₁₂
Nontronite-K	15.45	-3.66	-19.12	K ₁ ·33Fe ₂ Al ₁ ·33Si ₃ ·67H ₂ O ₁₂
Nontronite-Mg	16.57	-3.54	-20.11	Mg ₁ ·65Fe ₂ Al ₁ ·33Si ₃ ·67H ₂ O ₁₂
Nontronite-Na	15.74	-3.34	-19.08	Na ₁ ·33Fe ₂ Al ₁ ·33Si ₃ ·67H ₂ O ₁₂
O ₂ (g)	-2.99	-5.36	-2.36	O ₂
Okenite	-6.49	2.63	9.12	CaSi ₂ O ₄ (OH) 2:2H ₂ O
Oxychloride-Mg	-20.75	4.73	25.48	Mg ₂ Cl ₂ (OH) 3:4H ₂ O
Paragonite	0.41	-9.79	-10.20	NaAl ₃ Si ₃ O ₁₀ (OH) 2
Pargasite	-2.16	18.25	20.41	NaCa ₂ Al ₃ Mg ₄ Si ₆ O ₂₂ (OH) 2
Pentahydrite	-8.06	-9.69	-1.64	MgSO ₄ ·5H ₂ O
Periclase	-3.41	5.26	8.67	MgO
Phlogopite	2.04	10.32	8.29	KAlMg ₃ Si ₃ O ₁₀ (OH) 2
Picromerite	-15.34	-20.08	-4.74	K ₂ Mg (SO ₄) ₂ ·6H ₂ O
Pirssonite	-16.06	-4.84	11.22	Na ₂ Ca (CO ₃) ₂ ·2H ₂ O
Polysialite	-23.41	-37.82	-14.41	K ₂ MgCa ₂ (SO ₄) ₄ ·2H ₂ O
Portlandite	-5.62	6.03	11.65	Ca (OH) ₂
Prehnite	-0.43	1.68	2.11	Ca ₂ Al ₂ Si ₃ O ₁₀ (OH) 2
Pseudowollastonite	-1.95	4.34	6.29	CaSiO ₃
Pyrite	-92.99	-112.64	-19.65	FeS ₂
Pyrophyllite	0.89	-12.09	-12.98	Al ₂ Si ₄ O ₁₀ (OH) 2

Pyrrhotite	-54.15	-60.72	-6.56	FeS
Quartz	0.31	-1.70	-2.00	SiO2
Rankinite	-9.44	14.71	24.15	Ca3Si2O7
Ripidolite-14A	3.87	12.46	8.59	Mg3Fe2Al2Si3O10 (OH) 8
Ripidolite-7A	1.53	12.46	10.92	Mg3Fe2Al2Si3O10 (OH) 8
Rutile	6.99	-2.56	-9.55	TiO2
S	-43.01	-66.93	-23.92	S
S2(g)	-89.22	-103.84	-14.62	S2
Sanidine_high	-0.27	-5.46	-5.20	KAlSi3O8
Saponite-Ca	3.97	9.68	5.72	Ca.165Mg3Al.33Si3.67O10 (OH) 2
Saponite-H	3.19	8.69	5.50	H.33Mg3Al.33Si3.67O10 (OH) 2
Saponite-K	2.97	9.44	6.47	K.33Mg3Al.33Si3.67O10 (OH) 2
Saponite-Mg	4.08	9.56	5.48	Mg3.165Al.33Si3.67O10 (OH) 2
Saponite-Na	3.27	9.76	6.49	Na.33Mg3Al.33Si3.67O10 (OH) 2
Scolecite	1.07	-4.37	-5.44	CaAl2Si3O10:3H2O
Sepiolite	-3.41	10.83	14.23	Mg4Si6O15 (OH) 2:6H2O
Si	-70.09	3.66	73.75	Si
Si(g)	-104.01	3.66	107.67	Si
Siderite	-0.39	-5.14	-4.74	FeCO3
Sillimanite	-0.50	-6.99	-6.50	Al2SiO5
SiO2(am)	-0.10	-1.70	-1.59	SiO2
Smectite-high-Fe-Mg	3.22	-0.23	-3.45	Ca.025Na.1K.2Fe.5Fe.2Mg1.15Al1.25Si3.5H2O12
Smectite-low-Fe-Mg	2.63	-2.63	-5.26	Ca.02Na.15K.2Fe.29Fe.16Mg.9Al1.25Si3.75H2O12
SO2(g)	-18.44	-19.40	-0.96	SO2
Spinel	-2.17	-0.03	2.14	Al2MgO4
Starkeyite	-8.49	-9.69	-1.20	MgSO4:4H2O
Stilbite	1.73	-10.79	-12.52	Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O
Sylvite	-4.11	-3.49	0.62	KCl
Syngenite	-11.62	-19.27	-7.65	K2Ca (SO4) 2:H2O
Tachyhydrite	-34.62	-18.08	16.54	Mg2CaCl6:12H2O
Talc	3.31	9.00	5.69	Mg3Si4O10 (OH) 2
Thenardite	-4.91	-8.42	-3.51	Na2SO4
Thermonatrite	-10.40	-2.19	8.21	Na2CO3:H2O
Ti	-146.60	2.80	149.40	Ti
Ti(g)	-221.65	2.80	224.45	Ti
Ti2O3	-45.62	-2.43	43.19	Ti2O3
Ti3O5	-39.94	-4.99	34.96	Ti3O5
TiC	-182.48	-0.52	181.96	TiC
TiCl2	-82.48	-11.39	71.09	TiCl2
TiCl3	-57.98	-18.49	39.48	TiCl3
TiCl4(g)	-53.84	-25.59	28.25	TiCl4
TiO(alpha)	-61.11	0.12	61.23	TiO
TiO(g)	-145.55	0.12	145.67	TiO
Titanite	-717.85	1.78	719.63	CaTiSiO5
Tobermorite-11A	-16.98	19.96	36.94	Ca5Si6H11O22.5
Tobermorite-14A	-22.31	19.92	42.23	Ca5Si6H21O27.5
Tobermorite-9A	-16.03	19.98	36.01	Ca5Si6H6O20
Tremolite	4.31	24.82	20.50	Ca2Mg5Si8O22 (OH) 2
Tridymite	-0.51	-1.70	-1.18	SiO2
Troilite	-54.08	-60.72	-6.64	FeS
Trona-K	-21.07	-9.58	11.49	K2NaH (CO3) 2:2H2O
Wairakite	0.77	-6.06	-6.83	CaAl2Si4O10 (OH) 4
Wollastonite	-1.95	4.34	6.29	CaSiO3
Wustite	-0.32	3.12	3.44	Fe.9470
Xonotlite	-26.24	26.03	52.27	Ca6Si6O17 (OH) 2
Zoisite	-0.08	-0.97	-0.88	Ca2Al3 (SiO4) 3OH

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

TIME STEP 5 HOURS

Reaction step 5.

WARNING: No data for rate Magnetite in KINETICS keyword.

Using solution 1. Sileri 2300p10
Using pure phase assemblage 1. Reservoir
Using kinetics 1.

Kinetics 1.

Time step: 3600 seconds (Incremented time: 18000 seconds)

Rate name	Delta	Moles	Total Moles	Reactant	Coefficient
Quartz	4.596e-02	4.298e+01		SiO2	1
Anorthite	2.055e-03	2.550e+01		CaAl2 (SiO4) 2	1
Albite	-3.730e-03	2.252e+01		NaAlSi3O8	1
K-Feldspar	-3.831e-04	1.312e+01		KAlSi3O8	1
Diopside	-1.877e-02	3.706e+00		CaMgSi2O6	1
Enstatite	1.216e-03	3.375e+01		MgSiO3	1
Ilmenite	1.450e-04	1.739e+00		FeTiO3	1
Actinolite	-5.390e-05	1.470e+00		Ca2Mg2.5Fe2.5Si8O22 (OH) 2	1
Calcite	-0.000e+00	0.000e+00		CaCO3	1
Dolomite	1.829e-02	4.044e-01		CaMg (CO3) 2	1
Magnesite	-0.000e+00	0.000e+00		MgCO3	1

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

Phase	SI	log IAP	log K(T, P)	Initial	Moles in assemblage	
					Final	Delta
CO2(g)	1.65	-0.42	-2.07	0.000e+00	0	0.000e+00

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

Elements	Molality	Moles
Al	2.203e-05	2.203e-05
C	3.973e-01	3.972e-01
Ca	3.981e-03	3.981e-03
Cl	1.925e-01	1.925e-01
Fe	2.949e-05	2.949e-05
K	1.651e-02	1.651e-02
Mg	3.712e-03	3.712e-03
Na	1.657e-01	1.657e-01
S	3.036e-03	3.036e-03
Si	1.129e-02	1.129e-02

Ti		1.142e-03	1.142e-03				
-----Description of solution-----							
		pH	=	5.088	Charge balance		
		pe	=	4.814	Adjusted to redox equilibrium		
		Density (g/cm³)	=	0.72996			
		Volume (L)	=	1.41113			
		Activity of water	=	0.988			
		Ionic strength (mol/kgw)	=	1.446e-01			
		Mass of water (kg)	=	9.999e-01			
		Total alkalinity (eq/kg)	=	4.274e-04			
		Total CO2 (mol/kg)	=	3.973e-01			
		Temperature (°C)	=	300.00			
		Pressure (atm)	=	223.00			
		Electrical balance (eq)	=	-1.241e-03			
Percent error, 100*(Cat-[An])/([Cat+[An])			=	-0.43			
		Iterations	=	256			
		Total H	=	1.110499e+02			
		Total O	=	5.635666e+01			
-----Distribution of species-----							
	Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	
						mole V cm³/mol	
Al	H+	1.289e-05	8.174e-06	-4.890	-5.088	-0.198	0.00
	OH-	1.417e-06	7.032e-07	-5.849	-6.153	-0.304	(0)
	H2O	5.553e+01	9.876e-01	1.744	-0.005	0.000	24.39
	NaAlO2	9.903e-06	9.903e-06	-5.004	-5.004	0.000	(0)
	AlO2-	6.111e-06	3.134e-06	-5.214	-5.504	-0.290	(0)
	HALO2	6.007e-06	6.007e-06	-5.221	-5.221	0.000	(0)
	Al(OH)2+	6.848e-09	3.512e-09	-8.164	-8.454	-0.290	(0)
	AlOH+2	6.814e-12	5.310e-13	-11.167	-12.275	-1.108	(0)
	Al+3	9.895e-17	1.646e-18	-16.005	-17.784	-1.779	(0)
	AlSO4+	2.915e-20	1.495e-20	-19.535	-19.825	-0.290	(0)
	Al(SO4)2-	2.009e-23	1.030e-23	-22.697	-22.987	-0.290	(0)
	Al2(OH)2+4	1.194e-29	1.016e-33	-28.923	-32.993	-4.070	(0)
	Al3(OH)4+5	0.000e+00	0.000e+00	-40.594	-46.703	-6.109	(0)
	Al13O4(OH)24+7	0.000e+00	0.000e+00	-153.893	-165.867	-11.974	(0)
	C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-118.943	-118.943	0.000	(0)	
C(-3)	0.000e+00						
C2H6	0.000e+00	0.000e+00	-103.114	-103.114	0.000	(0)	
C(-4)	0.000e+00						
CH4	0.000e+00	0.000e+00	-64.096	-64.096	0.000	(0)	
C(2)	2.717e-21	2.717e-21	-20.566	-20.566	0.000	(0)	
CO	3.973e-01						
C(4)	3.973e-01						
CO2	3.710e-01	3.836e-01	-0.431	-0.416	0.014	145.38	
(CO2)2	1.285e-02	1.328e-02	-1.891	-1.877	0.014	290.77	
HCO3-	2.776e-04	1.424e-04	-3.557	-3.847	-0.290	(0)	
CaHCO3+	2.592e-04	1.329e-04	-3.586	-3.876	-0.290	(0)	
MgHCO3+	4.094e-05	2.100e-05	-4.388	-4.678	-0.290	(0)	
CaCO3	2.654e-07	2.654e-07	-6.576	-6.576	0.000	(0)	
FeHCO3+	7.651e-08	3.924e-08	-7.116	-7.406	-0.290	(0)	
NaHCO3	5.775e-08	5.775e-08	-7.238	-7.238	0.000	(0)	
MgCO3	4.131e-09	4.131e-09	-8.384	-8.384	0.000	(0)	
CO3-2	7.972e-10	6.212e-11	-9.098	-10.207	-1.108	(0)	
FeCO3	2.304e-11	2.304e-11	-10.638	-10.638	0.000	(0)	
FeCO3+	8.432e-13	4.324e-13	-12.074	-12.364	-0.290	(0)	
NaCO3-	2.528e-15	1.296e-15	-14.597	-14.887	-0.290	(0)	
Ca	3.981e-03						
CaCl+	1.350e-03	6.925e-04	-2.870	-3.160	-0.290	(0)	
Ca+2	1.242e-03	1.309e-04	-2.906	-3.883	-0.977	(0)	
CaCl2	9.594e-04	9.594e-04	-3.018	-3.018	0.000	(0)	
CaHCO3+	2.592e-04	1.329e-04	-3.586	-3.876	-0.290	(0)	
CaSO4	1.697e-04	1.697e-04	-3.770	-3.770	0.000	(0)	
CaCO3	2.654e-07	2.654e-07	-6.576	-6.576	0.000	(0)	
CaOH+	4.886e-12	2.506e-12	-11.311	-11.601	-0.290	(0)	
Cl(-1)	1.925e-01						
Cl-	1.428e-01	6.837e-02	-0.845	-1.165	-0.320	(0)	
NaCl	4.281e-02	4.281e-02	-1.368	-1.368	0.000	(0)	
KCl	2.421e-03	2.421e-03	-2.616	-2.616	0.000	(0)	
CaCl+	1.350e-03	6.925e-04	-2.870	-3.160	-0.290	(0)	
MgCl+	1.129e-03	5.790e-04	-2.947	-3.237	-0.290	(0)	
CaCl2	9.594e-04	9.594e-04	-3.018	-3.018	0.000	(0)	
FeCl+	1.870e-05	9.589e-06	-4.728	-5.018	-0.290	(0)	
HCl	1.605e-05	1.605e-05	-4.795	-4.795	0.000	(0)	
FeCl4-2	5.218e-06	3.609e-07	-5.282	-6.443	-1.160	(0)	
FeCl2	5.016e-07	5.016e-07	-6.300	-6.300	0.000	(0)	
FeCl4+2	4.144e-09	3.229e-10	-8.383	-9.491	-1.108	(0)	
FeCl2+	3.415e-14	1.751e-14	-13.467	-13.757	-0.290	(0)	
FeCl4-	1.919e-19	9.842e-20	-18.717	-19.007	-0.290	(0)	
Cl(1)	5.722e-13						
HClO	5.686e-13	5.686e-13	-12.245	-12.245	0.000	(0)	
ClO-	3.657e-15	1.876e-15	-14.437	-14.727	-0.290	(0)	
Cl(3)	3.134e-22						
ClO2-	3.115e-22	1.597e-22	-21.507	-21.797	-0.290	(0)	
HClO2	1.930e-24	1.930e-24	-23.714	-23.714	0.000	(0)	
Cl(5)	4.846e-22						
ClO3-	4.846e-22	2.405e-22	-21.315	-21.619	-0.304	(0)	
Cl(7)	3.187e-25						
ClO4-	3.187e-25	1.582e-25	-24.497	-24.801	-0.304	(0)	
Fe(2)	2.948e-05						
FeCl+	1.870e-05	9.589e-06	-4.728	-5.018	-0.290	(0)	
FeCl4-2	5.218e-06	3.609e-07	-5.282	-6.443	-1.160	(0)	
Fe+2	4.986e-06	5.252e-07	-5.302	-6.280	-0.977	(0)	
FeCl2	5.016e-07	5.016e-07	-6.300	-6.300	0.000	(0)	
FeHCO3+	7.651e-08	3.924e-08	-7.116	-7.406	-0.290	(0)	
FeSO4	7.388e-10	7.388e-10	-9.131	-9.131	0.000	(0)	
FeOH+	4.390e-11	2.251e-11	-10.358	-10.648	-0.290	(0)	
FeCO3	2.304e-11	2.304e-11	-10.638	-10.638	0.000	(0)	
Fe(OH)2	2.424e-17	2.424e-17	-16.615	-16.615	0.000	(0)	
Fe(OH)3-	2.551e-22	1.308e-22	-21.593	-21.883	-0.290	(0)	
Fe(OH)4-2	2.564e-31	1.773e-32	-30.591	-31.751	-1.160	(0)	
Fe(3)	9.455e-09						

FeCl+2	4.144e-09	3.229e-10	-8.383	-9.491	-1.108	(0)
FeSO4+	2.799e-09	1.435e-09	-8.553	-8.843	-0.290	(0)
Fe (OH) 2+	2.128e-09	1.091e-09	-8.672	-8.962	-0.290	(0)
FeOH+2	3.120e-10	2.431e-11	-9.506	-10.614	-1.108	(0)
Fe (OH) 3	6.919e-11	6.919e-11	-10.160	-10.160	0.000	(0)
Fe+3	1.670e-12	2.778e-14	-11.777	-13.556	-1.779	(0)
FeCO3+	8.432e-13	4.324e-13	-12.074	-12.364	-0.290	(0)
FeCl2+	3.415e-14	1.751e-14	-13.467	-13.757	-0.290	(0)
Fe (OH) 4-	4.594e-15	2.356e-15	-14.338	-14.628	-0.290	(0)
Fe2 (OH) 2+4	1.869e-16	1.591e-20	-15.728	-19.798	-4.070	(0)
FeCl4-	1.919e-19	9.842e-20	-18.717	-19.007	-0.290	(0)
Fe (SO4) 2-	6.980e-21	3.580e-21	-20.156	-20.446	-0.290	(0)
Fe3 (OH) 4+5	4.662e-21	3.628e-27	-20.331	-26.440	-6.109	(0)
H (0)	4.164e-19					
H2	2.082e-19	2.259e-19	-18.682	-18.646	0.035	(0)
K	1.651e-02					
K+	1.395e-02	6.677e-03	-1.855	-2.175	-0.320	(0)
KCl	2.421e-03	2.421e-03	-2.616	-2.616	0.000	(0)
KSO4-	1.345e-04	6.899e-05	-3.871	-4.161	-0.290	(0)
KHSO4	4.827e-06	4.827e-06	-5.316	-5.316	0.000	(0)
KOH	3.139e-12	3.139e-12	-11.503	-11.503	0.000	(0)
Mg	3.712e-03					
MgSO4	2.387e-03	2.387e-03	-2.622	-2.622	0.000	(0)
MgCl+	1.129e-03	5.790e-04	-2.947	-3.237	-0.290	(0)
Mg+2	1.552e-04	2.220e-05	-3.809	-4.654	-0.844	(0)
MgHCO3+	4.094e-05	2.100e-05	-4.388	-4.678	-0.290	(0)
MgCO3	4.131e-09	4.131e-09	-8.384	-8.384	0.000	(0)
Mg4 (OH) 4+4	1.714e-34	1.459e-38	-33.766	-37.836	-4.070	(0)
Na	1.657e-01					
Na+	1.229e-01	6.303e-02	-0.910	-1.200	-0.290	(0)
NaCl	4.281e-02	4.281e-02	-1.368	-1.368	0.000	(0)
NaAlO2	9.903e-06	9.903e-06	-5.004	-5.004	0.000	(0)
NaSO4-	7.208e-06	3.696e-06	-5.142	-5.432	-0.290	(0)
NaHSiO3	1.545e-06	1.545e-06	-5.811	-5.811	0.000	(0)
NaOH	1.082e-06	1.082e-06	-5.966	-5.966	0.000	(0)
NaHCO3	5.775e-08	5.775e-08	-7.238	-7.238	0.000	(0)
NaCO3-	2.528e-15	1.296e-15	-14.597	-14.887	-0.290	(0)
O (0)	8.145e-06					
O2	4.072e-06	4.419e-06	-5.390	-5.355	0.035	(0)
S (-2)	0.000e+00					
H2S	0.000e+00	0.000e+00	-57.028	-57.028	0.000	(0)
HS-	0.000e+00	0.000e+00	-59.174	-59.478	-0.304	(0)
S-2	0.000e+00	0.000e+00	-60.899	-61.960	-1.061	(0)
S2-2	0.000e+00	0.000e+00	-106.372	-107.532	-1.160	(0)
S3-2	0.000e+00	0.000e+00	-148.989	-150.149	-1.160	(0)
S4-2	0.000e+00	0.000e+00	-191.713	-192.873	-1.160	(0)
S5-2	0.000e+00	0.000e+00	-234.559	-235.720	-1.160	(0)
S (2)	0.000e+00					
S2O3-2	0.000e+00	0.000e+00	-62.890	-64.051	-1.160	(0)
HS2O3-	0.000e+00	0.000e+00	-67.834	-68.124	-0.290	(0)
S (3)	0.000e+00					
S2O4-2	0.000e+00	0.000e+00	-59.492	-60.553	-1.061	(0)
S (4)	2.828e-20					
SO2	1.984e-20	1.984e-20	-19.703	-19.703	0.000	(0)
HSO3-	8.438e-21	4.327e-21	-20.074	-20.364	-0.290	(0)
SO3-2	1.222e-25	9.521e-27	-24.913	-26.021	-1.108	(0)
H2SO3	1.039e-27	1.039e-27	-26.983	-26.983	0.000	(0)
S2O6-2	5.879e-34	4.066e-35	-33.231	-34.391	-1.160	(0)
S3O6-2	0.000e+00	0.000e+00	-77.905	-79.065	-1.160	(0)
S4O6-2	0.000e+00	0.000e+00	-110.972	-112.132	-1.160	(0)
S5O6-2	0.000e+00	0.000e+00	-165.593	-166.753	-1.160	(0)
S (5)	0.000e+00					
S2O5-2	0.000e+00	0.000e+00	-45.697	-46.857	-1.160	(0)
S (6)	3.036e-03					
MgSO4	2.387e-03	2.387e-03	-2.622	-2.622	0.000	(0)
HSO4-	2.046e-04	1.049e-04	-3.689	-3.979	-0.290	(0)
CaSO4	1.697e-04	1.697e-04	-3.770	-3.770	0.000	(0)
KSO4-	1.345e-04	6.899e-05	-3.871	-4.161	-0.290	(0)
SO4-2	1.283e-04	8.878e-06	-3.892	-5.052	-1.160	(0)
NaSO4-	7.208e-06	3.696e-06	-5.142	-5.432	-0.290	(0)
KHSO4	4.827e-06	4.827e-06	-5.316	-5.316	0.000	(0)
FeSO4+	2.799e-09	1.435e-09	-8.553	-8.843	-0.290	(0)
FeSO4	7.388e-10	7.388e-10	-9.131	-9.131	0.000	(0)
H2SO4	5.652e-17	5.652e-17	-16.248	-16.248	0.000	(0)
AlSO4+	2.915e-20	1.495e-20	-19.535	-19.825	-0.290	(0)
Fe (SO4) 2-	6.980e-21	3.580e-21	-20.156	-20.446	-0.290	(0)
Al (SO4) 2-	2.009e-23	1.030e-23	-22.697	-22.987	-0.290	(0)
S (7)	7.384e-25					
S2O8-2	3.692e-25	2.553e-26	-24.433	-25.593	-1.160	(0)
S (8)	1.786e-16					
HSO5-	1.786e-16	9.161e-17	-15.748	-16.038	-0.290	(0)
Si	1.129e-02					
SiO2	1.128e-02	1.128e-02	-1.948	-1.948	0.000	(0)
NaHSiO3	1.545e-06	1.545e-06	-5.811	-5.811	0.000	(0)
HSiO3-	1.173e-06	6.017e-07	-5.931	-6.221	-0.290	(0)
H6 (H2SiO4) 4-2	1.826e-10	1.263e-11	-9.738	-10.899	-1.160	(0)
H2SiO4-2	3.287e-14	2.273e-15	-13.483	-14.643	-1.160	(0)
H4 (H2SiO4) 4-4	4.141e-19	9.474e-24	-18.383	-23.023	-4.641	(0)
Ti	1.142e-03					
Ti (OH) 4	1.142e-03	1.142e-03	-2.942	-2.942	0.000	(0)

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

Phase	SI**	log IAP	log K (573 K, 223 atm)	
Actinolite	-0.00	20.50	20.50	Ca2Mg2.5Fe2.5Si8O22 (OH) 2
Afwillite	-16.92	14.95	31.87	Ca3Si2O4 (OH) 6
Akermanite	-4.75	14.19	18.95	Ca2MgSi2O7
Al	-65.72	1.49	67.21	Al
Al (g)	-89.13	1.49	90.62	Al
Al2 (SO4) 3	-25.11	-50.72	-25.62	Al2 (SO4) 3
Al2 (SO4) 3:6H2O	-23.27	-50.76	-27.48	Al2 (SO4) 3:6H2O
Albite	-0.00	-4.49	-4.48	NaAlSi3O8
Albite high	-0.40	-4.49	-4.09	NaAlSi3O8
Albite_low	-0.01	-4.49	-4.48	NaAlSi3O8
Alum-K	-18.39	-30.13	-11.74	KAl (SO4) 2:12H2O
Alunite	-5.29	-35.14	-29.84	KAl3 (OH) 6 (SO4) 2
Amesite-14A	4.55	8.03	3.48	Mg4Al4Si2O10 (OH) 8

Analcime	-0.50	-2.68	-2.18	Na.96Al.96Si2.0406:H2O
Analcime-dehy	-3.21	-2.67	0.54	Na.96Al.96Si2.0406
Anatase	5.53	-2.93	-8.46	TiO2
Andalusite	-0.41	-7.01	-6.60	Al2SiO5
Andradite	13.59	16.41	2.82	Ca3Fe2(SiO4)3
Anhydrite	0.99	-8.94	-9.92	CaSO4
Ankerite	-0.28	-7.19	-6.92	CaMg0.3Fe0.7(CO3)2
Annite	2.36	6.20	3.84	KFe3AlSi3O10(OH)2
Anorthite	0.02	-2.67	-2.68	CaAl2(SiO4)2
Antarcticite	-10.04	-6.25	3.79	CaCl2:6H2O
Anthophyllite	3.04	23.03	19.99	Mg7Si8O22(OH)2
Antigorite	24.66	198.39	173.73	Mg48Si34O85(OH)62
Aphthalite	-13.94	-17.83	-3.89	NaK3(SO4)2
Aragonite	-0.61	-2.64	-2.03	CaCO3
Arcanite	-5.91	-9.40	-3.49	K2SO4
Artinite	-5.78	2.08	7.86	Mg2CO3(OH)2:3H2O
Bassanite	0.28	-8.94	-9.21	CaSO4:0.5H2O
Beidellite-Ca	1.02	-12.01	-13.02	Ca.165Al2.33Si3.67O10(OH)2
Beidellite-H	0.20	-13.05	-13.24	H.33Al2.33Si3.67O10(OH)2
Beidellite-K	0.19	-12.09	-12.28	K.33Al2.33Si3.67O10(OH)2
Beidellite-Mg	1.15	-12.14	-13.28	Mg.165Al2.33Si3.67O10(OH)2
Beidellite-Na	0.48	-11.76	-12.25	Na.33Al2.33Si3.67O10(OH)2
Bischofite	-11.11	-7.02	4.09	MgCl2:6H2O
Bloedite	-14.50	-17.18	-2.68	Na2Mg(SO4)2:4H2O
Boehmite	0.34	-2.53	-2.87	AlO2H
Brucite	-1.59	5.51	7.10	Mg(OH)2
Burkeite	-25.55	-16.07	9.49	Na6CO3(SO4)2
C	-31.66	-3.57	28.09	C
C(g)	-89.42	-3.57	85.84	C
Ca	-60.70	8.96	69.67	Ca
Ca(g)	-71.34	8.96	80.30	Ca
Ca-Al_Pyroxene	-3.26	-0.72	2.54	CaAl2SiO6
Ca2Al2O5:8H2O	-51.45	7.47	58.92	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-26.08	0.06	26.14	Ca2Cl2(OH)2:H2O
Ca3Al2O6	-28.98	13.80	42.78	Ca3Al2O6
Ca4Al2Fe2O10	-20.47	23.48	43.95	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-86.24	20.02	106.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-82.40	19.98	102.38	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-54.82	12.56	67.38	Ca4Cl2(OH)6:13H2O
CaAl2O4	-6.58	1.23	7.81	CaAl2O4
CaAl2O4:10H2O	-36.12	1.17	37.29	CaAl2O4:10H2O
CaAl4O7	-10.52	-3.83	6.69	CaAl4O7
Calcite	-0.44	-2.64	-2.20	CaCO3
Carnallite	-14.33	-10.36	3.97	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	0.32	-8.94	-9.26	CaSO4:0.5H2O
Celadonite	0.20	-1.90	-2.10	KMgAlSi4O10(OH)2
CH4(g)	-61.60	-64.10	-2.49	CH4
Chalcedony	-0.08	-1.95	-1.86	SiO2
Chamosite-7A	1.42	0.76	-0.66	Fe2Al2SiO5(OH)4
Chloromagnesite	-11.79	-6.98	4.80	MgCl2
Chrysotile	1.03	12.64	11.62	Mg3Si2O5(OH)4
Cl2(g)	-11.50	-15.18	-3.67	Cl2
Clinocllore-14A	4.63	16.66	12.03	Mg5Al2Si3O10(OH)8
Clinocllore-7A	2.27	16.66	14.39	Mg5Al2Si3O10(OH)8
Clinoptilolite-Ca	2.78	-26.16	-28.94	Ca1.7335Al3.45Fe.017Si14.533O36:10.922H2O
Clinoptilolite-dehy-Ca	-11.68	-26.10	-14.42	Ca1.7335Al3.45Fe.017Si14.533O36
Clinoptilolite-dehy-K	-20.69	-26.91	-6.22	K3.467Al3.45Fe.017Si14.533O36
Clinoptilolite-dehy-Na	-17.10	-23.53	-6.43	Na3.467Al3.45Fe.017Si14.533O36
Clinoptilolite-hy-Ca	1.98	-26.17	-28.15	Ca1.7335Al3.45Fe.017Si14.533O36:11.645H2O
Clinoptilolite-hy-K	-3.34	-26.95	-23.62	K3.467Al3.45Fe.017Si14.533O36:7.499H2O
Clinoptilolite-hy-Na	-2.73	-23.59	-20.86	Na3.467Al3.45Fe.017Si14.533O36:10.877H2O
Clinoptilolite-K	-6.59	-26.97	-20.39	K3.467Al3.45Fe.017Si14.533O36:10.922H2O
Clinoptilolite-Na	-2.77	-23.59	-20.82	Na3.467Al3.45Fe.017Si14.533O36:10.922H2O
Clinozoisite	0.03	-0.86	-0.89	Ca2Al3Si3O12(OH)
CO(g)	-18.39	-20.57	-2.17	CO
CO2(g)	1.65	-0.42	-2.07	CO2
Coesite	-0.40	-1.95	-1.55	SiO2
Cordierite_anhyd	-0.60	-8.82	-8.22	Mg2Al4Si5O18
Cordierite_hydr	0.22	-8.83	-9.05	Mg2Al4Si5O18:H2O
Corundum	4.70	-5.06	-9.76	Al2O3
Cristobalite(alpha)	-0.18	-1.95	-1.77	SiO2
Cristobalite(beta)	-0.33	-1.95	-1.62	SiO2
Cronstedtite-7A	16.76	9.22	-7.54	Fe2Fe2SiO5(OH)4
Daphnite-14A	4.73	8.53	3.80	Fe5AlAlSi3O10(OH)8
Daphnite-7A	2.48	8.53	6.05	Fe5AlAlSi3O10(OH)8
Dawsonite	-5.42	-7.58	-2.16	NaAlCO3(OH)2
Diaspore	0.45	-2.53	-2.98	AlHO2
Dicalcium_silicate	-6.97	10.63	17.59	Ca2SiO4
Diopside	-0.00	7.91	7.91	CaMgSi2O6
Dolomite	0.00	-6.06	-6.06	CaMg(CO3)2
Dolomite-dis	-0.51	-6.06	-5.55	CaMg(CO3)2
Dolomite-ord	0.01	-6.06	-6.07	CaMg(CO3)2
Enstatite	0.00	3.57	3.57	MgSiO3
Epidote	8.66	3.37	-5.29	Ca2FeAl2Si3O12OH
Epidote-ord	8.62	3.37	-5.26	FeCa2Al2(OH)(SiO4)3
Epsomite	-7.43	-9.74	-2.31	MgSO4:7H2O
Etringite	-55.51	-13.18	42.33	Ca6Al2(SO4)3(OH)12:26H2O
Fayalite	0.78	5.83	5.05	Fe2SiO4
Fe	-20.22	6.57	26.78	Fe
Fe(OH)2	-1.90	3.88	5.79	Fe(OH)2
Fe(OH)3	3.72	1.69	-2.03	Fe(OH)3
Fe2(SO4)3	-10.49	-42.27	-31.78	Fe2(SO4)3
FeO	-0.44	3.89	4.33	FeO
Ferrite-Ca	12.79	9.68	-3.10	CaFe2O4
Ferrite-Dicalcium	1.77	15.97	14.20	Ca2Fe2O5
Ferrite-Mg	13.78	8.91	-4.87	MgFe2O4
Ferrosilite	0.39	1.94	1.55	FeSiO3
FeSO4	-3.88	-11.33	-7.45	FeSO4
Forsterite	-0.63	9.08	9.71	Mg2SiO4
Foshagite	-13.45	19.30	32.74	Ca4Si3O9(OH)2:0.5H2O
Gaylussite	-14.74	-3.83	10.91	CaNa2(CO3)2:5H2O
Gehlenite	-6.28	5.57	11.84	Ca2Al2SiO7
Gibbsite	0.00	-2.54	-2.62	Al(OH)3
Gismondine	-46.25	-5.38	40.87	Ca22Al4Si4O16:9H2O
Glauberite	-10.92	-16.39	-5.47	Na2Ca(SO4)2
Goethite	6.42	1.70	-4.72	FeOOH
Greenalite	0.90	7.76	6.86	Fe3Si2O5(OH)4
Grossular	-2.59	7.96	10.55	Ca3Al2(SiO4)3

Gypsum	-0.58	-8.95	-8.37	CaSO4:2H2O
Gyrolite	-7.13	6.72	13.85	Ca2Si3O7(OH)2:1.5H2O
H2(g)	-16.26	-18.65	-2.39	H2
H2O(g)	1.85	-0.01	-1.85	H2O
H2S(g)	-55.57	-64.57	-8.99	H2S
Halite	-2.85	-2.37	0.48	NaCl
Hatrurite	-18.34	16.91	35.25	Ca3SiO5
HCl(g)	-5.10	-6.25	-1.15	HCl
Hedenbergite	-0.80	6.28	7.08	CaFe(SiO3)2
Hematite	16.28	3.40	-12.89	Fe2O3
Hercynite	1.17	-1.17	-2.34	FeAl2O4
Hexahydrite	-7.71	-9.74	-2.03	MgSO4:6H2O
Hillebrandite	-8.18	10.62	18.80	Ca2SiO3(OH)2:0.17H2O
Huntite	-1.98	-12.88	-10.90	CaMg3(CO3)4
Hydromagnesite	-8.15	-8.16	-0.02	Mg5(CO3)4(OH)2:4H2O
Hydrophillite	-7.25	-6.21	1.04	CaCl2
Ice	-1.35	-0.01	1.35	H2O
Illite	0.75	-9.51	-10.27	K0.6Mg0.25Al1.8Al0.5Si3.5O10(OH)2
Ilmenite	0.00	0.96	0.95	FeTiO3
Jadeite	-1.70	-2.54	-0.84	NaAl(SiO3)2
Jarosite	7.39	-22.46	-29.84	KFe3(SO4)2(OH)6
Jarosite-Na	-15.73	-21.48	-5.75	NaFe3(SO4)2(OH)6
K	-33.45	4.25	37.70	K
K(g)	-36.91	4.25	41.16	K
K-Feldspar	-0.00	-5.46	-5.46	KAlSi3O8
K2CO3:1.5H2O	-16.42	-3.12	13.30	K2CO3:1.5H2O
K2O	-42.41	5.82	48.23	K2O
K3H(SO4)2	-18.09	-21.72	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-57.88	-30.32	27.56	K8H4(CO3)6:3H2O
Kainite	-12.60	-13.06	-0.46	KMgClSO4:3H2O
KAl(SO4)2	-13.00	-30.06	-17.06	KAl(SO4)2
Kallicinite	-6.31	-6.02	0.28	KRCO3
Kalsilite	-1.68	-1.57	0.12	KAlSiO4
Kaolinite	0.04	-8.96	-9.00	Al2Si2O5(OH)4
Katoite	-64.58	13.77	78.34	Ca3Al2Si2H2O12
Kieserite	-9.39	-9.71	-0.32	MgSO4:H2O
KMgCl3	-16.84	-10.32	6.51	KMgCl3
KMgCl3:2H2O	-15.52	-10.34	5.19	KMgCl3:2H2O
KNaCO3:6H2O	-12.13	-2.17	9.96	KNaCO3:6H2O
Kyanite	-0.49	-7.01	-6.51	Al2SiO5
Lansfordite	-8.03	-3.44	4.59	MgCO3:5H2O
Larnite	-7.45	10.63	18.07	Ca2SiO4
Laumontite	-0.23	-6.58	-6.35	CaAl2Si4O12:4H2O
Lawrencite	-6.68	-8.61	-1.93	FeCl2
Lawsonite	-0.98	-2.68	-1.70	CaAl2Si2O7(OH)2:H2O
Leonite	-14.82	-19.13	-4.31	K2Mg(SO4)2:4H2O
Lime	-9.73	6.29	16.01	CaO
Magnesite	-0.32	-3.41	-3.09	MgCO3
Magnetite	17.43	7.29	-10.14	Fe3O4
Margarite	0.58	-7.73	-8.31	CaAl4Si2O10(OH)2
Maximum Microcline	0.00	-5.46	-5.46	KAlSi3O8
Mayenite	-109.77	40.03	149.80	Ca12Al14O33
Melanterite	-7.85	-11.37	-3.52	FeSO4:7H2O
Mercallite	-10.88	-12.31	-1.44	KHSO4
Merwinite	-9.48	20.48	29.96	MgCa3(SiO4)2
Mesolite	0.50	-4.15	-4.65	Na.676Ca.657Al1.99Si3.01O10:2.647H2O
Mg	-50.84	8.19	59.03	Mg
Mg(g)	-58.57	8.19	66.76	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-1.72	-8.33	-6.61	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-1.84	-6.95	-5.11	Mg1.5SO4(OH)
MgCl2:2H2O	-8.81	-6.99	1.82	MgCl2:2H2O
MgCl2:4H2O	-7.90	-7.01	0.90	MgCl2:4H2O
MgCl2:H2O	-9.63	-6.99	2.64	MgCl2:H2O
MgOHCl	-4.92	-0.74	4.19	MgOHCl
MgSO4	-3.08	-9.71	-6.62	MgSO4
Minnesotaite	2.43	3.87	1.45	Fe3Si4O10(OH)2
Mirabilite	-18.12	-7.51	10.62	Na2SO4:10H2O
Misenite	-72.22	-83.29	-11.08	K8H6(SO4)7
Molybite	-11.16	-17.05	-5.89	FeCl3
Monohydrocalcite	-3.41	-2.65	0.77	CaCO3:H2O
Monticellite	-2.20	9.85	12.05	CaMgSiO4
Montmor-Ca	1.44	-9.16	-10.60	Ca.165Mg.33Al1.67Si4O10(OH)2
Montmor-K	0.77	-9.24	-10.01	K.33Mg.33Al1.67Si4O10(OH)2
Montmor-Mg	1.59	-9.29	-10.88	Mg.495Al1.67Si4O10(OH)2
Montmor-Na	0.94	-8.92	-9.86	Na.33Mg.33Al1.67Si4O10(OH)2
Mordenite	-0.86	-9.03	-8.16	Ca.2895Na.361Al.94Si5.06O12:3.468H2O
Mordenite-dehy	-6.70	-9.01	-2.31	Ca.2895Na.361Al.94Si5.06O12
Muscovite	1.26	-10.53	-11.78	KAl3Si3O10(OH)2
Na	-30.18	5.22	35.40	Na
Na(g)	-34.96	5.22	40.18	Na
Na2CO3	-8.01	-1.16	6.85	Na2CO3
Na2CO3:7H2O	-18.44	-1.20	17.25	Na2CO3:7H2O
Na2O	-30.86	7.77	38.63	Na2O
Na2SiO3	-9.46	5.82	15.28	Na2SiO3
Na3H(SO4)2	-17.90	-18.79	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-17.86	-23.85	-5.99	Na4Ca(SO4)3:2H2O
Na4SiO4	-30.28	13.59	43.87	Na4SiO4
Na6Si2O7	-43.18	19.41	62.59	Na6Si2O7
NaFeO2	-0.97	5.58	6.55	NaFeO2
Nahcolite	-5.13	-5.05	0.08	NaHCO3
Natrolite	-2.89	-3.14	-0.25	Na2Al2Si3O10:2H2O
Natron	-16.72	-1.21	15.51	Na2CO3:10H2O
Natrosilite	-9.10	3.87	12.97	Na2Si2O5
Nepheline	-1.63	-0.59	1.04	NaAlSiO4
Nesquehonite	-6.74	-3.43	3.31	MgCO3:3H2O
Nontronite-Ca	16.31	-3.55	-19.86	Ca.165Fe2Al.33Si3.67H2O12
Nontronite-H	15.59	-4.59	-20.18	H.33Fe2Al.33Si3.67H2O12
Nontronite-K	15.49	-3.63	-19.12	K.33Fe2Al.33Si3.67H2O12
Nontronite-Mg	16.43	-3.68	-20.11	Mg.165Fe2Al.33Si3.67H2O12
Nontronite-Na	15.77	-3.31	-19.08	Na.33Fe2Al.33Si3.67H2O12
O2(g)	-2.99	-5.35	-2.36	O2
Okenite	-6.74	2.38	9.12	CaSi2O4(OH)2:H2O
Oxychloride-Mg	-20.73	4.75	25.48	Mg2Cl(OH)3:4H2O
Paragonite	0.65	-9.55	-10.20	NaAl3Si3O10(OH)2
Pargasite	-1.17	19.24	20.41	NaCa2Al3Mg4Si6O22(OH)2
Pentahydrite	-8.10	-9.73	-1.64	MgSO4:5H2O
Periclase	-3.16	5.52	8.67	MgO
Phlogopite	2.79	11.08	8.29	KAlMg3Si3O10(OH)2

Picromerite	-14.40	-19.14	-4.74	K2Mg(SO4)2:6H2O
Pirssonite	-15.04	-3.81	11.22	Na2Ca(CO3)2:2H2O
Polyhalite	-22.58	-36.99	-14.41	K2MgCa2(SO4)4:2H2O
Portlandite	-5.37	6.28	11.65	Ca(OH)2
Prehnite	-0.44	1.67	2.11	Ca2Al2Si3O10(OH)2
Pseudowollastonite	-1.95	4.34	6.29	CaSiO3
Pyrite	-93.24	-112.90	-19.65	FeS2
Pyrophyllite	0.13	-12.85	-12.98	Al2Si4O10(OH)2
Pyrrhotite	-54.11	-60.67	-6.56	FeS
Quartz	0.06	-1.95	-2.00	SiO2
Rankinite	-9.18	14.96	24.15	Ca3Si2O7
Ripidolite-14A	4.82	13.41	8.59	Mg3Fe2Al2Si3O10(OH)8
Ripidolite-7A	2.49	13.41	10.92	Mg3Fe2Al2Si3O10(OH)8
Rutile	6.61	-2.93	-9.55	TiO2
S	-43.32	-67.24	-23.92	S
S2(g)	-89.83	-104.45	-14.62	S2
Sanidine_high	-0.27	-5.46	-5.20	KAlSi3O8
Saponite-Ca	3.88	9.60	5.72	Ca.165Mg3Al.33Si3.67O10(OH)2
Saponite-H	3.06	8.56	5.50	H.33Mg3Al.33Si3.67O10(OH)2
Saponite-K	3.05	9.52	6.47	K.33Mg3Al.33Si3.67O10(OH)2
Saponite-Mg	3.99	9.47	5.48	Mg3.165Al.33Si3.67O10(OH)2
Saponite-Na	3.35	9.84	6.49	Na.33Mg3Al.33Si3.67O10(OH)2
Scolecite	0.81	-4.63	-5.44	CaAl2Si3O10:3H2O
Sepiolite	-3.89	10.34	14.23	Mg4Si6O15(OH)2:6H2O
Si	-70.35	3.41	73.75	Si
Si(g)	-104.26	3.41	107.67	Si
Siderite	-0.29	-5.04	-4.74	FeCO3
Sillimanite	-0.51	-7.01	-6.50	Al2SiO5
SiO2(am)	-0.36	-1.95	-1.59	SiO2
Smectite-high-Fe-Mg	3.22	-0.23	-3.45	Ca.025Na.1K.2Fe.5Fe.2Mg1.15Al1.25Si3.5H2O12
Smectite-low-Fe-Mg	2.45	-2.82	-5.26	Ca.02Na.15K.2Fe.29Fe.16Mg.9Al1.25Si3.75H2O12
SO2(g)	-18.74	-19.70	-0.96	SO2
Spinel	-1.68	0.46	2.14	Al2MgO4
Starkeyite	-8.53	-9.73	-1.20	MgSO4:4H2O
Stilbite	0.63	-11.88	-12.52	Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O
Sylvite	-3.96	-3.34	0.62	KCl
Syngenite	-10.69	-18.34	-7.65	K2Ca(SO4)2:H2O
Tachyhydrite	-36.79	-20.25	16.54	Mg2CaCl6:12H2O
Talc	3.06	8.75	5.69	Mg3Si4O10(OH)2
Thenardite	-3.94	-7.45	-3.51	Na2SO4
Thermonatrite	-9.37	-1.17	8.21	Na2CO3:H2O
Ti	-146.97	2.42	149.40	Ti
Ti(g)	-222.03	2.42	224.45	Ti
Ti2O3	-46.37	-3.19	43.19	Ti2O3
Ti3O5	-41.07	-6.12	34.96	Ti3O5
TiC	-183.11	-1.15	181.96	TiC
TiCl2	-83.84	-12.75	71.09	TiCl2
TiCl3	-59.83	-20.34	39.48	TiCl3
TiCl4(g)	-56.18	-27.93	28.25	TiCl4
TiO(alpha)	-61.48	-0.25	61.23	TiO
TiO(g)	-145.93	-0.25	145.67	TiO
Titanite	-718.23	1.41	719.63	CaTiSiO5
Tobermorite-11A	-17.22	19.72	36.94	Ca5Si6H11O22.5
Tobermorite-14A	-22.54	19.69	42.23	Ca5Si6H21O27.5
Tobermorite-9A	-16.28	19.73	36.01	Ca5Si6H6O20
Tremolite	4.07	24.57	20.50	Ca2Mg5Si8O22(OH)2
Tridymite	-0.77	-1.95	-1.18	SiO2
Troilite	-54.04	-60.67	-6.64	FeS
Trona-K	-19.66	-8.17	11.49	K2NaH(CO3)2:2H2O
Wairakite	0.25	-6.57	-6.83	CaAl2Si4O10(OH)4
Wollastonite	-1.95	4.34	6.29	CaSiO3
Wustite	0.01	3.45	3.44	Fe.947O
Xonotlite	-26.24	26.03	52.27	Ca6Si6O17(OH)2
Zoisite	0.02	-0.86	-0.88	Ca2Al3(SiO4)3OH

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

End of simulation.

APPENDIX G

EQUILIBRIUM MODELING RESULT IN AWIBENGKOK FIELD

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\l1n1.dat

Reading data base.

LLNL AQUEOUS MODEL PARAMETERS
NAMED EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\l1n1.dat
SOLUTION_SPECIES
CO3-2 + 2 H+ = CO2 + H2O
log_k 16.681
delta_h -5.738 kcal
analytical_expression 464.1965 0.09344813 -26986.16 -165.75951 2248628.9
dw 1.92e-9
vm 7.29 0.92 2.07 -1.23 -1.60 # ref. 1 + McBride et al. 2015, JCED 60, 171
2CO2 = (CO2)2 # activity correction for CO2 solubility at high P, T
log_k -1.8
analytical_expression 8.68 -0.0103 -2190
vm 14.58 1.84 4.14 -2.46 -3.20
END

End of simulation.

Reading input data for simulation 2.

PHASES
CO2(g)
CO2 = CO2
log_k -1.468
delta_h -4.776 kcal
analytical_expression 10.5624 -2.3547e-2 -3972.8 0 5.8746e5 1.9194e-5
t_c 304.2 # critical T, K
p_c 72.86 # critical P, atm
omega 0.225 # acentric factor
Ankerite
CaMg0.3Fe0.7(CO3)2 + 2H+ = Ca++ + 0.3Mg++ + 0.7Fe++ + 2HCO3-
log_k 1.54
delta_h 0
analytical_expression -1.8649e+03 -2.9583e-01 1.0468e+05 6.7554e+02 -6.0514e+06
END

End of simulation.

Reading input data for simulation 3.

SOLUTION 1 AWI 1-2 1600
temp 250
pH 6.92
pe 4
redox pe
units ppm
density 1
C(4) 96.2
Ca 227
Cl 6700
Mg 0.71
Na 3680
S(6) 23.6
K 630
B 245
Li 13.5
F 1.82
Si 498
water 1 # kg
pressure 155 atm
EQUILIBRIUM PHASES 1 Reservoir
Albite 0 30.98
Anhydrite 0 0
Ankerite 0 0
Anorthite 0 19.45
Aragonite 0 0
Calcite 0 7.9
Chamosite-7A 0 11.73
Dawsonite 0 0
Diopside 0 0.66
Dolomite 0 0
Enstatite 0 10.18
Epidote 0 1.53
Fluorapatite 0 0.35
Gypsum 0 0
Hematite 0 6.37

```

Ilmenite 0 0.38
K-Feldspar 0 7.87
Magnesite 0 0
Quartz 0 48.09
Siderite 0 0
Titanite 0 1.99
Zircon 0 0.01
CO2(g) 2.20 0.9
SELECTED_OUTPUT 1
file D:\20182 SPRING\Thesis PHREEQC\4. Awibengkok\equilibrium modeling salak.sel
reset false
solution true
ph true
pe true
temperature true
molalities K+ Na+ Ca+2 Mg+2
HCO3- SO4-2 Cl- CO3-2
saturation_indices Anhydrite Gypsum Aragonite Calcite
Dolomite Magnesite CO2(g)
END
-----
Beginning of initial solution calculations.
-----
Initial solution 1. AWI 1-2 1600
-----Solution composition-----

```

Elements	Molality	Moles
B	2.294e-02	2.294e-02
C (4)	1.596e-03	1.596e-03
Ca	5.733e-03	5.733e-03
Cl	1.913e-01	1.913e-01
F	9.697e-05	9.697e-05
K	1.631e-02	1.631e-02
Li	1.969e-03	1.969e-03
Mg	2.957e-05	2.957e-05
Na	1.620e-01	1.620e-01
S (6)	2.487e-04	2.487e-04
Si	8.392e-03	8.392e-03

```

-----Description of solution-----
pH = 6.920
pe = 4.000
Density (g/cm³) = 0.82270
Volume (L) = 1.23182
Activity of water = 0.993
Ionic strength (mol/kgw) = 1.688e-01
Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = 1.045e-03
Total CO2 (mol/kg) = 1.596e-03
Temperature (°C) = 250.00
Pressure (atm) = 155.00
Electrical balance (eq) = -1.101e-03
Percent error, 100*(Cat-An)/ (Cat+|An|) = -0.33
Iterations = 7
Total H = 1.111192e+02
Total O = 5.561551e+01
-----Distribution of species-----

```

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	1.013e-04	5.697e-05	-3.994	-4.244	-0.250	(0)
H+	1.734e-07	1.202e-07	-6.761	-6.920	-0.159	0.00
H2O	5.553e+01	9.935e-01	1.744	-0.003	0.000	22.19
B(-5)	0.000e+00					
BH4-	0.000e+00	0.000e+00	-115.047	-115.285	-0.238	(0)
B(3)	2.294e-02					
B(OH)3	2.259e-02	2.259e-02	-1.646	-1.646	0.000	(0)
BO2-	3.211e-04	1.858e-04	-3.493	-3.731	-0.238	(0)
NaB(OH)4	1.721e-05	1.721e-05	-4.764	-4.764	0.000	(0)
CaB(OH)4+	7.615e-06	4.405e-06	-5.118	-5.356	-0.238	(0)
MgB(OH)4+	1.888e-08	1.092e-08	-7.724	-7.962	-0.238	(0)
BF2(OH)2-	2.090e-11	1.209e-11	-10.680	-10.918	-0.238	(0)
B2O(OH)5-	1.516e-15	8.768e-16	-14.819	-15.057	-0.238	(0)
BF4-	7.836e-20	4.533e-20	-19.106	-19.344	-0.238	(0)
BF3OH-	8.184e-40	4.734e-40	-39.087	-39.325	-0.238	(0)
C(4)	1.596e-03					
CO2	1.271e-03	1.321e-03	-2.896	-2.879	0.017	79.97
HCO3-	1.816e-04	1.051e-04	-3.741	-3.979	-0.238	(0)
CaHCO3+	1.273e-04	7.362e-05	-3.895	-4.133	-0.238	(0)
CaCO3	1.561e-05	1.561e-05	-4.807	-4.807	0.000	(0)
MgHCO3+	2.639e-07	1.526e-07	-6.579	-6.816	-0.238	(0)
(CO2)2	2.140e-07	2.225e-07	-6.670	-6.653	0.017	159.93
NaHCO3	1.762e-07	1.762e-07	-6.754	-6.754	0.000	(0)
CO3-2	9.187e-08	1.095e-08	-7.037	-7.961	-0.924	(0)
MgCO3	3.660e-09	3.660e-09	-8.437	-8.437	0.000	(0)
NaCO3-	2.040e-12	1.180e-12	-11.690	-11.928	-0.238	(0)
Ca	5.733e-03					
Ca+2	3.735e-03	5.760e-04	-2.428	-3.240	-0.812	(0)
CaCl+	1.308e-03	7.568e-04	-2.883	-3.121	-0.238	(0)
CaCl2	4.168e-04	4.168e-04	-3.380	-3.380	0.000	(0)
CaHCO3+	1.273e-04	7.362e-05	-3.895	-4.133	-0.238	(0)
CaSO4	9.503e-05	9.503e-05	-4.022	-4.022	0.000	(0)
CaF+	2.787e-05	1.612e-05	-4.555	-4.793	-0.238	(0)
CaCO3	1.561e-05	1.561e-05	-4.807	-4.807	0.000	(0)
CaB(OH)4+	7.615e-06	4.405e-06	-5.118	-5.356	-0.238	(0)
CaOH+	1.259e-09	7.280e-10	-8.900	-9.138	-0.238	(0)
Cl(-1)	1.913e-01					
Cl-	1.645e-01	8.971e-02	-0.784	-1.047	-0.263	(0)
NaCl	2.325e-02	2.325e-02	-1.634	-1.634	0.000	(0)
CaCl+	1.308e-03	7.568e-04	-2.883	-3.121	-0.238	(0)
KCl	1.242e-03	1.242e-03	-2.906	-2.906	0.000	(0)
CaCl2	4.168e-04	4.168e-04	-3.380	-3.380	0.000	(0)
LiCl	1.073e-04	1.073e-04	-3.970	-3.970	0.000	(0)
MgCl+	1.224e-05	7.082e-06	-4.912	-5.150	-0.238	(0)
HCl	3.921e-08	3.921e-08	-7.407	-7.407	0.000	(0)
Cl(1)	5.926e-15					

HC1O	4.271e-15	4.271e-15	-14.370	-14.370	0.000	(0)
ClO-	1.656e-15	9.578e-16	-14.781	-15.019	-0.238	(0)
Cl(3)	4.975e-23					
ClO2-	4.974e-23	2.877e-23	-22.303	-22.541	-0.238	(0)
HC1O2	5.114e-27	5.114e-27	-26.291	-26.291	0.000	(0)
Cl(5)	1.295e-22					
ClO3-	1.295e-22	7.285e-23	-21.888	-22.138	-0.250	(0)
Cl(7)	1.143e-25					
ClO4-	1.143e-25	6.427e-26	-24.942	-25.192	-0.250	(0)
F	9.697e-05					
F-	6.044e-05	3.399e-05	-4.219	-4.469	-0.250	(0)
CaF+	2.787e-05	1.612e-05	-4.555	-4.793	-0.238	(0)
NaF	7.317e-06	7.317e-06	-5.136	-5.136	0.000	(0)
HF	1.186e-06	1.186e-06	-5.926	-5.926	0.000	(0)
MgF+	1.589e-07	9.190e-08	-6.799	-7.037	-0.238	(0)
HF2-	2.105e-11	1.217e-11	-10.677	-10.915	-0.238	(0)
BF2(OH)2-	2.090e-11	1.209e-11	-10.680	-10.918	-0.238	(0)
H2F2	9.791e-17	9.791e-17	-16.009	-16.009	0.000	(0)
BF4-	7.836e-20	4.533e-20	-19.106	-19.344	-0.238	(0)
SiF6-2	1.872e-30	2.015e-31	-29.728	-30.696	-0.968	(0)
BF3OH-	8.184e-40	4.734e-40	-39.087	-39.325	-0.238	(0)
H(0)	8.977e-22					
H2	4.489e-22	4.857e-22	-21.348	-21.314	0.034	(0)
K	1.631e-02					
K+	1.503e-02	8.193e-03	-1.823	-2.087	-0.263	(0)
KCl	1.242e-03	1.242e-03	-2.906	-2.906	0.000	(0)
KSO4-	4.010e-05	2.320e-05	-4.397	-4.635	-0.238	(0)
KHSO4	4.618e-09	4.618e-09	-8.336	-8.336	0.000	(0)
KOH	2.542e-10	2.542e-10	-9.595	-9.595	0.000	(0)
Li	1.969e-03					
Li+	1.862e-03	1.178e-03	-2.730	-2.929	-0.199	(0)
LiCl	1.071e-04	1.071e-04	-3.970	-3.970	0.000	(0)
LiSO4-	1.201e-07	6.945e-08	-6.921	-7.158	-0.238	(0)
LiOH	2.415e-10	2.415e-10	-9.617	-9.617	0.000	(0)
Mg	2.957e-05					
MgCl+	1.224e-05	7.082e-06	-4.912	-5.150	-0.238	(0)
MgSO4	1.088e-05	1.088e-05	-4.963	-4.963	0.000	(0)
Mg+2	5.998e-06	1.200e-06	-5.222	-5.921	-0.699	(0)
MgHCO3+	2.639e-07	1.526e-07	-6.579	-6.816	-0.238	(0)
MgF+	1.589e-07	9.190e-08	-6.799	-7.037	-0.238	(0)
MgB(OH)4+	1.888e-08	1.092e-08	-7.724	-7.962	-0.238	(0)
MgCO3	3.660e-09	3.660e-09	-8.437	-8.437	0.000	(0)
Mg4(OH)4+4	5.957e-33	2.364e-36	-32.225	-35.626	-3.401	(0)
Na	1.620e-01					
Na+	1.386e-01	8.018e-02	-0.858	-1.096	-0.238	(0)
NaCl	2.325e-02	2.325e-02	-1.634	-1.634	0.000	(0)
NaHSiO3	1.212e-04	1.212e-04	-3.916	-3.916	0.000	(0)
NaOH	2.095e-05	2.095e-05	-4.679	-4.679	0.000	(0)
NaB(OH)4	1.721e-05	1.721e-05	-4.764	-4.764	0.000	(0)
NaSO4-	9.167e-06	5.302e-06	-5.038	-5.276	-0.238	(0)
NaF	7.317e-06	7.317e-06	-5.136	-5.136	0.000	(0)
NaHCO3	1.762e-07	1.762e-07	-6.754	-6.754	0.000	(0)
NaCO3-	2.040e-12	1.180e-12	-11.690	-11.928	-0.238	(0)
O(0)	4.432e-06					
O2	2.216e-06	2.398e-06	-5.654	-5.620	0.034	(0)
S(6)	2.487e-04					
CaSO4	9.503e-05	9.503e-05	-4.022	-4.022	0.000	(0)
SO4-2	9.302e-05	1.001e-05	-4.031	-5.000	-0.968	(0)
KSO4-	4.010e-05	2.320e-05	-4.397	-4.635	-0.238	(0)
MgSO4	1.088e-05	1.088e-05	-4.963	-4.963	0.000	(0)
NaSO4-	9.167e-06	5.302e-06	-5.038	-5.276	-0.238	(0)
HSO4-	4.101e-07	2.372e-07	-6.387	-6.625	-0.238	(0)
LiSO4-	1.201e-07	6.945e-08	-6.921	-7.158	-0.238	(0)
KHSO4	4.618e-09	4.618e-09	-8.336	-8.336	0.000	(0)
H2SO4	1.379e-20	1.379e-20	-19.860	-19.860	0.000	(0)
Si	8.392e-03					
SiO2	8.154e-03	8.154e-03	-2.089	-2.089	0.000	(0)
NaHSiO3	1.212e-04	1.212e-04	-3.916	-3.916	0.000	(0)
HSiO3-	1.159e-04	6.703e-05	-3.936	-4.174	-0.238	(0)
H6(H2SiO4)4-2	1.168e-07	1.257e-08	-6.933	-7.901	-0.968	(0)
H2SiO4-2	6.653e-11	7.159e-12	-10.177	-11.145	-0.968	(0)
H4(H2SiO4)4-4	3.382e-13	4.358e-17	-12.471	-16.361	-3.890	(0)
SiF6-2	1.872e-30	2.015e-31	-29.728	-30.696	-0.968	(0)

-----Saturation indices-----					
Phase	SI**	log IAP	log K(523 K, 155 atm)		
Afwillite	-7.36	27.61	34.96	Ca3Si2O4(OH)6	
Akermanite	3.02	24.93	21.92	Ca2MgSi2O7	
Anhydrite	0.29	-8.24	-8.52	CaSO4	
Antarcticite	-9.24	-5.35	3.89	CaCl2:6H2O	
Anthophyllite	13.52	38.70	25.18	Mg7Si8O22(OH)2	
Antigorite	101.62	308.88	207.27	Mg48Si34O85(OH)62	
Aphthitalite	-13.47	-17.35	-3.89	NaK3(SO4)2	
Aragonite	0.90	-0.30	-1.20	CaCO3	
Arcanite	-6.58	-9.17	-2.59	K2SO4	
Artinite	-4.52	4.93	9.45	Mg2CO3(OH)2:3H2O	
B	-57.56	2.57	60.13	B	
B(g)	-106.38	2.57	108.96	B	
B2O3	-6.32	-3.28	3.03	B2O3	
Bassanite	-0.41	-8.24	-7.83	CaSO4:0.5H2O	
BF3(g)	-22.92	-35.80	-12.88	BF3	
Bischofite	-12.22	-8.03	4.18	MgCl2:6H2O	
Bloedite	-15.51	-18.12	-2.62	Na2Mg(SO4)2:4H2O	
Borax	-13.50	5.05	18.55	Na2(B4O5(OH)4):8H2O	
Boric_acid	-2.86	-1.65	1.22	B(OH)3	
Brucite	-0.19	7.91	8.11	Mg(OH)2	
Burkeite	-23.12	-13.63	9.49	Na6CO3(SO4)2	
C	-37.63	-5.28	32.36	C	
C(g)	-101.42	-5.28	96.15	C	
Ca	-63.74	13.41	77.15	Ca	
Ca(g)	-75.79	13.41	89.20	Ca	
Ca2Cl2(OH)2:2H2O	-20.93	5.26	26.19	Ca2Cl2(OH)2:2H2O	
Ca4Cl2(OH)6:13H2O	-41.26	26.41	67.67	Ca4Cl2(OH)6:13H2O	
Calcite	1.06	-0.30	-1.36	CaCO3	
Carnallite	-15.23	-11.17	4.06	KMgCl3:6H2O	
CaSO4:0.5H2O(beta)	-0.40	-8.24	-7.84	CaSO4:0.5H2O	
Chalcedony	-0.02	-2.09	-2.07	SiO2	

Chloromagnesite	-15.36	-8.02	7.35	MgCl2
Chrysotile	5.79	19.57	13.77	Mg3Si2O5(OH)4
Cl2(g)	-16.12	-18.74	-2.62	Cl2
CO2(g)	-0.80	-2.88	-2.08	CO2
Coesite	-0.35	-2.09	-1.73	SiO2
Colemanite	-10.25	11.33	21.58	Ca2B6O11:5H2O
Cristobalite(alpha)	-0.13	-2.09	-1.96	SiO2
Cristobalite(beta)	-0.31	-2.09	-1.78	SiO2
Dicalcium_silicate	-0.70	19.11	19.80	Ca2SiO4
Diopside	4.95	14.34	9.39	CaMgSi2O6
Dolomite	1.08	-3.28	-4.36	CaMg(CO3)2
Dolomite-dis	0.46	-3.28	-3.74	CaMg(CO3)2
Dolomite-ord	1.09	-3.28	-4.37	CaMg(CO3)2
Enstatite	1.40	5.83	4.43	MgSiO3
Epsomite	-8.74	-10.94	-2.20	MgSO4:7H2O
F2(g)	-50.51	-25.58	24.93	F2
Fluorite	-0.57	-12.18	-11.60	CaF2
Forsterite	2.02	13.74	11.72	Mg2SiO4
Foshagite	-0.34	36.12	36.46	Ca4Si3O9(OH)2:0.5H2O
Gaylussite	-10.55	0.44	10.99	CaNa2(CO3)2:5H2O
Glauberite	-9.96	-15.43	-5.47	Na2Ca(SO4)2
Gypsum	-1.07	-8.24	-7.17	CaSO4:2H2O
Gyrolite	0.07	14.92	14.85	Ca2Si3O7(OH)2:1.5H2O
H2(g)	-18.71	-21.31	-2.61	H2
H2O(g)	1.56	-0.00	-1.56	H2O
Halite	-3.05	-2.14	0.91	NaCl
Hatrurite	-9.79	29.70	39.49	Ca3SiO5
HCl(g)	-7.78	-7.97	-0.18	HCl
Hexahydrite	-9.00	-10.94	-1.93	MgSO4:6H2O
Hillebrandite	-1.70	19.10	20.80	Ca2SiO3(OH)2:0.17H2O
Huntite	-2.12	-9.24	-7.11	CaMg3(CO3)4
Hydroboracite	-11.75	8.65	20.40	MgCaB6O11:6H2O
Hydromagnesite	-8.70	-4.02	4.68	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-8.29	-5.33	2.95	CaCl2
Ice	-1.14	-0.00	1.14	H2O
K	-34.99	6.24	41.23	K
K(g)	-39.10	6.24	45.34	K
K2CO3:1.5H2O	-14.56	-1.24	13.33	K2CO3:1.5H2O
K2O	-42.29	9.66	51.96	K2O
K3H(SO4)2	-19.56	-23.18	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-54.34	-26.73	27.61	K8H4(CO3)6:3H2O
Kainite	-13.65	-14.06	-0.42	KMgClSO4:3H2O
Kalinite	-6.35	-6.07	0.28	KHCO3
Kieserite	-10.62	-10.92	-0.30	MgSO4:H2O
KMgCl3	-19.80	-11.15	8.65	KMgCl3
KMgCl3:2H2O	-17.70	-11.15	6.54	KMgCl3:2H2O
KNaCO3:6H2O	-10.31	-0.26	10.05	KNaCO3:6H2O
Lansfordite	-7.66	-2.99	4.67	MgCO3:5H2O
Larnite	-1.26	19.11	20.36	Ca2SiO4
Leonite	-15.85	-20.10	-4.25	K2Mg(SO4)2:4H2O
Li	-35.91	5.39	41.30	Li
Li(g)	-46.28	5.39	51.68	Li
Lime	-7.23	10.60	17.83	CaO
Magnesite	-0.84	-2.98	-2.14	MgCO3
Mercallite	-12.57	-14.01	-1.44	KHSO4
Merwinite	1.22	35.53	34.32	MgCa3(SiO4)2
Mg	-55.07	10.73	65.79	Mg
Mg(g)	-63.93	10.73	74.66	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-4.36	-8.94	-4.59	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-4.17	-6.96	-2.80	Mg1.5SO4(OH)
MgCl2:2H2O	-11.69	-8.02	3.67	MgCl2:2H2O
MgCl2:4H2O	-10.24	-8.03	2.22	MgCl2:4H2O
MgCl2:H2O	-12.79	-8.02	4.78	MgCl2:H2O
MgOHC1	-5.86	-0.05	5.81	MgOHC1
MgSO4	-6.28	-10.92	-4.64	MgSO4
Mirabilite	-15.98	-7.22	8.76	Na2SO4:10H2O
Misenite	-82.13	-93.21	-11.08	K8H6(SO4)7
Monohydrocalcite	-1.36	-0.30	1.06	CaCO3:H2O
Monticellite	2.40	16.43	14.03	CaMgSiO4
Na	-31.52	7.23	38.75	Na
Na(g)	-37.12	7.23	44.35	Na
Na2CO3	-6.83	0.75	7.58	Na2CO3
Na2CO3:7H2O	-15.12	0.73	15.85	Na2CO3:7H2O
Na2O	-29.90	11.65	41.54	Na2O
Na2SiO3	-6.36	9.56	15.92	Na2SiO3
Na3H(SO4)2	-19.32	-20.21	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.66	-22.63	-5.96	Na4Ca(SO4)3:2H2O
Na4SiO4	-25.29	21.20	46.49	Na4SiO4
Na6Si2O7	-35.66	30.76	66.42	Na6Si2O7
Nahcolite	-5.50	-5.07	0.42	NaHCO3
Natron	-14.08	0.72	14.80	Na2CO3:10H2O
Natrosilite	-5.95	7.47	13.41	Na2Si2O5
Nesquehonite	-6.96	-2.99	3.97	MgCO3:3H2O
O2(g)	-2.98	-5.62	-2.64	O2
Okenite	-2.60	6.41	9.02	CaSi2O4(OH)2:2H2O
Oxychloride-Mg	-17.74	7.85	25.59	Mg2Cl(OH)3:4H2O
Pentahydrite	-9.37	-10.93	-1.56	MgSO4:5H2O
Periclase	-2.14	7.92	10.06	MgO
Picromerite	-15.46	-20.11	-4.65	K2Mg(SO4)2:6H2O
Pirssonite	-10.81	0.45	11.25	Na2Ca(CO3)2:2H2O
Polyhalite	-22.20	-36.58	-14.38	K2MgCa2(SO4)4:2H2O
Portlandite	-2.27	10.59	12.86	Ca(OH)2
Pseudowollastonite	1.34	8.51	7.16	CaSiO3
Quartz	0.13	-2.09	-2.22	SiO2
Rankinite	0.32	27.62	27.30	Ca3Si2O7
Sellaite	-2.21	-14.86	-12.65	MgF2
Sepiolite	3.24	19.11	15.88	Mg4Si6O15(OH)2:6H2O
Si	-78.28	3.53	81.81	Si
Si(g)	-115.73	3.53	119.26	Si
SiF4(g)	-25.73	-47.64	-21.90	SiF4
SiO2(am)	-0.38	-2.09	-1.71	SiO2
Starkeyite	-9.79	-10.93	-1.14	MgSO4:4H2O
Sylvite	-4.12	-3.13	0.99	KCl
Synogenite	-9.78	-17.41	-7.63	K2Ca(SO4)2:H2O
Tachyhydrite	-38.13	-21.40	16.73	Mg2CaCl6:12H2O
Talc	7.99	15.39	7.40	Mg3Si4O10(OH)2
Thenardite	-4.66	-7.19	-2.54	Na2SO4
Thermonatrite	-7.92	0.75	8.67	Na2CO3:H2O

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Tobermorite-11A  0.31    40.44   40.14   Ca5Si6H11O22.5
Tobermorite-14A -4.03    40.43   44.46   Ca5Si6H21O27.5
Tobermorite-9A  0.64    40.45   39.80   Ca5Si6H6O20
Tremolite       18.96    44.06   25.10   Ca2Mg5Si8O22(OH)2
Tridymite       -0.39    -2.09   -1.70   SiO2
Trona-K         -17.83   -6.31   11.52   K2NaH(CO3)2·2H2O
Wollastonite    1.37     8.51    7.14    CaSiO3
Xonotlite       -3.77    51.05   54.82   Ca6Si6O17(OH)2

**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 1.      ANI 1-2 1600
Using pure phase assemblage 1.      Reservoir

-----Phase assemblage-----
Phase              SI  log IAP  log K(T, P)      Moles in assemblage
                   SI  log IAP  log K(T, P)      Initial      Final      Delta
Albite             0.00   -3.57   -3.57   3.098e+01   3.101e+01   3.124e-02
Anhydrite          -1.34   -9.87   -8.52   0.000e+00   0           0.000e+00
Ankerite           -1.72   -6.86   -5.14   0.000e+00   0           0.000e+00
Anorthite          0.00    0.90    0.90   1.945e+01   1.085e+01   -8.601e+00
Aragonite          -1.21   -2.41   -1.20   0.000e+00   0           0.000e+00
CO2(g)             1.29   -0.78   -2.08   9.000e-01   0           -9.000e-01
Calcite            -1.05   -2.41   -1.36   7.900e+00   0           -7.900e+00
Chamosite-7A       0.00    3.46    3.46   1.173e+01   1.074e+01   -9.934e-01
Dawsonite          -4.33   -5.71   -1.38   0.000e+00   0           0.000e+00
Diopside           -0.80    8.59    9.39   6.600e-01   0           -6.600e-01
Dolomite           -0.20   -4.56   -4.36   0.000e+00   0           0.000e+00
Enstatite          -0.00    4.43    4.43   1.018e+01   2.178e+00   -8.002e+00
Epidote            -0.00   -0.46   -0.46   1.530e+00   1.111e+01   9.575e+00
Fluorapatite       0.00   -42.42  -42.42   3.500e-01   3.500e-01   -2.503e-09
Gypsum            -2.70   -9.87   -7.17   0.000e+00   0           0.000e+00
Hematite           0.00   -11.04  -11.04   6.370e+00   1.582e+00   -4.788e+00
Ilmenite           0.00    0.94    0.94   3.800e-01   2.366e+00   1.986e+00
K-Feldspar         0.00   -4.71   -4.71   7.870e+00   7.877e+00   6.975e-03
Magnesite          0.00   -2.14   -2.14   0.000e+00   8.644e+00   8.644e+00
Quartz             0.00   -2.22   -2.22   4.809e+01   4.876e+01   6.701e-01
Siderite           -1.57   -5.43   -3.86   0.000e+00   0           0.000e+00
Titanite           -717.88  1.74    719.62   1.990e+00   0           -1.990e+00
Zircon             -0.00  -11.75  -11.75   1.000e-02   1.000e-02   -1.938e-11

-----Solution composition-----
Elements           Molality      Moles
Al                 2.562e-05    2.432e-05
B                  2.416e-02    2.294e-02
C                  1.659e-01    1.575e-01
Ca                 6.492e-03    6.164e-03
Cl                 2.015e-01    1.913e-01
F                  1.021e-04    9.697e-05
Fe                 9.870e-06    9.371e-06
K                  9.833e-03    9.336e-03
Li                 2.074e-03    1.969e-03
Mg                 1.937e-02    1.839e-02
Na                 1.378e-01    1.308e-01
P                  7.910e-09    7.510e-09
S                  2.620e-04    2.487e-04
Si                 5.988e-03    5.685e-03
Ti                 3.688e-03    3.502e-03
Zr                 2.042e-11    1.938e-11

-----Description of solution-----
pH = 4.785
pe = -1.657      Charge balance
Density (g/cm³) = 0.82018      Adjusted to redox equilibrium
Volume (L) = 1.18196
Activity of water = 0.991
Ionic strength (mol/kgw) = 1.761e-01
Mass of water (kg) = 9.494e-01
Total alkalinity (eq/kg) = 5.764e-04
Total CO2 (mol/kg) = 1.659e-01
Temperature (°C) = 250.00
Pressure (atm) = 155.00
Electrical balance (eq) = -1.101e-03
Percent error, 100*(Cat-[An])/([Cat]+[An]) = -0.35
Iterations = 18
Total H = 1.055173e+02
Total O = 5.312757e+01

-----Distribution of species-----
Species           Molality      Activity      Log Molality      Log Activity      Log Gamma      mole V
H+                2.374e-05    1.642e-05    -4.625    -4.785    -0.160    0.00
OH-               7.454e-07    4.161e-07    -6.128    -6.381    -0.253    (0)
H2O               5.553e+01    9.909e-01    1.744    -0.004    0.000    22.19
Al                2.562e-05
AlO2              1.191e-05    1.191e-05    -4.924    -4.924    0.000    (0)
AlO2-             9.182e-06    5.276e-06    -5.037    -5.278    -0.241    (0)
NaAlO2            4.462e-06    4.462e-06    -5.351    -5.351    0.000    (0)
Al(OH)2+          6.462e-08    3.713e-08    -7.190    -7.430    -0.241    (0)
AlOH+2            3.329e-10    3.866e-11    -9.478    -10.413    -0.935    (0)
AlF+2             9.579e-13    1.112e-13    -12.019    -12.954    -0.935    (0)
AlF2+             6.299e-13    3.619e-13    -12.201    -12.441    -0.241    (0)
Al+3              4.204e-14    1.361e-15    -13.376    -14.866    -1.490    (0)
AlF3              3.723e-14    3.723e-14    -13.429    -13.429    0.000    (0)
AlF4-             1.330e-16    7.641e-17    -15.876    -16.117    -0.241    (0)
AlSO4+            5.006e-19    2.876e-19    -18.301    -18.541    -0.241    (0)
AlHPO4+           7.006e-20    4.026e-20    -19.155    -19.395    -0.241    (0)
Al(SO4)2-         8.023e-24    4.610e-24    -23.096    -23.336    -0.241    (0)
Al2(OH)2+4        4.449e-25    1.616e-28    -24.352    -27.792    -3.440    (0)

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AlH2PO4+2	2.852e-28	3.312e-29	-27.545	-28.480	-0.935	(0)
Al3 (OH) 4+5	8.765e-35	6.067e-40	-34.057	-39.217	-5.160	(0)
Al13O4 (OH) 24+7	0.000e+00	0.000e+00	-127.901	-138.020	-10.119	(0)
B (-5)	0.000e+00					
BH4-	0.000e+00	0.000e+00	-54.810	-55.051	-0.241	(0)
B (3)	2.416e-02					
B (OH) 3	2.416e-02	2.416e-02	-1.617	-1.617	0.000	(0)
BO2-	2.538e-06	1.458e-06	-5.595	-5.836	-0.241	(0)
MgB (OH) 4+	1.520e-07	8.733e-08	-6.818	-7.059	-0.241	(0)
NaB (OH) 4	1.137e-07	1.137e-07	-6.944	-6.944	0.000	(0)
CaB (OH) 4+	6.857e-08	3.940e-08	-7.164	-7.405	-0.241	(0)
BF2 (OH) 2-	1.780e-10	1.023e-10	-9.750	-9.990	-0.241	(0)
BF4-	7.226e-16	4.152e-16	-15.141	-15.382	-0.241	(0)
B2O (OH) 5-	1.278e-17	7.342e-18	-16.894	-17.134	-0.241	(0)
BF3OH-	2.293e-37	1.318e-37	-36.640	-36.880	-0.241	(0)
C (-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-40.127	-40.127	0.000	(0)
C (-3)	1.429e-07					
C2H6	7.143e-08	7.143e-08	-7.146	-7.146	0.000	(0)
C (-4)	8.162e-11					
CH4	8.162e-11	8.162e-11	-10.088	-10.088	0.000	(0)
C (2)	5.889e-09					
CO	5.889e-09	5.889e-09	-8.230	-8.230	0.000	(0)
C (4)	1.659e-01					
CO2	1.587e-01	1.652e-01	-0.800	-0.782	0.018	79.97
(CO2) 2	3.341e-03	3.479e-03	-2.476	-2.459	0.018	159.93
MgHCO3+	2.484e-04	1.427e-04	-3.605	-3.845	-0.241	(0)
HCO3-	1.670e-04	9.597e-05	-3.777	-4.018	-0.241	(0)
CaHCO3+	1.340e-04	7.701e-05	-3.873	-4.113	-0.241	(0)
NaHCO3	1.362e-07	1.362e-07	-6.866	-6.866	0.000	(0)
CaCO3	1.196e-07	1.196e-07	-6.922	-6.922	0.000	(0)
FeHCO3+	5.517e-08	3.170e-08	-7.258	-7.499	-0.241	(0)
MgCO3	2.507e-08	2.507e-08	-7.601	-7.601	0.000	(0)
CO3 2-	6.308e-10	7.325e-11	-9.200	-10.135	-0.935	(0)
FeCO3	9.268e-12	9.268e-12	-11.033	-11.033	0.000	(0)
NaCO3-	1.163e-14	6.681e-15	-13.935	-14.175	-0.241	(0)
FeCO3+	1.286e-20	7.387e-21	-19.891	-20.132	-0.241	(0)
Ca	6.492e-03					
Ca+2	4.363e-03	6.596e-04	-2.360	-3.181	-0.821	(0)
CaCl+	1.508e-03	8.664e-04	-2.822	-3.062	-0.241	(0)
CaCl2	4.770e-04	4.770e-04	-3.322	-3.322	0.000	(0)
CaHCO3+	1.340e-04	7.701e-05	-3.873	-4.113	-0.241	(0)
CaF+	7.722e-06	4.437e-06	-5.112	-5.353	-0.241	(0)
CaSO4	2.245e-06	2.245e-06	-5.649	-5.649	0.000	(0)
CaCO3	1.196e-07	1.196e-07	-6.922	-6.922	0.000	(0)
CaB (OH) 4+	6.857e-08	3.940e-08	-7.164	-7.405	-0.241	(0)
CaOH+	1.060e-11	6.090e-12	-10.975	-11.215	-0.241	(0)
CaHPO4	4.267e-13	4.267e-13	-12.370	-12.370	0.000	(0)
CaPO4-	1.132e-16	6.502e-17	-15.946	-16.187	-0.241	(0)
CaH2PO4+	5.572e-19	3.202e-19	-18.254	-18.495	-0.241	(0)
Ca2PO7 2-	9.218e-24	9.639e-25	-23.035	-24.016	-0.981	(0)
Cl (-1)	2.015e-01					
Cl-	1.659e-01	8.968e-02	-0.780	-1.047	-0.267	(0)
NaCl	1.967e-02	1.967e-02	-1.706	-1.706	0.000	(0)
MgCl+	1.262e-02	7.249e-03	-1.899	-2.140	-0.241	(0)
CaCl+	1.508e-03	8.664e-04	-2.822	-3.062	-0.241	(0)
KCl	7.443e-04	7.443e-04	-3.128	-3.128	0.000	(0)
CaCl2	4.770e-04	4.770e-04	-3.322	-3.322	0.000	(0)
LiCl	1.123e-04	1.123e-04	-3.950	-3.950	0.000	(0)
HCl	5.352e-06	5.352e-06	-5.271	-5.271	0.000	(0)
FeCl+	5.114e-06	2.938e-06	-5.291	-5.532	-0.241	(0)
FeCl4 2-	4.887e-07	5.110e-08	-6.311	-7.292	-0.981	(0)
FeCl2	4.885e-08	4.885e-08	-7.311	-7.311	0.000	(0)
FeCl4 2-	1.058e-16	1.228e-17	-15.976	-16.911	-0.935	(0)
FeCl2+	2.566e-20	1.474e-20	-19.591	-19.831	-0.241	(0)
FeCl4-	2.481e-25	1.425e-25	-24.605	-24.846	-0.241	(0)
Cl (1)	1.519e-28					
HClO	1.514e-28	1.514e-28	-27.820	-27.820	0.000	(0)
ClO-	4.329e-31	2.488e-31	-30.364	-30.604	-0.241	(0)
Cl (3)	0.000e+00					
ClO2-	0.000e+00	0.000e+00	-53.471	-53.712	-0.241	(0)
HClO2	0.000e+00	0.000e+00	-55.327	-55.327	0.000	(0)
Cl (5)	0.000e+00					
ClO3-	0.000e+00	0.000e+00	-68.641	-68.894	-0.253	(0)
Cl (7)	0.000e+00					
ClO4-	0.000e+00	0.000e+00	-87.280	-87.534	-0.253	(0)
F	1.021e-04					
MgF+	3.936e-05	2.262e-05	-4.405	-4.646	-0.241	(0)
HF	3.893e-05	3.893e-05	-4.410	-4.410	0.000	(0)
F-	1.464e-05	8.171e-06	-4.835	-5.088	-0.253	(0)
CaF+	7.722e-06	4.437e-06	-5.112	-5.353	-0.241	(0)
NaF	1.488e-06	1.488e-06	-5.827	-5.827	0.000	(0)
FeF+	2.051e-10	1.178e-10	-9.688	-9.929	-0.241	(0)
BF2 (OH) 2-	1.780e-10	1.023e-10	-9.750	-9.990	-0.241	(0)
HF2-	1.672e-10	9.605e-11	-9.777	-10.018	-0.241	(0)
AlF+2	9.579e-13	1.112e-13	-12.019	-12.954	-0.935	(0)
AlF2+	6.299e-13	3.619e-13	-12.201	-12.441	-0.241	(0)
H2F2	1.055e-13	1.055e-13	-12.977	-12.977	0.000	(0)
AlF3	3.723e-14	3.723e-14	-13.429	-13.429	0.000	(0)
PO3F 2-	2.227e-14	2.329e-15	-13.652	-14.633	-0.981	(0)
HPO3F-	8.366e-16	4.807e-16	-15.077	-15.318	-0.241	(0)
BF4-	7.226e-16	4.152e-16	-15.141	-15.382	-0.241	(0)
AlF4-	1.330e-16	7.641e-17	-15.876	-16.117	-0.241	(0)
FeF2+	6.770e-17	3.890e-17	-16.169	-16.410	-0.241	(0)
FeF2	2.389e-17	2.774e-18	-16.622	-17.557	-0.935	(0)
H2PO3F	5.047e-20	5.047e-20	-19.297	-19.297	0.000	(0)
ZrF2+2	1.029e-22	1.195e-23	-21.987	-22.922	-0.935	(0)
ZrF3+	5.915e-23	3.399e-23	-22.228	-22.469	-0.241	(0)
ZrF4	1.275e-23	1.275e-23	-22.895	-22.895	0.000	(0)
ZrF+3	1.069e-23	1.026e-25	-22.971	-24.989	-2.018	(0)
ZrF5-	4.238e-24	2.435e-24	-23.373	-23.614	-0.241	(0)
ZrF6 2-	9.736e-25	1.018e-25	-24.012	-24.992	-0.981	(0)
SiF6 2-	9.535e-26	9.971e-27	-25.021	-26.001	-0.981	(0)
BF3OH-	2.293e-37	1.318e-37	-36.640	-36.880	-0.241	(0)
Fe (2)	9.870e-06					
FeCl+	5.114e-06	2.938e-06	-5.291	-5.532	-0.241	(0)
Fe+2	4.163e-06	6.294e-07	-5.381	-6.201	-0.821	(0)
FeCl4 2-	4.887e-07	5.110e-08	-6.311	-7.292	-0.981	(0)

FeHCO3+	5.517e-08	3.170e-08	-7.258	-7.499	-0.241	(0)
FeCl2	4.885e-08	4.885e-08	-7.311	-7.311	0.000	(0)
FeF+	2.051e-10	1.178e-10	-9.688	-9.929	-0.241	(0)
FeOH+	2.264e-11	1.301e-11	-10.645	-10.886	-0.241	(0)
FeSO4	2.059e-11	2.059e-11	-10.686	-10.686	0.000	(0)
FeCO3	9.268e-12	9.268e-12	-11.033	-11.033	0.000	(0)
FeHPO4	2.949e-15	2.949e-15	-14.530	-14.530	0.000	(0)
Fe (OH) 2	6.754e-18	6.754e-18	-17.170	-17.170	0.000	(0)
FePO4-	3.187e-18	1.831e-18	-17.497	-17.737	-0.241	(0)
FeH2PO4+	1.061e-20	6.096e-21	-19.974	-20.215	-0.241	(0)
Fe (OH) 3-	3.059e-23	1.757e-23	-22.514	-22.755	-0.241	(0)
Fe (OH) 4-2	1.098e-32	1.149e-33	-31.959	-32.940	-0.981	(0)
Fe (3)	4.674e-16					
Fe (OH) 2+	2.160e-16	1.241e-16	-15.666	-15.906	-0.241	(0)
FeCl+2	1.058e-16	1.228e-17	-15.976	-16.911	-0.935	(0)
FeF2+	6.770e-17	3.890e-17	-16.169	-16.410	-0.241	(0)
FeOH+2	4.938e-17	5.734e-18	-16.306	-17.242	-0.935	(0)
FeF+2	2.389e-17	2.774e-18	-16.622	-17.557	-0.935	(0)
Fe (OH) 3	3.794e-18	3.794e-18	-17.421	-17.421	0.000	(0)
Fe+3	4.196e-19	1.359e-20	-18.377	-19.867	-1.490	(0)
FeSO4+	3.569e-19	2.050e-19	-18.447	-18.688	-0.241	(0)
FeCl2+	2.566e-20	1.474e-20	-19.591	-19.831	-0.241	(0)
FeCO3+	1.286e-20	7.387e-21	-19.891	-20.132	-0.241	(0)
FeHPO4+	4.214e-22	2.421e-22	-21.375	-21.616	-0.241	(0)
Fe (OH) 4-	1.084e-22	6.229e-23	-21.965	-22.206	-0.241	(0)
FeCl4-	2.481e-25	1.425e-25	-24.605	-24.846	-0.241	(0)
Fe2 (OH) 2+4	2.437e-30	8.851e-34	-29.613	-33.053	-3.440	(0)
Fe (SO4) 2-	1.649e-30	9.474e-31	-29.783	-30.023	-0.241	(0)
FeH2PO4+2	3.344e-32	3.884e-33	-31.476	-32.411	-0.935	(0)
Fe3 (OH) 4+5	0.000e+00	0.000e+00	-41.479	-46.639	-5.160	(0)
H (0)	3.436e-06					
H2	1.718e-06	1.864e-06	-5.765	-5.729	0.036	(0)
K	9.833e-03					
K+	9.088e-03	4.913e-03	-2.042	-2.309	-0.267	(0)
KCl	7.443e-04	7.443e-04	-3.128	-3.128	0.000	(0)
KSO4-	4.994e-07	2.869e-07	-6.302	-6.542	-0.241	(0)
KHSO4	7.799e-09	7.799e-09	-8.108	-8.108	0.000	(0)
KOH	1.113e-12	1.113e-12	-11.953	-11.953	0.000	(0)
KHP04-	6.065e-14	3.485e-14	-13.217	-13.458	-0.241	(0)
KP207-3	4.412e-19	2.697e-21	-18.355	-20.569	-2.214	(0)
Li	2.074e-03					
Li+	1.961e-03	1.236e-03	-2.707	-2.908	-0.201	(0)
LiCl	1.123e-04	1.123e-04	-3.950	-3.950	0.000	(0)
LiSO4-	2.615e-09	1.502e-09	-8.583	-8.823	-0.241	(0)
LiOH	1.850e-12	1.850e-12	-11.733	-11.733	0.000	(0)
Mg	1.937e-02					
MgCl+	1.262e-02	7.249e-03	-1.899	-2.140	-0.241	(0)
Mg+2	6.232e-03	1.229e-03	-2.205	-2.911	-0.705	(0)
MgHCO3+	2.484e-04	1.427e-04	-3.605	-3.845	-0.241	(0)
MgSO4	2.299e-04	2.299e-04	-3.639	-3.639	0.000	(0)
MgF+	3.936e-05	2.262e-05	-4.405	-4.646	-0.241	(0)
MgB (OH) 4+	1.520e-07	8.733e-08	-6.818	-7.059	-0.241	(0)
MgCO3	2.507e-08	2.507e-08	-7.601	-7.601	0.000	(0)
MgHPO4	1.176e-12	1.176e-12	-11.930	-11.930	0.000	(0)
MgPO4-	2.837e-16	1.630e-16	-15.547	-15.788	-0.241	(0)
MgH2PO4+	1.889e-18	1.085e-18	-17.724	-17.964	-0.241	(0)
MgP207-2	1.171e-18	1.224e-19	-17.932	-18.912	-0.981	(0)
Mg4 (OH) 4+4	2.037e-29	7.397e-33	-28.691	-32.131	-3.440	(0)
Na	1.378e-01					
Na+	1.181e-01	6.785e-02	-0.928	-1.168	-0.241	(0)
NaCl	1.967e-02	1.967e-02	-1.706	-1.706	0.000	(0)
NaAlO2	4.462e-06	4.462e-06	-5.351	-5.351	0.000	(0)
NaF	1.488e-06	1.488e-06	-5.827	-5.827	0.000	(0)
NaHSiO3	5.503e-07	5.503e-07	-6.259	-6.259	0.000	(0)
NaSO4-	1.611e-07	9.255e-08	-6.793	-7.034	-0.241	(0)
NaHCO3	1.362e-07	1.362e-07	-6.866	-6.866	0.000	(0)
NaOH	1.295e-07	1.295e-07	-6.888	-6.888	0.000	(0)
NaB (OH) 4	1.137e-07	1.137e-07	-6.944	-6.944	0.000	(0)
NaHPO4-	1.156e-12	6.643e-13	-11.937	-12.178	-0.241	(0)
NaCO3-	1.163e-14	6.681e-15	-13.935	-14.175	-0.241	(0)
NaHP207-2	9.733e-23	1.018e-23	-22.012	-22.992	-0.981	(0)
NaP207-3	5.013e-25	3.064e-27	-24.300	-26.514	-2.214	(0)
Na2P207-2	1.579e-25	1.651e-26	-24.802	-25.782	-0.981	(0)
O (0)	2.982e-37					
O2	1.491e-37	1.618e-37	-36.826	-36.791	0.036	(0)
P (-3)	0.000e+00					
PH4+	0.000e+00	0.000e+00	-165.202	-165.442	-0.241	(0)
P (5)	7.910e-09					
H2PO4-	7.518e-09	4.319e-09	-8.124	-8.365	-0.241	(0)
H3PO4	3.778e-10	3.778e-10	-9.423	-9.423	0.000	(0)
HPO4-2	1.126e-11	1.177e-12	-10.949	-11.929	-0.981	(0)
MgHPO4	1.176e-12	1.176e-12	-11.930	-11.930	0.000	(0)
NaHPO4-	1.156e-12	6.643e-13	-11.937	-12.178	-0.241	(0)
CaHPO4	4.267e-13	4.267e-13	-12.370	-12.370	0.000	(0)
KHP04-	6.065e-14	3.485e-14	-13.217	-13.458	-0.241	(0)
HP207-3	3.767e-14	2.303e-16	-13.424	-15.638	-2.214	(0)
PO3F-2	2.227e-14	2.329e-15	-13.652	-14.633	-0.981	(0)
FeHPO4	2.949e-15	2.949e-15	-14.530	-14.530	0.000	(0)
HPO3F-	8.366e-16	4.807e-16	-15.077	-15.318	-0.241	(0)
MgPO4-	2.837e-16	1.630e-16	-15.547	-15.788	-0.241	(0)
H2P207-2	2.176e-16	2.275e-17	-15.662	-16.643	-0.981	(0)
CaPO4-	1.132e-16	6.502e-17	-15.946	-16.187	-0.241	(0)
H3P207-	4.788e-18	2.751e-18	-17.320	-17.561	-0.241	(0)
H4P207	3.873e-18	3.873e-18	-17.412	-17.412	0.000	(0)
FePO4	3.187e-18	1.831e-18	-17.497	-17.737	-0.241	(0)
MgH2PO4+	1.889e-18	1.085e-18	-17.724	-17.964	-0.241	(0)
PO4-3	1.661e-18	1.015e-20	-17.780	-19.993	-2.214	(0)
MgP207-2	1.171e-18	1.224e-19	-17.932	-18.912	-0.981	(0)
CaH2PO4+	5.572e-19	3.202e-19	-18.254	-18.495	-0.241	(0)
P207-4	4.982e-19	5.716e-23	-18.303	-22.243	-3.940	(0)
KP207-3	4.412e-19	2.697e-21	-18.355	-20.569	-2.214	(0)
AlHPO4+	7.006e-20	4.026e-20	-19.155	-19.395	-0.241	(0)
H2PO3F	5.047e-20	5.047e-20	-19.297	-19.297	0.000	(0)
FeH2PO4+	1.061e-20	6.096e-21	-19.974	-20.215	-0.241	(0)
FeHPO4+	4.214e-22	2.421e-22	-21.375	-21.616	-0.241	(0)
NaHP207-2	9.733e-23	1.018e-23	-22.012	-22.992	-0.981	(0)
CaP207-2	9.218e-24	9.639e-25	-23.035	-24.016	-0.981	(0)
NaP207-3	5.013e-25	3.064e-27	-24.300	-26.514	-2.214	(0)

	Na2P2O7-2	1.579e-25	1.651e-26	-24.802	-25.782	-0.981	(0)
	AlH2PO4+2	2.852e-28	3.312e-29	-27.545	-28.480	-0.935	(0)
	FeH2PO4+2	3.344e-32	3.884e-33	-31.476	-32.411	-0.935	(0)
S (-2)	2.607e-05						
	H2S	2.582e-05	2.582e-05	-4.588	-4.588	0.000	(0)
	HS-	2.496e-07	1.393e-07	-6.603	-6.856	-0.253	(0)
	S-2	2.617e-10	3.345e-11	-9.582	-10.476	-0.893	(0)
	S2-2	1.221e-15	1.277e-16	-14.913	-15.894	-0.981	(0)
	S3-2	4.788e-19	5.007e-20	-18.320	-19.300	-0.981	(0)
	S4-2	1.369e-22	1.431e-23	-21.864	-22.844	-0.981	(0)
	S5-2	2.937e-26	3.072e-27	-25.532	-26.513	-0.981	(0)
S (2)	1.210e-12						
	S2O3-2	6.049e-13	6.325e-14	-12.218	-13.199	-0.981	(0)
	HS2O3-	1.866e-17	1.072e-17	-16.729	-16.970	-0.241	(0)
S (3)	7.261e-24						
	S2O4-2	3.630e-24	4.639e-25	-23.440	-24.334	-0.893	(0)
S (4)	1.670e-09						
	HSO3-	9.345e-10	5.369e-10	-9.029	-9.270	-0.241	(0)
	SO2	7.352e-10	7.352e-10	-9.134	-9.134	0.000	(0)
	SO3-2	3.598e-14	4.178e-15	-13.444	-14.379	-0.935	(0)
	H2SO3	1.840e-15	1.840e-15	-14.735	-14.735	0.000	(0)
	S4O6-2	1.437e-24	1.503e-25	-23.843	-24.823	-0.981	(0)
	S2O6-2	1.688e-25	1.765e-26	-24.773	-25.753	-0.981	(0)
	S3O6-2	5.198e-31	5.436e-32	-30.284	-31.265	-0.981	(0)
	S5O6-2	3.027e-40	0.000e+00	-39.519	-40.500	-0.981	(0)
S (5)	7.912e-24						
	S2O5-2	3.956e-24	4.137e-25	-23.403	-24.383	-0.981	(0)
S (6)	2.359e-04						
	MgSO4	2.299e-04	2.299e-04	-3.639	-3.639	0.000	(0)
	CaSO4	2.245e-06	2.245e-06	-5.649	-5.649	0.000	(0)
	SO4-2	1.974e-06	2.065e-07	-5.705	-6.685	-0.981	(0)
	HSO4-	1.163e-06	6.681e-07	-5.934	-6.175	-0.241	(0)
	KSO4-	4.994e-07	2.869e-07	-6.302	-6.542	-0.241	(0)
	NaSO4-	1.611e-07	9.255e-08	-6.793	-7.034	-0.241	(0)
	RHSO4	7.799e-09	7.799e-09	-8.108	-8.108	0.000	(0)
	LiSO4	2.615e-09	1.502e-09	-8.583	-8.823	-0.241	(0)
	FeSO4	2.059e-11	2.059e-11	-10.686	-10.686	0.000	(0)
	H2SO4	5.302e-18	5.302e-18	-17.276	-17.276	0.000	(0)
	AlSO4+	5.006e-19	2.876e-19	-18.301	-18.541	-0.241	(0)
	FeSO4+	3.569e-19	2.050e-19	-18.447	-18.688	-0.241	(0)
	Al (SO4) 2-	8.023e-24	4.610e-24	-23.096	-23.336	-0.241	(0)
	Fe (SO4) 2-	1.649e-30	9.474e-31	-29.783	-30.023	-0.241	(0)
	ZrSO4+2	2.352e-31	2.732e-32	-30.628	-31.564	-0.935	(0)
	Zr (SO4) 2	2.763e-36	2.763e-36	-35.559	-35.559	0.000	(0)
	Zr (SO4) 3-2	0.000e+00	0.000e+00	-40.259	-41.240	-0.981	(0)
S (7)	0.000e+00						
	S2O8-2	0.000e+00	0.000e+00	-45.725	-46.705	-0.981	(0)
S (8)	1.925e-35						
	HSO5-	1.925e-35	1.106e-35	-34.716	-34.956	-0.241	(0)
Si	5.988e-03						
	SiO2	5.987e-03	5.987e-03	-2.223	-2.223	0.000	(0)
	HSiO3-	6.257e-07	3.595e-07	-6.204	-6.444	-0.241	(0)
	NaHSiO3	5.503e-07	5.503e-07	-6.259	-6.259	0.000	(0)
	H6 (H2SiO4) 4-2	1.835e-12	1.919e-13	-11.736	-12.717	-0.981	(0)
	H2SiO4-2	2.682e-15	2.804e-16	-14.572	-15.552	-0.981	(0)
	H4 (H2SiO4) 4-4	3.110e-22	3.568e-26	-21.507	-25.448	-3.940	(0)
	SiF6-2	9.535e-26	9.971e-27	-25.021	-26.001	-0.981	(0)
Ti	3.688e-03						
	Ti (OH) 4	3.688e-03	3.688e-03	-2.433	-2.433	0.000	(0)
Zr	2.042e-11						
	Zr (OH) 4	2.041e-11	2.041e-11	-10.690	-10.690	0.000	(0)
	Zr (OH) 3+	3.408e-15	1.958e-15	-14.467	-14.708	-0.241	(0)
	Zr (OH) 2+2	6.957e-19	8.079e-20	-18.158	-19.093	-0.935	(0)
	Zr (OH) 5-	7.196e-21	4.134e-21	-20.143	-20.384	-0.241	(0)
	ZrOH+3	2.478e-22	2.378e-24	-21.606	-23.624	-2.018	(0)
	ZrF2+2	1.029e-22	1.195e-23	-21.987	-22.922	-0.935	(0)
	ZrF3+	5.915e-23	3.399e-23	-22.228	-22.469	-0.241	(0)
	ZrF4	1.275e-23	1.275e-23	-22.895	-22.895	0.000	(0)
	ZrF+3	1.069e-23	1.026e-25	-22.971	-24.989	-2.018	(0)
	ZrF5-	4.238e-24	2.435e-24	-23.373	-23.614	-0.241	(0)
	ZrF6-2	9.736e-25	1.018e-25	-24.012	-24.992	-0.981	(0)
	Zr+4	7.267e-27	3.275e-29	-26.139	-28.485	-2.346	(0)
	ZrSO4+2	2.352e-31	2.732e-32	-30.628	-31.564	-0.935	(0)
	Zr (SO4) 2	2.763e-36	2.763e-36	-35.559	-35.559	0.000	(0)
	Zr (SO4) 3-2	0.000e+00	0.000e+00	-40.259	-41.240	-0.981	(0)
	Zr3 (OH) 4+8	0.000e+00	0.000e+00	-53.555	-66.773	-13.218	(0)
	Zr4 (OH) 8+8	0.000e+00	0.000e+00	-68.159	-81.377	-13.218	(0)

-----Saturation indices-----				
Phase	SI**	log IAP	log K (523 K, 155 atm)	
Afwillite	-20.27	14.70	34.96	Ca3Si2O4 (OH) 6
Akermanite	-6.94	14.98	21.92	Ca2MgSi2O7
Al	-49.13	27.08	76.20	Al
Al (g)	-75.22	27.08	102.29	Al
Al2 (SO4) 3	-31.51	-49.79	-18.28	Al2 (SO4) 3
Al2 (SO4) 3:6H2O	-27.77	-49.81	-22.04	Al2 (SO4) 3:6H2O
Albite	0.00	-3.57	-3.57	NaAlSi3O8
Albite_high	-0.49	-3.57	-3.08	NaAlSi3O8
Albite_low	-0.00	-3.57	-3.57	NaAlSi3O8
AlF3	-6.21	-30.13	-23.92	AlF3
Alum-K	-21.58	-30.59	-9.01	KAl (SO4) 2:12H2O
Alunite	-6.95	-31.59	-24.65	KAl3 (OH) 6 (SO4) 2
Amesite-14A	7.96	20.09	12.13	Mg4Al4Si2O10 (OH) 8
Analcime	-0.39	-1.57	-1.17	Na.96Al.96Si2.04O6:H2O
Analcime-dehy	-3.51	-1.56	1.95	Na.96Al.96Si2.04O6
Anatase	6.06	-2.43	-8.49	TiO2
Andalusite	0.52	-3.26	-3.77	Al2SiO5
Andradite	-5.28	1.45	6.73	Ca3Fe2 (SiO4) 3
Anhydrite	-1.34	-9.87	-8.52	CaSO4
Ankerite	-1.72	-6.86	-5.14	CaMg0.3Fe0.7 (CO3) 2
Annite	-1.59	5.38	6.97	KFe3AlSi3O10 (OH) 2
Anorthite	0.00	0.90	0.90	CaAl2 (SiO4) 2
Antarcticite	-9.19	-5.30	3.89	CaCl2:6H2O
Anthophyllite	3.62	28.80	25.18	Mg7Si8O22 (OH) 2
Antigorite	36.47	243.74	207.27	Mg48Si34O85 (OH) 62
Aphthitalite	-17.58	-21.46	-3.89	NaK3 (SO4) 2
Aragonite	-1.21	-2.41	-1.20	CaCO3

Arcanite	-8.71	-11.30	-2.59	K2SO4
Artinite	-4.95	4.50	9.45	Mg2CO3(OH)2·3H2O
B	-34.15	25.98	60.13	B
B(g)	-82.98	25.98	108.96	B
B2O3	-6.26	-3.22	3.03	B2O3
Baddeleyite	-1.81	-9.52	-7.72	ZrO2
Bassanite	-2.04	-9.87	-7.83	CaSO4·0.5H2O
Beidellite-Ca	2.28	-8.31	-10.59	Ca.165Al2.33Si3.67O10(OH)2
Beidellite-H	1.54	-9.37	-10.91	H.33Al2.33Si3.67O10(OH)2
Beidellite-K	1.41	-8.55	-9.97	K.33Al2.33Si3.67O10(OH)2
Beidellite-Mg	2.56	-8.27	-10.83	Mg.165Al2.33Si3.67O10(OH)2
Beidellite-Na	1.74	-8.18	-9.92	Na.33Al2.33Si3.67O10(OH)2
Berlinite	-3.96	-22.01	-18.05	AlPO4
BF3(g)	-18.34	-31.22	-12.88	BF3
Bischofite	-9.21	-5.03	4.18	MgCl2·6H2O
Bloedite	-16.02	-18.63	-2.62	Na2Mg(SO4)2·4H2O
Boehmite	1.03	-0.52	-1.55	AlO2H
Borax	-17.81	0.74	18.55	Na2(B4O5(OH)4)·8H2O
Boric acid	-2.83	-1.62	1.22	B(OH)3
Brucite	-1.46	6.65	8.11	Mg(OH)2
Brushite	-21.60	-15.12	6.48	CaHPO4·2H2O
Burkeite	-29.10	-19.61	9.49	Na6CO3(SO4)2
C	-4.37	27.99	32.36	C
C(g)	-68.16	27.99	96.15	C
Ca	-52.37	24.78	77.15	Ca
Ca(g)	-64.42	24.78	89.20	Ca
Ca-Al Pyroxene	-3.47	3.13	6.59	CaAl2SiO6
Ca2Al2O5·8H2O	-47.42	11.70	59.12	Ca2Al2O5·8H2O
Ca2Cl2(OH)2·H2O	-25.08	1.10	26.19	Ca2Cl2(OH)2·H2O
Ca3Al2O6	-32.19	18.12	50.31	Ca3Al2O6
Ca4Al2Fe2O10	-40.93	13.47	54.40	Ca4Al2Fe2O10
Ca4Al2O7·13H2O	-82.11	24.45	106.56	Ca4Al2O7·13H2O
Ca4Al2O7·19H2O	-78.35	24.43	102.78	Ca4Al2O7·19H2O
Ca4Cl2(OH)6·13H2O	-53.86	13.82	67.67	Ca4Cl2(OH)6·13H2O
CaAl2O4	-7.13	5.35	12.48	CaAl2O4
CaAl2O4·10H2O	-32.20	5.31	37.51	CaAl2O4·10H2O
CaAl4O7	-9.28	4.31	13.59	CaAl4O7
Calcite	-1.05	-2.41	-1.36	CaCO3
Carnallite	-12.45	-8.39	4.06	KMgCl3·6H2O
CaSO4·0.5H2O(beta)	-2.03	-9.87	-7.84	CaSO4·0.5H2O
CaZrO3	84.88	-3.14	-88.02	CaZrO3
Celadonite	0.67	-0.28	-0.95	KMgAlSi4O10(OH)2
CH4(g)	-7.48	-10.09	-2.60	CH4
Chalcedony	-0.15	-2.22	-2.07	SiO2
Chamosite-7A	0.00	3.46	3.46	Fe2Al2SiO5(OH)4
Chloromagnesite	-12.35	-5.01	7.35	MgCl2
Chrysotile	1.74	15.51	13.77	Mg3Si2O5(OH)4
Cl2(g)	-27.43	-30.06	-2.62	Cl2
Clinocllore-14A	7.07	25.55	18.48	Mg5Al2Si3O10(OH)8
Clinocllore-7A	4.61	25.55	20.94	Mg5Al2Si3O10(OH)8
Clinoptilolite-Ca	2.40	-23.16	-25.56	Ca1.7335Al3.45Fe.0178Si14.533036:10.922H2O
Clinoptilolite-dehy-Ca	-14.02	-23.12	-9.09	Ca1.7335Al3.45Fe.0178Si14.533036
Clinoptilolite-dehy-K	-23.32	-25.61	-2.29	K3.467Al3.45Fe.0178Si14.533036
Clinoptilolite-dehy-Na	-19.42	-21.65	-2.24	Na3.467Al3.45Fe.0178Si14.533036
Clinoptilolite-hy-Ca	1.69	-23.16	-24.85	Ca1.7335Al3.45Fe.0178Si14.533036:11.645H2O
Clinoptilolite-hy-K	-4.27	-25.64	-21.37	K3.467Al3.45Fe.0178Si14.533036:7.499H2O
Clinoptilolite-hy-Na	-3.08	-21.70	-18.62	Na3.467Al3.45Fe.0178Si14.533036:10.877H2O
Clinoptilolite-K	-7.21	-25.65	-18.44	K3.467Al3.45Fe.0178Si14.533036:10.922H2O
Clinoptilolite-Na	-3.11	-21.70	-18.58	Na3.467Al3.45Fe.0178Si14.533036:10.922H2O
Clinzoisite	-0.02	4.55	4.56	Ca2Al3Si3O12(OH)
CO(g)	-5.72	-8.23	-2.51	CO
CO2(g)	1.29	-0.78	-2.08	CO2
Coesite	-0.49	-2.22	-1.73	SiO2
Colemanite	-18.50	3.08	21.58	Ca2B6O11·5H2O
Cordierite_anhyd	1.04	0.12	-0.91	Mg2Al4Si5O18
Cordierite_hydr	2.04	0.12	-1.92	Mg2Al4Si5O18·H2O
Corundum	4.67	-1.04	-5.71	Al2O3
Cristobalite(alpha)	-0.27	-2.22	-1.96	SiO2
Cristobalite(beta)	-0.44	-2.22	-1.78	SiO2
Cronstedtite-7A	-2.16	-6.54	-4.38	Fe2Fe2SiO5(OH)4
Daphnite-14A	-0.61	9.10	9.71	Fe5AlAlSi3O10(OH)8
Daphnite-7A	-2.97	9.10	12.08	Fe5AlAlSi3O10(OH)8
Dawsonite	-4.33	-5.71	-1.38	NaAlCO3(OH)2
Diaspore	1.18	-0.52	-1.70	AlHO2
Dicalcium silicate	-9.26	10.55	19.80	Ca2SiO4
Diopside	-0.80	8.59	9.39	CaMgSi2O6
Dolomite	-0.20	-4.56	-4.36	CaMg(CO3)2
Dolomite-dis	-0.82	-4.56	-3.74	CaMg(CO3)2
Dolomite-ord	-0.19	-4.56	-4.37	CaMg(CO3)2
Enstatite	-0.00	4.43	4.43	MgSiO3
Epidote	-0.00	-0.46	-0.46	Ca2FeAl2Si3O12OH
Epidote-ord	-0.04	-0.46	-0.42	FeCa2Al2(OH)(SiO4)3
Epsomite	-7.42	-9.62	-2.20	MgSO4·7H2O
Etringite	-54.96	-11.61	43.35	Ca6Al2(SO4)3(OH)12·26H2O
Eucryptite	-2.80	-0.87	1.93	LiAlSiO4
F2(g)	-63.06	-38.14	24.93	F2
Fayalite	-2.18	4.51	6.68	Fe2SiO4
Fe	-8.57	21.76	30.33	Fe
Fe(OH)2	-3.35	3.36	6.71	Fe(OH)2
Fe(OH)3	-4.49	-5.52	-1.03	Fe(OH)3
Fe2(SO4)3	-34.30	-59.79	-25.49	Fe2(SO4)3
FeF2	-7.67	-16.38	-8.71	FeF2
FeF3	-11.61	-35.13	-23.52	FeF3
FeO	-2.03	3.36	5.39	FeO
Ferrite-Ca	-4.70	-4.65	0.04	CaFe2O4
Ferrite-Dicalcium	-17.59	1.73	19.33	Ca2Fe2O5
Ferrite-Mg	-2.79	-4.38	-1.59	MgFe2O4
Ferrosilite	-1.10	1.14	2.25	FeSiO3
FeSO4	-7.27	-12.89	-5.61	FeSO4
Fluorapatite	0.00	-42.42	-42.42	Ca5(PO4)3F
Fluorite	-1.75	-13.36	-11.60	CaF2
Forsterite	-0.64	11.09	11.72	Mg2SiO4
Foshagite	-17.60	18.86	36.46	Ca4Si3O9(OH)2·0.5H2O
Gaylussite	-15.00	-4.00	10.99	CaNa2(CO3)2·5H2O
Gehlenite	-7.62	9.51	17.14	Ca2Al2SiO7
Gibbsite	0.65	-0.52	-1.17	Al(OH)3
Gismondine	-39.36	1.77	41.13	Ca2Al4Si4O16·9H2O
Glauberite	-13.42	-18.89	-5.47	Na2Ca(SO4)2

Goethite	-1.40	-5.52	-4.13	FeOOH
Greenalite	-3.08	5.64	8.72	Fe3Si2O5(OH)4
Grossular	-4.12	11.45	15.57	Ca3Al2(SiO4)3
Gypsum	-2.70	-9.87	-7.17	CaSO4·2H2O
Gyrolite	-8.76	6.09	14.85	Ca2Si3O7(OH)2·1.5H2O
H2(g)	-3.12	-5.73	-2.61	H2
H2O(g)	1.56	-0.00	-1.56	H2O
H2S(g)	-3.05	-11.64	-8.59	H2S
Halite	-3.12	-2.22	0.91	NaCl
Hatrurite	-22.56	16.93	39.49	Ca3SiO5
HCl(g)	-5.65	-5.83	-0.18	HCl
Hedenbergite	-3.25	5.30	8.55	CaFe(SiO3)2
Hematite	0.00	-11.04	-11.04	Fe2O3
Hercynite	0.86	2.33	1.46	FeAl2O4
Hexahydrite	-7.69	-9.62	-1.93	MgSO4·6H2O
Hillebrandite	-10.26	10.54	20.80	Ca2SiO3(OH)2·0.17H2O
Huntite	-1.73	-8.84	-7.11	CaMg3(CO3)4
Hydroboracite	-17.05	3.35	20.40	MgCaB6O11·6H2O
Hydromagnesite	-6.62	-1.94	4.68	Mg5(CO3)4(OH)2·4H2O
Hydrophilite	-8.23	-5.28	2.95	CaCl2
Hydroxylapatite	-5.64	-32.56	-26.92	Ca5(OH)(PO4)3
Ice	-1.14	-0.00	1.14	H2O
Illite	1.90	-5.83	-7.73	K0.6Mg0.25Al1.8Al0.5Si3.5O10(OH)2
Ilmenite	0.00	0.94	0.94	FeTiO3
Jadeite	-1.64	-1.35	0.29	NaAl(SiO3)2
Jarosite	-19.68	-46.59	-26.91	KFe3(SO4)2(OH)6
Jarosite-Na	-39.80	-45.45	-5.66	NaFe3(SO4)2(OH)6
K	-29.56	11.67	41.23	K
K(g)	-33.67	11.67	45.34	K
K-Feldspar	0.00	-4.71	-4.71	KAlSi3O8
KZCO3·1.5H2O	-17.18	-3.86	13.33	KZCO3·1.5H2O
K2O	-47.01	4.95	51.96	K2O
K3H(SO4)2	-21.46	-25.08	-3.62	K3H(SO4)2
K8H4(CO3)6·3H2O	-60.62	-33.02	27.61	K8H4(CO3)6·3H2O
Kainite	-12.55	-12.96	-0.42	KMgCl3SO4·3H2O
KAl(SO4)2	-17.32	-30.54	-13.22	KAl(SO4)2
Kalclinite	-6.61	-6.33	0.28	KHCO3
Kalsilite	-1.73	-0.27	1.46	KAlSiO4
Kaolinite	1.46	-5.49	-6.95	Al2Si2O5(OH)4
Katoite	-60.43	18.09	78.53	Ca3Al2H12O12
Kieserite	-9.30	-9.60	-0.30	MgSO4·H2O
KMgCl3	-17.01	-8.36	8.65	KMgCl3
KMgCl3·2H2O	-14.91	-8.37	6.54	KMgCl3·2H2O
KNaCO3·6H2O	-12.79	-2.73	10.05	KNaCO3·6H2O
Kyanite	0.46	-3.26	-3.72	Al2SiO5
Lansfordite	-6.83	-2.16	4.67	MgCO3·5H2O
Larnite	-9.82	10.55	20.36	Ca2SiO4
Laumontite	0.30	-3.56	-3.86	CaAl2Si4O12·4H2O
Lawrencite	-8.31	-8.30	0.02	FeCl2
Lawsonite	-0.40	0.90	1.30	CaAl2Si2O7(OH)2·H2O
Leonite	-16.66	-20.91	-4.25	K2Mg(SO4)2·4H2O
Li	-30.23	11.07	41.30	Li
Li(g)	-40.60	11.07	51.68	Li
Lime	-11.45	6.38	17.83	CaO
Magnesite	0.00	-2.14	-2.14	MgCO3
Magnetite	-0.28	-7.67	-7.40	Fe3O4
Margarite	2.02	-0.14	-2.15	CaAl4Si2O10(OH)2
Maximum Microcline	0.02	-4.71	-4.73	KAlSi3O8
Mayenite	-117.81	69.37	187.18	Ca12Al14O33
Melanterite	-10.07	-12.91	-2.85	FeSO4·7H2O
Mercallite	-12.34	-13.78	-1.44	KHSO4
Merwinite	-12.95	21.36	34.32	MgCa3(SiO4)2
Mesolite	1.36	-1.09	-2.45	Na.676Ca.657Al1.99Si3.01O10·2.647H2O
Mg	-40.74	25.05	65.79	Mg
Mg(g)	-49.61	25.05	74.66	Mg
Mg1.25SO4(OH)0.5·0.5H2O	-3.35	-7.93	-4.59	Mg1.25SO4(OH)0.5·0.5H2O
Mg1.5SO4(OH)	-3.47	-6.27	-2.80	Mg1.5SO4(OH)
MgCl2·2H2O	-8.68	-5.01	3.67	MgCl2·2H2O
MgCl2·4H2O	-7.24	-5.02	2.22	MgCl2·4H2O
MgCl2·H2O	-9.78	-5.01	4.78	MgCl2·H2O
MgOHCl	-4.99	0.82	5.81	MgOHCl
MgSO4	-4.95	-9.60	-4.64	MgSO4
Minnesotaite	-1.76	1.20	2.96	Fe3Si4O10(OH)2
Mirabilite	-17.82	-9.06	8.76	Na2SO4·10H2O
Misenite	-82.90	-93.97	-11.08	K8H6(SO4)7
Molysite	-20.45	-23.01	-2.56	FeCl3
Monohydrocalcite	-3.47	-2.42	1.06	CaCO3·H2O
Monticellite	-3.21	10.82	14.03	CaMgSiO4
Montmor-Ca	2.33	-6.51	-8.84	Ca.165Mg.33Al1.67Si4O10(OH)2
Montmor-K	1.60	-6.75	-8.35	K.33Mg.33Al1.67Si4O10(OH)2
Montmor-Mg	2.64	-6.47	-9.11	Mg.495Al1.67Si4O10(OH)2
Montmor-Na	1.84	-6.37	-8.21	Na.33Mg.33Al1.67Si4O10(OH)2
Mordenite	-0.86	-8.59	-7.73	Ca.2895Na.361Al.94Si5.06O12·3.468H2O
Mordenite-dehy	-7.77	-8.58	-0.81	Ca.2895Na.361Al.94Si5.06O12
Muscovite	2.74	-5.75	-8.50	KAl3Si3O10(OH)2
Na	-25.94	12.81	38.75	Na
Na(g)	-31.54	12.81	44.35	Na
Na2CO3	-9.15	-1.57	7.58	Na2CO3
Na2CO3·7H2O	-17.45	-1.60	15.85	Na2CO3·7H2O
Na2O	-34.32	7.23	41.54	Na2O
Na2SiO3	-10.91	5.01	15.92	Na2SiO3
Na3H(SO4)2	-20.77	-21.66	-0.89	Na3H(SO4)2
Na4Ca(SO4)3·2H2O	-21.96	-27.92	-5.96	Na4Ca(SO4)3·2H2O
Na4SiO4	-34.26	12.23	46.49	Na4SiO4
Na6Si2O7	-49.18	17.24	66.42	Na6Si2O7
NaFeO2	-9.83	-1.90	7.92	NaFeO2
Nahcolite	-5.61	-5.19	0.42	NaHCO3
Natrolite	-2.50	-0.48	2.01	Na2Al2Si3O10·2H2O
Natron	-16.41	-1.61	14.80	Na2CO3·10H2O
Natrosilite	-10.63	2.78	13.41	Na2Si2O5
Nepheline	-1.69	0.87	2.56	NaAlSiO4
Nesquehonite	-6.13	-2.16	3.97	MgCO3·3H2O
Nontronite-Ca	0.19	-18.32	-18.50	Ca.165Fe2Al.33Si3.67H2O12
Nontronite-H	-0.49	-19.37	-18.88	H.33Fe2Al.33Si3.67H2O12
Nontronite-K	-0.68	-18.55	-17.88	K.33Fe2Al.33Si3.67H2O12
Nontronite-Mg	0.47	-18.27	-18.74	Mg.165Fe2Al.33Si3.67H2O12
Nontronite-Na	-0.35	-18.18	-17.83	Na.33Fe2Al.33Si3.67H2O12
O2(g)	-34.15	-36.79	-2.64	O2

Okenite	-7.08	1.93	9.02	CaSi2O4 (OH) 2:H2O
Oxychloride-Mg	-18.13	7.46	25.59	Mg2Cl (OH) 3:4H2O
P	-39.33	24.50	63.83	P
Paragonite	2.10	-4.61	-6.71	NaAl3Si3O10 (OH) 2
Pargasite	-1.81	28.11	29.92	NaCa2Al3Mg4Si6O22 (OH) 2
Pentahydrate	-8.06	-9.62	-1.56	MgSO4:5H2O
Periclase	-3.40	6.65	10.06	MgO
Petalite	0.37	-7.53	-7.90	LiAlSi4O10
Phlogopite	3.56	15.25	11.69	KAlMg3Si3O10 (OH) 2
Picromerite	-16.28	-20.92	-4.65	K2Mg (SO4) 2:6H2O
Pirssonite	-15.25	-3.99	11.25	Na2Ca (CO3) 2:2H2O
Polyhalite	-26.26	-40.64	-14.38	K2MgCa2 (SO4) 4:2H2O
Portlandite	-6.48	6.38	12.86	Ca (OH) 2
Prehnite	-0.86	5.06	5.92	Ca2Al2Si3O10 (OH) 2
Pseudowollastonite	-3.00	4.16	7.16	CaSiO3
Pyrite	-1.75	-21.06	-19.31	FeS2
Pyrophyllite	1.25	-9.93	-11.18	Al2Si4O10 (OH) 2
Pyrrhotite	-2.48	-8.27	-5.79	FeS
Quartz	0.00	-2.22	-2.22	SiO2
Rankinite	-12.59	14.71	27.30	Ca3Si2O7
Ripidolite-14A	4.16	18.97	14.81	Mg3Fe2Al2Si3O10 (OH) 8
Ripidolite-7A	1.73	18.97	17.25	Mg3Fe2Al2Si3O10 (OH) 8
Rutile	7.15	-2.43	-9.58	TiO2
S	-4.14	-30.03	-25.89	S
S2(g)	-12.59	-25.58	-12.99	S2
Sanidine_high	-0.35	-4.71	-4.36	KAlSi3O8
Saponite-Ca	4.62	12.69	8.07	Ca.165Mg3Al.33Si3.67O10 (OH) 2
Saponite-H	3.88	11.63	7.75	H.33Mg3Al.33Si3.67O10 (OH) 2
Saponite-K	3.76	12.45	8.69	K.33Mg3Al.33Si3.67O10 (OH) 2
Saponite-Mg	4.89	12.73	7.84	Mg3.165Al.33Si3.67O10 (OH) 2
Saponite-Na	4.08	12.83	8.75	Na.33Mg3Al.33Si3.67O10 (OH) 2
Scolecite	1.39	-1.33	-2.72	CaAl2Si3O10:3H2O
Sellaite	-0.44	-13.09	-12.65	MgF2
Sepiolite	-2.62	13.26	15.88	Mg4Si6O15 (OH) 2:6H2O
Si	-47.24	34.57	81.81	Si
Si(g)	-84.69	34.57	119.26	Si
Siderite	-1.57	-5.43	-3.86	FeCO3
SiF4(g)	-19.80	-41.70	-21.90	SiF4
Sillimanite	0.39	-3.26	-3.65	Al2SiO5
SiO2(am)	-0.51	-2.22	-1.71	SiO2
Smectite-high-Fe-Mg	1.70	0.82	-0.88	Ca.025Na.1K.2Fe.5Fe.2Mg1.15Al1.25Si3.5H2O12
Smectite-low-Fe-Mg	1.48	-1.74	-3.22	Ca.02Na.15K.2Fe.29Fe.16Mg.9Al1.25Si3.75H2O12
SO2(g)	-8.14	-9.13	-0.99	SO2
Spinel	-0.78	5.62	6.40	Al2MgO4
Spodumene	-1.68	-3.09	-1.41	LiAlSi2O6
Starkeyite	-8.47	-9.61	-1.14	MgSO4:4H2O
Stilbite	1.39	-9.30	-10.69	Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O
Strengite	-9.80	-27.02	-17.22	FePO4:2H2O
Sylvite	-4.34	-3.36	0.99	KCl
Syngenite	-13.54	-21.17	-7.63	K2Ca (SO4) 2:2H2O
Tachyhydrite	-32.06	-15.33	16.73	Mg2CaCl6:12H2O
Talc	3.67	11.07	7.40	Mg3Si4O10 (OH) 2
Thenardite	-6.49	-9.02	-2.54	Na2SO4
Thermonatrite	-10.25	-1.57	8.67	Na2CO3:H2O
Ti	-115.00	34.37	149.37	Ti
Ti(g)	-190.05	34.37	224.42	Ti
Ti2O3	-29.58	13.55	43.12	Ti2O3
Ti3O5	-23.74	11.12	34.86	Ti3O5
TiB2	-226.26	86.33	312.59	TiB2
TiC	-119.56	62.36	181.92	TiC
TiCl2	-66.73	4.31	71.04	TiCl2
TiCl3	-50.15	-10.72	39.43	TiCl3
TiCl4(g)	-53.94	-25.75	28.19	TiCl4
TiF4(am)	-29.60	-41.91	-12.30	TiF4
TiO(alpha)	-45.23	15.97	61.20	TiO
TiO(g)	-129.67	15.97	145.64	TiO
Titanite	-717.88	1.74	719.62	CaTiSiO5
Tobermorite-11A	-21.57	18.57	40.14	Ca5Si6H11O22.5
Tobermorite-14A	-25.91	18.55	44.46	Ca5Si6H21O27.5
Tobermorite-9A	-21.23	18.58	39.80	Ca5Si6H6O20
Tremolite	3.16	28.26	25.10	Ca2Mg5Si8O22 (OH) 2
Tridymite	-0.52	-2.22	-1.70	SiO2
Troilite	-2.41	-8.27	-5.86	FeS
Trona-K	-20.56	-9.04	11.52	K2NaH (CO3) 2:2H2O
Vivianite	-27.92	-32.92	-5.00	Fe3 (PO4) 2:8H2O
Wairakite	0.22	-3.55	-3.77	CaAl2Si4O10 (OH) 4
Whitlockite	-4.61	-23.83	-19.22	Ca3 (PO4) 2
Wollastonite	-2.98	4.16	7.14	CaSiO3
Wustite	-2.24	2.24	4.48	Fe.947O
Xonotlite	-29.86	24.97	54.82	Ca6Si6O17 (OH) 2
Zircon	-0.00	-11.75	-11.75	ZrSiO4
Zoisite	-0.04	4.55	4.58	Ca2Al3 (SiO4) 3OH
Zr	-67.45	27.27	94.72	Zr
Zr(g)	-249.63	27.44	277.06	Zr
ZrB2	-155.93	-52.39	103.54	ZrB2
ZrC	-151.63	55.43	207.06	ZrC
ZrCl	-118.48	12.41	130.89	ZrCl
ZrCl2	-98.90	-2.62	96.29	ZrCl2
ZrCl3	-80.08	-17.65	62.43	ZrCl3
ZrCl4	-60.66	-32.67	27.98	ZrCl4
ZrF4(beta)	-21.08	-48.84	-27.76	ZrF4
ZrF4(g)	-191.79	-48.84	142.95	ZrF4
ZrH2	-152.39	45.83	198.22	ZrH2

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

End of simulation.

APPENDIX H

KINETIC MODELING RESULT IN AWIBENGKOK FIELD FOR 10 HOURS (0.001 YEAR) AND 1 YEAR TIME STEP

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\llnl.dat

Reading data base.

```
LLNL AQUEOUS MODEL PARAMETERS
NAMED EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END
```

Reading input data for simulation 1.

```
DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.3.7-11094\database\llnl.dat
SOLUTION_SPECIES
CO3-2 + 2 H+ = CO2 + H2O
log_k 16.681
delta_h -5.738 kcal
analytical_expression 464.1965 0.09344813 -26986.16 -165.75951 2248628.9
dw 1.92e-9
vm 7.29 0.92 2.07 -1.23 -1.60 # ref. 1 + McBride et al. 2015, JCED 60, 171
2CO2 = (CO2)2 # activity correction for CO2 solubility at high P, T
log_k -1.8
analytical_expression 8.68 -0.0103 -2190
vm 14.58 1.84 4.14 -2.46 -3.20
END
```

End of simulation.

Reading input data for simulation 2.

```
PHASES
CO2(g)
CO2 = CO2
log_k -1.468
delta_h -4.776 kcal
analytical_expression 10.5624 -2.3547e-2 -3972.8 0 5.8746e5 1.9194e-5
t_c 304.2 # critical T, K
p_c 72.86 # critical P, atm
omega 0.225 # acentric factor
Ankerite
CaMg0.3Fe0.7(CO3)2 + 2H+ = Ca++ + 0.3Mg++ + 0.7Fe++ + 2HCO3-
log_k 1.54
delta_h 0
analytical_expression -1.8649e+03 -2.9583e-01 1.0468e+05 6.7554e+02 -6.0514e+06
END
```

End of simulation.

Reading input data for simulation 3.

```
SOLUTION 1 AWI 1-2
temp 250
pH 6.92
pe 4
redox pe
units ppm
density 1
C(4) 96.2
Ca 227
Cl 6700
Mg 0.71
Na 3680
S(6) 23.6
K 630
B 245
Li 13.5
F 1.82
Si 498
water 1 # kg
pressure 155 atm
EQUILIBRIUM_PHASES 1 Reservoir
CO2(g) 2.20 0.9
RATES
Quartz
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_qtz = SI("Quartz")
30 if (M <= 0 and si_qtz < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_qtz > 0) then SA = 1e-05 #nucleation
60 k_acid = 0
70 k_neut = 10^(-13.40)*EXP(-90.90e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_qtz))
```

```

190 moles = r * TIME
200 SAVE moles
end
Anorthite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_anort = SI("Anorthite")
30 if (M <= 0 and si_anort < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_anort > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-3.5)*EXP(-16.60e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.411)
70 k_neut = 10^(-9.82)*EXP(-31.50e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_anort))
190 moles = r * TIME
200 SAVE moles
end
Albite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_alb = SI("Albite")
30 if (M <= 0 and si_alb < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_alb > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-10.16)*EXP(-65.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.457)
70 k_neut = 10^(-12.56)*EXP(-69.80e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-15.60)*EXP(-71.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.572)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_alb))
190 moles = r * TIME
200 SAVE moles
end
K-Feldspar
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_kfeld = SI("K-Feldspar")
30 if (M <= 0 and si_kfeld < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_kfeld > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-10.06)*EXP(-51.70e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.500)
70 k_neut = 10^(-12.41)*EXP(-38.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-21.20)*EXP(-94.10e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.823)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_kfeld))
190 moles = r * TIME
200 SAVE moles
end
Diopside
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_diopsi = SI("Diopside")
30 if (M <= 0 and si_diopsi < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_diopsi > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-6.36)*EXP(-96.10e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.710)
70 k_neut = 10^(-11.11)*EXP(-40.60e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_diopsi))
190 moles = r * TIME
200 SAVE moles
end
Enstatite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_enst = SI("Enstatite")
30 if (M <= 0 and si_enst < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_enst > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-9.02)*EXP(-80.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.600)
70 k_neut = 10^(-12.72)*EXP(-80.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_enst))
190 moles = r * TIME
200 SAVE moles
end
Ilmenite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_ilmen = SI("Ilmenite")
30 if (M <= 0 and si_ilmen < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_ilmen > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-8.35)*EXP(-37.90e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.421)
70 k_neut = 10^(-11.16)*EXP(-37.90e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_ilmen))
190 moles = r * TIME
200 SAVE moles
end
Titanite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_titan = SI("Titanite") #kyanite
30 if (M <= 0 and si_titan < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_titan > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-10.17)*EXP(-53.90e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.268)
70 k_neut = 10^(-17.44)*EXP(-53.90e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_titan))
190 moles = r * TIME
200 SAVE moles
end

```

```

Hematite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_hema = SI("Hematite")
30 if (M <= 0 and si_hema < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_hema > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-9.39)*EXP(-66.20e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.000)
70 k_neut = 10^(-14.60)*EXP(-66.20e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_hema))
190 moles = r * TIME
200 SAVE moles
end

Epidote
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_epidt = SI("Epidote")
30 if (M <= 0 and si_epidt < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_epidt > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-10.60)*EXP(-71.10e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.338)
70 k_neut = 10^(-11.99)*EXP(-70.70e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 10^(-17.33)*EXP(-79.10e+03/8.314*(1.0/TK-1.0/298.15))*ACT("OH-")^(-0.556)
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_epidt))
190 moles = r * TIME
200 SAVE moles
end

Chamosite-7A
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_cham = SI("Chamosite-7A")
30 if (M <= 0 and si_cham < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_cham > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-11.11)*EXP(-88.00e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.500)
70 k_neut = 10^(-12.52)*EXP(-88.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_cham))
190 moles = r * TIME
200 SAVE moles
end

Calcite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_calc = SI("Calcite")
30 if (M <= 0 and si_calc < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_calc > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-0.30)*EXP(-14.40e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.000)
70 k_neut = 10^(-5.81)*EXP(-23.50e+03/8.314*(1.0/TK-1.0/298.15))
80 k_carb = 10^(-3.48)*EXP(-35.40e+03/8.314*(1.0/TK-1.0/298.15))*PR_P("CO2(g)")^(1.000)
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_calc))
190 moles = r * TIME
200 SAVE moles
end

Dolomite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_dolo = SI("Dolomite")
30 if (M <= 0 and si_dolo < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_dolo > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-3.76)*EXP(-56.70e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.500)
70 k_neut = 10^(-9.60)*EXP(-95.30e+03/8.314*(1.0/TK-1.0/298.15))
80 k_carb = 10^(-5.37)*EXP(-45.70e+03/8.314*(1.0/TK-1.0/298.15))*PR_P("CO2(g)")^(0.500)
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_dolo))
190 moles = r * TIME
200 SAVE moles
end

Magnesite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_magnes = SI("Magnesite")
30 if (M <= 0 and si_magnes < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_magnes > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-6.38)*EXP(-14.40e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(1.000)
70 k_neut = 10^(-9.34)*EXP(-23.50e+03/8.314*(1.0/TK-1.0/298.15))
80 k_carb = 10^(-5.22)*EXP(-62.80e+03/8.314*(1.0/TK-1.0/298.15))*PR_P("CO2(g)")^(1.000)
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_magnes))
190 moles = r * TIME
200 SAVE moles
end

Siderite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_side = SI("Siderite")
30 if (M <= 0 and si_side < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_side > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-3.76)*EXP(-56.70e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.500)
70 k_neut = 10^(-8.60)*EXP(-95.30e+03/8.314*(1.0/TK-1.0/298.15))
80 k_carb = 10^(-5.37)*EXP(-45.70e+03/8.314*(1.0/TK-1.0/298.15))*PR_P("CO2(g)")^(0.500)
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_side))
190 moles = r * TIME
200 SAVE moles
end

Ankerite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]

```

```

20 si_anke = SI("Ankerite")
30 if (M <= 0 and si_anke < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_anke > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-3.76)*EXP(-56.70e+03/8.314*(1.0/TK-1.0/298.15))*ACT("H+")^(0.500)
70 k_neut = 10^(-8.60)*EXP(-95.30e+03/8.314*(1.0/TK-1.0/298.15))
80 k_carb = 10^(-5.37)*EXP(-45.70e+03/8.314*(1.0/TK-1.0/298.15))*PR_P("CO2(g)")^(0.500)
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_anke))
190 moles = r * TIME
200 SAVE moles
end
Dawsonite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_daws = SI("Dawsonite")
30 if (M <= 0 and si_daws < 0) then goto 200
40 SA = PARM(1) * M
50 if (M = 0 and si_daws > 0) then SA = 1e-05 #nucleation
60 k_acid = 10^(-4.48)*EXP(-49.43e+03/8.314*(1.0/TK-1.0/295.15))*ACT("H+")^(0.982)
70 k_neut = 10^(-6.89)*EXP(-63.82e+03/8.314*(1.0/TK-1.0/350.15))
80 k_carb = 0
90 k_rateconst = k_acid + k_neut + k_carb
100 r = k_rateconst * SA * (1-(10^si_daws))
190 moles = r * TIME
200 SAVE moles
end
Anhydrite
start
10 REM PARM(1) = MSA (Molar surface area) [m^2/mol]
20 si_anhyd = SI("Anhydrite")
30 if (M <= 0 and si_anhyd < 0) then goto 200
40 SA = PARM(1)*M
50 if (M = 0 and si_anhyd > 0) then SA = 1e-05 #nucleation
60 k_acid = 0
70 k_neut = 10^(-2.79)*EXP(-0.00e+03/8.314*(1.0/TK-1.0/298.15))
80 k_base = 0
90 k_rateconst = k_acid + k_neut + k_base
100 r = k_rateconst * SA * (1-(10^si_anhyd))
190 moles = r * TIME
200 SAVE moles
end
KINETICS 1
Quartz
formula SiO2 1
m 48.09
m0 48.09
parms 48.064
tol 1e-08
Anorthite
formula CaAl2(SiO4)2 1
m 19.45
m0 19.45
parms 5.548
tol 1e-08
Albite
formula NaAlSi3O8 1
m 30.98
m0 30.98
parms 5.26
tol 1e-08
K-Feldspar
formula KAlSi3O8 1
m 7.87
m0 7.87
parms 86.282
tol 1e-08
Diopside
formula CaMgSi2O6 1
m 0.66
m0 0.66
parms 25.122
tol 1e-08
Enstatite
formula MgSiO3 1
m 10.18
m0 10.18
parms 933.627
tol 1e-08
Ilmenite
formula FeTiO3 1
m 0.38
m0 0.38
parms 31.101
tol 1e-08
Titanite
formula CaTiSiO5 1
m 1.99
m0 1.99
parms 14.68 #0.08(Oelker,1994) and 183.49
tol 1e-08
Hematite
formula Fe2O3 1
m 6.37
m0 6.37
parms 3672.87
tol 1e-08
Epidote
formula Ca2FeAl2Si3O12OH 1
m 1.53
m0 1.53
parms 128.267 #519.3
tol 1e-08
Chamosite-7A
formula Fe2Al2SiO5(OH)4 1
m 11.73
m0 11.73
parms 107.92

```

```

tol      1e-08
Calcite
  formula CaCO3 1
  m        7.9
  m0       7.9
  parms    15.014
  tol      1e-08
Dolomite
  formula CaMg(CO3)2 1
  m        0
  m0       0
  parms    33.192
  tol      1e-08
Magnesite
  formula MgCO3 1
  m        0
  m0       0
  parms    1.096
  tol      1e-08
steps    3 30 300 3000 30000 300000 3000000 30000000 300000000 3000000000 30000000000 300000000000
cvscode  true
KNOBS
convergence_tolerance 1e-10
INCREMENTAL REACTIONS True
USER_GRAPH 1
  -headings      Time Quartz Anorthite Albite K-Feldspar Diopside Enstatite Ilmenite Titanite Hematite Epidote
Chamosite-7A Calcite Dolomite Magnesite
  -axis_titles   "Log10 Time" "kin" ""
  -initial_solutions false
  -connect_simulations true
  -plot_concentration_vs x
-start
10 GRAPH X log10(total_time)
20 GRAPH Y kin("Quartz"), kin("Anorthite"), kin("Albite"), kin("K-Feldspar"), kin("Diopside"), kin("Enstatite"),
kin("Ilmenite"), kin("Titanite"), kin("Hematite"), kin("Epidote"), kin("Chamosite-7A"), kin("Calcite"), kin("Dolomite"), kin("Magnesite")
-end
-active         true
SELECTED_OUTPUT 1
  file           D:\20182 SPRING\Thesis PHREEQC\4. Awibengkok\selected_output_kin salak.sel
  reset          false
  time           true
  step           true
  ph             true
  pe             true
  reaction       true
  totals         C(4)
  molalities     K+ Na+ Ca+2 Mg+2
               HCO3- SO4-2 Cl- CO3-2
  gases          CO2(g)
  kinetic_reactants Quartz Anorthite Albite K-Feldspar
                  Diopside Enstatite Ilmenite Titanite
                  Hematite Epidote Chamosite-7A Calcite
                  Dolomite Magnesite
END
-----
Beginning of initial solution calculations.
-----
Initial solution 1.      AWI 1-2
-----
-----Solution composition-----
Elements      Molality      Moles
B              2.294e-02    2.294e-02
C(4)           1.596e-03    1.596e-03
Ca             5.733e-03    5.733e-03
Cl            1.913e-01    1.913e-01
F             9.697e-05    9.697e-05
K             1.631e-02    1.631e-02
Li            1.969e-03    1.969e-03
Mg            2.957e-05    2.957e-05
Na            1.620e-01    1.620e-01
S(6)          2.487e-04    2.487e-04
Si            8.392e-03    8.392e-03
-----
-----Description of solution-----
pH = 6.920
pe = 4.000
Density (g/cm³) = 0.82270
Volume (L) = 1.23182
Activity of water = 0.993
Ionic strength (mol/kgw) = 1.688e-01
Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = 1.045e-03
Total CO2 (mol/kg) = 1.596e-03
Temperature (°C) = 250.00
Pressure (atm) = 155.00
Electrical balance (eq) = -1.101e-03
Percent error, 100*(Cat-|An|)/(|Cat+|An|) = -0.33
Iterations = 8
Total H = 1.11192e+02
Total O = 5.561551e+01
-----
-----Distribution of species-----
Species      Molality      Activity      Log      Log      Log      mole V
              Molality      Activity      Molality      Activity      Gamma      cm³/mol
OH-          1.013e-04    5.697e-05    -3.994    -4.244    -0.250    (0)
H+           1.734e-07    1.202e-07    -6.761    -6.920    -0.159    0.00
H2O          5.553e+01    9.935e-01    1.744    -0.003    0.000    22.19
B(-5)        0.000e+00
BH4-         0.000e+00    0.000e+00    -115.047    -115.285    -0.238    (0)
B(3)         2.294e-02
B(OH)3       2.259e-02    2.259e-02    -1.646    -1.646    0.000    (0)
BO2-         3.211e-04    1.858e-04    -3.493    -3.731    -0.238    (0)
NaB(OH)4     1.721e-05    1.721e-05    -4.764    -4.764    0.000    (0)
CaB(OH)4+    7.615e-06    4.405e-06    -5.118    -5.356    -0.238    (0)
MgB(OH)4+    1.888e-08    1.092e-08    -7.724    -7.962    -0.238    (0)
BF2(OH)2-    2.090e-11    1.209e-11    -10.680    -10.918    -0.238    (0)

```

B2O(OH) 5-	1.516e-15	8.768e-16	-14.819	-15.057	-0.238	(0)
BF4-	7.836e-20	4.533e-20	-19.106	-19.344	-0.238	(0)
BF3OH-	8.184e-40	4.734e-40	-39.087	-39.325	-0.238	(0)
C (4)	1.596e-03					
CO2	1.271e-03	1.321e-03	-2.896	-2.879	0.017	79.97
HCO3-	1.816e-04	1.051e-04	-3.741	-3.979	-0.238	(0)
CaHCO3+	1.273e-04	7.362e-05	-3.895	-4.133	-0.238	(0)
CaCO3	1.561e-05	1.561e-05	-4.807	-4.807	0.000	(0)
MgHCO3+	2.639e-07	1.526e-07	-6.579	-6.816	-0.238	(0)
(CO2) 2	2.140e-07	2.225e-07	-6.670	-6.653	0.017	159.93
NaHCO3	1.762e-07	1.762e-07	-6.754	-6.754	0.000	(0)
CO3-2	9.187e-08	1.095e-08	-7.037	-7.961	-0.924	(0)
MgCO3	3.660e-09	3.660e-09	-8.437	-8.437	0.000	(0)
NaCO3-	2.040e-12	1.180e-12	-11.690	-11.928	-0.238	(0)
Ca	5.733e-03					
Ca+2	3.735e-03	5.760e-04	-2.428	-3.240	-0.812	(0)
CaCl+	1.308e-03	7.569e-04	-2.883	-3.121	-0.238	(0)
CaCl2	4.168e-04	4.168e-04	-3.380	-3.380	0.000	(0)
CaHCO3+	1.273e-04	7.362e-05	-3.895	-4.133	-0.238	(0)
CaSO4	9.503e-05	9.503e-05	-4.022	-4.022	0.000	(0)
CaF+	2.787e-05	1.612e-05	-4.555	-4.793	-0.238	(0)
CaCO3	1.561e-05	1.561e-05	-4.807	-4.807	0.000	(0)
CaB(OH) 4+	7.615e-06	4.405e-06	-5.118	-5.356	-0.238	(0)
CaOH+	1.259e-09	7.280e-10	-8.900	-9.138	-0.238	(0)
Cl (-1)	1.913e-01					
Cl-	1.645e-01	8.971e-02	-0.784	-1.047	-0.263	(0)
NaCl	2.325e-02	2.325e-02	-1.634	-1.634	0.000	(0)
CaCl+	1.308e-03	7.568e-04	-2.883	-3.121	-0.238	(0)
KCl	1.242e-03	1.242e-03	-2.906	-2.906	0.000	(0)
CaCl2	4.168e-04	4.168e-04	-3.380	-3.380	0.000	(0)
LiCl	1.071e-04	1.071e-04	-3.970	-3.970	0.000	(0)
MgCl+	1.224e-05	7.082e-06	-4.912	-5.150	-0.238	(0)
HCl	3.921e-08	3.921e-08	-7.407	-7.407	0.000	(0)
Cl (1)	5.926e-15					
HClO	4.271e-15	4.271e-15	-14.370	-14.370	0.000	(0)
ClO-	1.656e-15	9.578e-16	-14.781	-15.019	-0.238	(0)
Cl (3)	4.975e-23					
ClO2-	4.974e-23	2.877e-23	-22.303	-22.541	-0.238	(0)
HClO2	5.114e-27	5.114e-27	-26.291	-26.291	0.000	(0)
Cl (5)	1.295e-22					
ClO3-	1.295e-22	7.285e-23	-21.888	-22.138	-0.250	(0)
Cl (7)	1.143e-25					
ClO4-	1.143e-25	6.427e-26	-24.942	-25.192	-0.250	(0)
F	9.697e-05					
F-	6.044e-05	3.399e-05	-4.219	-4.469	-0.250	(0)
CaF+	2.787e-05	1.612e-05	-4.555	-4.793	-0.238	(0)
NaF	7.317e-06	7.317e-06	-5.136	-5.136	0.000	(0)
HF	1.186e-06	1.186e-06	-5.926	-5.926	0.000	(0)
MgF+	1.589e-07	9.190e-08	-6.799	-7.037	-0.238	(0)
HF2-	2.105e-11	1.217e-11	-10.677	-10.915	-0.238	(0)
BF2(OH) 2-	2.090e-11	1.209e-11	-10.680	-10.918	-0.238	(0)
H2F2	9.791e-17	9.791e-17	-16.009	-16.009	0.000	(0)
BF4-	7.836e-20	4.533e-20	-19.106	-19.344	-0.238	(0)
SiF6-2	1.872e-30	2.015e-31	-29.728	-30.696	-0.968	(0)
BF3OH-	8.184e-40	4.734e-40	-39.087	-39.325	-0.238	(0)
H (0)	8.977e-22					
H2	4.489e-22	4.857e-22	-21.348	-21.314	0.034	(0)
K	1.631e-02					
K+	1.503e-02	8.193e-03	-1.823	-2.087	-0.263	(0)
KCl	1.242e-03	1.242e-03	-2.906	-2.906	0.000	(0)
KSO4-	4.010e-05	2.320e-05	-4.397	-4.635	-0.238	(0)
KHSO4	4.618e-09	4.618e-09	-8.336	-8.336	0.000	(0)
KOH	2.542e-10	2.542e-10	-9.595	-9.595	0.000	(0)
Li	1.969e-03					
Li+	1.862e-03	1.178e-03	-2.730	-2.929	-0.199	(0)
LiCl	1.071e-04	1.071e-04	-3.970	-3.970	0.000	(0)
LiSO4-	1.201e-07	6.945e-08	-6.921	-7.158	-0.238	(0)
LiOH	2.415e-10	2.415e-10	-9.617	-9.617	0.000	(0)
Mg	2.957e-05					
MgCl+	1.224e-05	7.082e-06	-4.912	-5.150	-0.238	(0)
MgSO4	1.088e-05	1.088e-05	-4.963	-4.963	0.000	(0)
Mg+2	5.998e-06	1.200e-06	-5.222	-5.921	-0.699	(0)
MgHCO3+	2.639e-07	1.526e-07	-6.579	-6.816	-0.238	(0)
MgF+	1.589e-07	9.190e-08	-6.799	-7.037	-0.238	(0)
MgB(OH) 4+	1.888e-08	1.092e-08	-7.724	-7.962	-0.238	(0)
MgCO3	3.660e-09	3.660e-09	-8.437	-8.437	0.000	(0)
Mg4(OH) 4+4	5.957e-33	2.364e-36	-32.225	-35.626	-3.401	(0)
Na	1.620e-01					
Na+	1.386e-01	8.018e-02	-0.858	-1.096	-0.238	(0)
NaCl	2.325e-02	2.325e-02	-1.634	-1.634	0.000	(0)
NaHSiO3	1.212e-04	1.212e-04	-3.916	-3.916	0.000	(0)
NaOH	2.095e-05	2.095e-05	-4.679	-4.679	0.000	(0)
NaB(OH) 4	1.721e-05	1.721e-05	-4.764	-4.764	0.000	(0)
NaSO4-	9.167e-06	5.302e-06	-5.038	-5.276	-0.238	(0)
NaF	7.317e-06	7.317e-06	-5.136	-5.136	0.000	(0)
NaHCO3	1.762e-07	1.762e-07	-6.754	-6.754	0.000	(0)
NaCO3-	2.040e-12	1.180e-12	-11.690	-11.928	-0.238	(0)
O (0)	4.432e-06					
O2	2.216e-06	2.398e-06	-5.654	-5.620	0.034	(0)
S (6)	2.487e-04					
CaSO4	9.503e-05	9.503e-05	-4.022	-4.022	0.000	(0)
SO4-2	9.302e-05	1.001e-05	-4.031	-5.000	-0.968	(0)
KSO4-	4.010e-05	2.320e-05	-4.397	-4.635	-0.238	(0)
MgSO4	1.088e-05	1.088e-05	-4.963	-4.963	0.000	(0)
NaSO4-	9.167e-06	5.302e-06	-5.038	-5.276	-0.238	(0)
HSO4-	4.101e-07	2.372e-07	-6.387	-6.625	-0.238	(0)
LiSO4-	1.201e-07	6.945e-08	-6.921	-7.158	-0.238	(0)
KHSO4	4.618e-09	4.618e-09	-8.336	-8.336	0.000	(0)
H2SO4	1.379e-20	1.379e-20	-19.860	-19.860	0.000	(0)
Si	8.392e-03					
SiO2	8.154e-03	8.154e-03	-2.089	-2.089	0.000	(0)
NaHSiO3	1.212e-04	1.212e-04	-3.916	-3.916	0.000	(0)
HSiO3-	1.159e-04	6.703e-05	-3.936	-4.174	-0.238	(0)
H6(H2SiO4) 4-2	1.168e-07	1.257e-08	-6.933	-7.901	-0.968	(0)
H2SiO4-2	6.653e-11	7.159e-12	-10.177	-11.145	-0.968	(0)
H4(H2SiO4) 4-4	3.382e-13	4.358e-17	-12.471	-16.361	-3.890	(0)
SiF6-2	1.872e-30	2.015e-31	-29.728	-30.696	-0.968	(0)

-----Saturation indices-----				
Phase	SI**	log IAP	log K(523 K, 155 atm)	
Afwillite	-7.36	27.61	34.96	Ca3Si2O4(OH)6
Akermanite	3.02	24.93	21.92	Ca2MgSi2O7
Anhydrite	0.29	-8.24	-8.52	CaSO4
Antarcticite	-9.24	-5.35	3.89	CaCl2:6H2O
Anthophyllite	13.52	38.70	25.18	Mg7Si8O22(OH)2
Antigorite	101.62	308.88	207.27	Mg48Si34O85(OH)62
Aphthitalite	-13.47	-17.35	-3.89	NaK3(SO4)2
Aragonite	0.90	-0.30	-1.20	CaCO3
Arcanite	-6.58	-9.17	-2.59	K2SO4
Artinite	-4.52	4.93	9.45	Mg2CO3(OH)2:3H2O
B	-57.56	2.57	60.13	B
B(g)	-106.38	2.57	108.96	B
B2O3	-6.32	-3.28	3.03	B2O3
Bassanite	-0.41	-8.24	-7.83	CaSO4:0.5H2O
BF3(g)	-22.92	-35.80	-12.88	BF3
Bischofite	-12.22	-8.03	4.18	MgCl2:6H2O
Bloedite	-15.51	-18.12	-2.62	Na2Mg(SO4)2:4H2O
Borax	-13.50	5.05	18.55	Na2(B4O5(OH)4):8H2O
Boric_acid	-2.86	-1.65	1.22	B(OH)3
Brucite	-0.19	7.91	8.11	Mg(OH)2
Burkeite	-23.12	-13.63	9.49	Na6CO3(SO4)2
C	-37.63	-5.28	32.36	C
C(g)	-101.42	-5.28	96.15	C
Ca	-63.74	13.41	77.15	Ca
Ca(g)	-75.79	13.41	89.20	Ca
Ca2Cl2(OH)2:H2O	-20.93	5.26	26.19	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-41.26	26.41	67.67	Ca4Cl2(OH)6:13H2O
Calcite	1.06	-0.30	-1.36	CaCO3
Carnallite	-15.23	-11.17	4.06	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-0.40	-8.24	-7.84	CaSO4:0.5H2O
Chalcedony	-0.02	-2.09	-2.07	SiO2
Chloromagnesite	-15.36	-8.02	7.35	MgCl2
Chrysotile	5.79	19.57	13.77	Mg3Si2O5(OH)4
Cl2(g)	-16.12	-18.74	-2.62	Cl2
CO2(g)	-0.80	-2.88	-2.08	CO2
Coesite	-0.35	-2.09	-1.73	SiO2
Colemanite	-10.25	11.33	21.58	Ca2B6O11:5H2O
Cristobalite(alpha)	-0.13	-2.09	-1.96	SiO2
Cristobalite(beta)	-0.31	-2.09	-1.78	SiO2
Dicalcium_silicate	-0.70	19.11	19.80	Ca2SiO4
Diopside	4.95	14.34	9.39	CaMgSi2O6
Dolomite	1.08	-3.28	-4.36	CaMg(CO3)2
Dolomite-dis	0.46	-3.28	-3.74	CaMg(CO3)2
Dolomite-ord	1.09	-3.28	-4.37	CaMg(CO3)2
Enstatite	1.40	5.83	4.43	MgSiO3
Epsomite	-8.74	-10.94	-2.20	MgSO4:7H2O
F2(g)	-50.51	-25.58	24.93	F2
Fluorite	-0.57	-12.18	-11.60	CaF2
Forsterite	2.02	13.74	11.72	Mg2SiO4
Foshagite	-0.34	36.12	36.46	Ca4Si3O9(OH)2:0.5H2O
Gaylussite	-10.55	0.44	10.99	CaNa2(CO3)2:5H2O
Glauberite	-9.96	-15.43	-5.47	Na2Ca(SO4)2
Gypsum	-1.07	-8.24	-7.17	CaSO4:2H2O
Gyrolite	0.07	14.92	14.85	Ca2Si3O7(OH)2:1.5H2O
H2(g)	-18.71	-21.31	-2.61	H2
H2O(g)	1.56	-0.00	-1.56	H2O
Halite	-3.05	-2.14	0.91	NaCl
Hatrurite	-9.79	29.70	39.49	Ca3SiO5
HCl(g)	-7.78	-7.97	-0.18	HCl
Hexahydrite	-9.00	-10.94	-1.93	MgSO4:6H2O
Hillebrandite	-1.70	19.10	20.80	Ca2SiO3(OH)2:0.17H2O
Huntite	-2.12	-9.24	-7.11	CaMg3(CO3)4
Hydroboracite	-11.75	8.65	20.40	MgCaB6O11:6H2O
Hydromagnesite	-8.70	-4.02	4.68	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-8.29	-5.33	2.95	CaCl2
Ice	-1.14	-0.00	1.14	H2O
K	-34.99	6.24	41.23	K
K(g)	-39.10	6.24	45.34	K
K2CO3:1.5H2O	-14.56	-1.24	13.33	K2CO3:1.5H2O
K2O	-42.29	9.66	51.96	K2O
K3H(SO4)2	-19.56	-23.18	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-54.34	-26.73	27.61	K8H4(CO3)6:3H2O
Kainite	-13.65	-14.06	-0.42	KMgClSO4:3H2O
Kalinite	-6.35	-6.07	0.28	KHCO3
Kieserite	-10.62	-10.92	-0.30	MgSO4:H2O
KMgCl3	-19.80	-11.15	8.65	KMgCl3
KMgCl3:2H2O	-17.70	-11.15	6.54	KMgCl3:2H2O
KNaCO3:6H2O	-10.31	-0.26	10.05	KNaCO3:6H2O
Lansfordite	-7.66	-2.99	4.67	MgCO3:5H2O
Larnite	-1.26	19.11	20.36	Ca2SiO4
Leonite	-15.85	-20.10	-4.25	K2Mg(SO4)2:4H2O
Li	-35.91	5.39	41.30	Li
Li(g)	-46.28	5.39	51.68	Li
Lime	-7.23	10.60	17.83	CaO
Magnesite	-0.84	-2.98	-2.14	MgCO3
Mercallite	-12.57	-14.01	-1.44	KHSO4
Merwinite	1.22	35.53	34.32	MgCa3(SiO4)2
Mg	-55.07	10.73	65.79	Mg
Mg(g)	-63.93	10.73	74.66	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-4.36	-8.94	-4.59	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-4.17	-6.96	-2.80	Mg1.5SO4(OH)
MgCl2:2H2O	-11.69	-8.02	3.67	MgCl2:2H2O
MgCl2:4H2O	-10.24	-8.03	2.22	MgCl2:4H2O
MgCl2:H2O	-12.79	-8.02	4.78	MgCl2:H2O
MgOHCl	-5.86	-0.05	5.81	MgOHCl
MgSO4	-6.28	-10.92	-4.64	MgSO4
Mirabilite	-15.98	-7.22	8.76	Na2SO4:10H2O
Misenite	-82.13	-93.21	-11.08	K8H6(SO4)7
Monohydrocalcite	-1.36	-0.30	1.06	CaCO3:H2O
Monticellite	2.40	16.43	14.03	CaMgSiO4
Na	-31.52	7.23	38.75	Na
Na(g)	-37.12	7.23	44.35	Na
Na2CO3	-6.83	0.75	7.58	Na2CO3
Na2CO3:7H2O	-15.12	0.73	15.85	Na2CO3:7H2O
Na2O	-29.90	11.65	41.54	Na2O

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Na2SiO3      -6.36      9.56      15.92      Na2SiO3
Na3H(SO4)2   -19.32     -20.21     -0.89      Na3H(SO4)2
Na4Ca(SO4)3:2H2O -16.66    -22.63     -5.96      Na4Ca(SO4)3:2H2O
Na4SiO4      -25.29     21.20     46.49      Na4SiO4
Na6Si2O7     -35.66     30.76     66.42      Na6Si2O7
Nahcolite    -5.50      -5.07      0.42      NaHCO3
Natron       -14.08      0.72      14.80      Na2CO3:10H2O
Natrosilite  -5.95       7.47      13.41      Na2Si2O5
Nesquehonite -6.96      -2.99      3.97      MgCO3:3H2O
O2(g)        -2.98      -5.62     -2.64      O2
Okenite      -2.60       6.41      9.02      CaSi2O4(OH)2:2H2O
Oxychloride-Mg -17.74     7.85     25.59      Mg2Cl(OH)3:4H2O
Pentahydrate -9.37     -10.93     -1.56      MgSO4:5H2O
Periclase    -2.14       7.92     10.06      MgO
Picromerite  -15.46     -20.11     -4.65      K2Mg(SO4)2:6H2O
Pirssonite   -10.81      0.45     11.25      Na2Ca(CO3)2:2H2O
Polyhalite   -22.20     -36.58    -14.38      K2MgCa2(SO4)4:2H2O
Portlandite  -2.27      10.59     12.86      Ca(OH)2
Pseudowollastonite 1.34      8.51      7.16      CaSiO3
Quartz       0.13      -2.09     -2.22      SiO2
Rankinite    0.32      27.62     27.30      Ca3Si2O7
Sellaite     -2.21     -14.86    -12.65      MgF2
Sepiolite     3.24      19.11     15.88      Mg4Si6O15(OH)2:6H2O
Si          -78.28      3.53     81.81      Si
Si(g)       -115.73     3.53    119.26      Si
SiF4(g)     -25.73    -47.64    -21.90      SiF4
SiO2(am)    -0.38      -2.09     -1.71      SiO2
Starkeyite   -9.79     -10.93    -1.14      MgSO4:4H2O
Sylvite      -4.12      -3.13      0.99      KCl
Syngenite    -9.78     -17.41    -7.63      K2Ca(SO4)2:2H2O
Tachyhydrite -38.13    -21.40     16.73      Mg2CaCl6:12H2O
Talc        7.99      15.39      7.40      Mg3Si4O10(OH)2
Thenardite   -4.66     -7.19     -2.54      Na2SO4
Thermonatrite -7.32      0.75      8.67      Na2CO3:H2O
Tobermorite-11A 0.31      40.44     40.14      Ca5Si6H11O22.5
Tobermorite-14A -4.03      40.43     44.46      Ca5Si6H21O27.5
Tobermorite-9A 0.64      40.45     39.80      Ca5Si6H6O20
Tremolite    18.96     44.06     25.10      Ca2Mg5Si8O22(OH)2
Tridymite    -0.39      -2.09     -1.70      SiO2
Trona-K      -17.83     -6.31     11.52      K2NaH(CO3)2:2H2O
Wollastonite 1.37       8.51      7.14      CaSiO3
Xonotlite    -3.77      51.05     54.82      Ca6Si6O17(OH)2

**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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TIME STEP 10 HOURS (0.001 YEAR)
Reaction step 7.

Using solution 1.      ANI 1-2
Using pure phase assemblage 1.      Reservoir
Using kinetics 1.

Kinetics 1.
Time step: 3e+06 seconds (Incremented time: 3.33333e+06 seconds)

Rate name      Delta Moles Total Moles      Reactant      Coefficient
Quartz         4.573e-01    4.880e+01      SiO2           1
Anorthite     -4.781e+00    1.384e+01      CaAl2(SiO4)2   1
Albite        1.532e-02     3.099e+01      NaAlSi3O8       1
K-Feldspar    1.083e-03     7.876e+00      KAlSi3O8        1
Diopside     -0.000e+00     0.000e+00      CaMgSi2O6       1
Enstatite    -1.602e+00     5.157e+00      MgSiO3          1
Ilmenite     -8.757e-04     3.778e-01      FeTiO3          1
Titanite     -3.277e-05     1.990e+00      CaTiSiO5        1
Hematite     -3.301e+00     3.572e+00      Fe2O3           1
Epidote      2.943e+00     7.129e+00      Ca2FeAl2Si3O12OH 1
Chamosite-7A 1.830e+00     1.173e+01      Fe2Al2SiO5(OH)4 1
Calcite      -0.000e+00     0.000e+00      CaCO3           1
Dolomite     -1.106e+00     2.971e+00      CaMg(CO3)2      1
Magnesite    2.702e+00     2.702e+00      MgCO3           1

-----Phase assemblage-----
Phase      SI  log IAP  log K(T, P)  Initial      Moles in assemblage
CO2(g)     1.29 -0.78   -2.08      0.000e+00      Final      Delta
0          0          0.000e+00

-----Solution composition-----
Elements      Molality      Moles
Al            2.018e-05     1.916e-05
B             2.416e-02     2.294e-02
C            1.661e-01     1.577e-01
Ca           5.469e-03     5.193e-03
Cl           2.015e-01     1.913e-01
F            1.021e-04     9.697e-05
Fe           8.199e-06     7.785e-06
K            1.115e-02     1.059e-02
Li           2.074e-03     1.969e-03
Mg           1.019e-02     9.675e-03
Na           1.565e-01     1.486e-01
S            2.620e-04     2.487e-04
Si           5.989e-03     5.686e-03
Ti           2.348e-03     2.229e-03

-----Description of solution-----
pH = 4.926      Charge balance
pe = -2.006     Adjusted to redox equilibrium
Density (g/cm³) = 0.82023
Volume (L) = 1.18204
Activity of water = 0.991
Ionic strength (mol/kgw) = 1.755e-01

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Mass of water (kg) = 9.495e-01
Total alkalinity (eq/kg) = 5.865e-04
Total CO2 (mol/kg) = 1.659e-01
Temperature (°C) = 250.00
Pressure (atm) = 155.00
Electrical balance (eq) = -1.101e-03
Percent error, 100*(Cat-|An|)/ (Cat+|An|) = -0.34
Iterations = 28813
Total H = 1.055207e+02
Total O = 5.312579e+01

-----Distribution of species-----						
Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.713e-05	1.185e-05	-4.766	-4.926	-0.160	0.00
OH-	1.032e-06	5.764e-07	-5.986	-6.239	-0.253	(0)
H2O	5.553e+01	9.907e-01	1.744	-0.004	0.000	22.19
Al	2.018e-05					
AlO2-	8.099e-06	4.656e-06	-5.092	-5.332	-0.240	(0)
HAIO2	7.585e-06	7.585e-06	-5.120	-5.120	0.000	(0)
NaAlO2	4.462e-06	4.462e-06	-5.351	-5.351	0.000	(0)
Al(OH)2+	2.969e-08	1.707e-08	-7.527	-7.768	-0.240	(0)
AlOH+2	1.103e-10	1.283e-11	-9.958	-10.892	-0.934	(0)
AlF+2	3.280e-13	3.817e-14	-12.484	-13.418	-0.934	(0)
AlF2+	3.093e-13	1.778e-13	-12.510	-12.750	-0.240	(0)
AlF3	2.619e-14	2.619e-14	-13.582	-13.582	0.000	(0)
Al+3	1.005e-14	3.262e-16	-13.998	-15.487	-1.489	(0)
AlF4-	1.339e-16	7.699e-17	-15.873	-16.114	-0.240	(0)
AlSO4+	4.184e-20	2.405e-20	-19.378	-19.619	-0.240	(0)
Al(SO4)2-	2.341e-25	1.346e-25	-24.631	-24.871	-0.240	(0)
Al2(OH)2+4	4.867e-26	1.780e-29	-25.313	-28.750	-3.437	(0)
Al3(OH)4+5	4.394e-36	0.000e+00	-35.357	-40.513	-5.156	(0)
Al13O4(OH)24+7	0.000e+00	0.000e+00	-131.448	-141.558	-10.111	(0)
B(-5)	0.000e+00					
BH4-	0.000e+00	0.000e+00	-53.007	-53.248	-0.240	(0)
B(3)	2.416e-02					
B(OH)3	2.416e-02	2.416e-02	-1.617	-1.617	0.000	(0)
BO2-	3.515e-06	2.021e-06	-5.454	-5.694	-0.240	(0)
NaB(OH)4	1.785e-07	1.785e-07	-6.748	-6.748	0.000	(0)
MgB(OH)4+	1.096e-07	6.301e-08	-6.960	-7.201	-0.240	(0)
CaB(OH)4+	7.883e-08	4.532e-08	-7.103	-7.344	-0.240	(0)
BF2(OH)2-	2.633e-10	1.514e-10	-9.579	-9.820	-0.240	(0)
BF4-	1.143e-15	6.568e-16	-14.942	-15.183	-0.240	(0)
B2O(OH)5-	1.769e-17	1.017e-17	-16.752	-16.993	-0.240	(0)
BF3OH-	3.508e-37	2.016e-37	-36.455	-36.695	-0.240	(0)
C(-2)	4.642e-38					
C2H4	2.321e-38	2.321e-38	-37.634	-37.634	0.000	(0)
C(-3)	1.155e-04					
C2H6	5.776e-05	5.776e-05	-4.238	-4.238	0.000	(0)
C(-4)	3.744e-09					
CH4	3.744e-09	3.744e-09	-8.427	-8.427	0.000	(0)
C(2)	1.533e-08					
CO	1.533e-08	1.533e-08	-7.814	-7.814	0.000	(0)
C(4)	1.659e-01					
CO2	1.587e-01	1.652e-01	-0.799	-0.782	0.018	79.97
(CO2)2	3.342e-03	3.480e-03	-2.476	-2.458	0.018	159.93
HCO3-	2.313e-04	1.330e-04	-3.636	-3.876	-0.240	(0)
MgHCO3+	1.792e-04	1.030e-04	-3.747	-3.987	-0.240	(0)
CaHCO3+	1.541e-04	8.860e-05	-3.812	-4.053	-0.240	(0)
NaHCO3	2.138e-07	2.138e-07	-6.670	-6.670	0.000	(0)
CaCO3	1.906e-07	1.906e-07	-6.720	-6.720	0.000	(0)
FeHCO3+	6.250e-08	3.593e-08	-7.204	-7.445	-0.240	(0)
MgCO3	2.507e-08	2.507e-08	-7.601	-7.601	0.000	(0)
CO3-2	1.208e-09	1.406e-10	-8.918	-9.852	-0.934	(0)
FeCO3	1.456e-11	1.456e-11	-10.837	-10.837	0.000	(0)
NaCO3-	2.528e-14	1.453e-14	-13.597	-13.838	-0.240	(0)
FeCO3+	9.030e-21	5.191e-21	-20.044	-20.285	-0.240	(0)
Ca	5.469e-03					
Ca+2	5.469e-03	5.478e-04	-2.442	-3.261	-0.820	(0)
CaCl+	1.276e-03	7.334e-04	-2.894	-3.135	-0.240	(0)
CaCl2	4.115e-04	4.115e-04	-3.386	-3.386	0.000	(0)
CaHCO3+	1.541e-04	8.860e-05	-3.812	-4.053	-0.240	(0)
CaF+	9.179e-06	5.276e-06	-5.037	-5.278	-0.240	(0)
CaSO4	6.506e-07	6.506e-07	-6.187	-6.187	0.000	(0)
CaCO3	1.906e-07	1.906e-07	-6.720	-6.720	0.000	(0)
CaB(OH)4+	7.883e-08	4.532e-08	-7.103	-7.344	-0.240	(0)
CaOH+	1.219e-11	7.005e-12	-10.914	-11.155	-0.240	(0)
Cl(-1)	2.015e-01					
Cl-	1.690e-01	9.141e-02	-0.772	-1.039	-0.267	(0)
NaCl	2.272e-02	2.272e-02	-1.644	-1.644	0.000	(0)
MgCl+	6.697e-03	3.850e-03	-2.174	-2.415	-0.240	(0)
CaCl+	1.276e-03	7.334e-04	-2.894	-3.135	-0.240	(0)
KCl	8.598e-04	8.598e-04	-3.066	-3.066	0.000	(0)
CaCl2	4.115e-04	4.115e-04	-3.386	-3.386	0.000	(0)
LiCl	1.144e-04	1.144e-04	-3.942	-3.942	0.000	(0)
FeCl+	4.263e-06	2.450e-06	-5.370	-5.611	-0.240	(0)
HCl	3.938e-06	3.938e-06	-5.405	-5.405	0.000	(0)
FeCl4-2	4.307e-07	4.514e-08	-6.366	-7.345	-0.980	(0)
FeCl2	4.153e-08	4.153e-08	-7.382	-7.382	0.000	(0)
FeCl+2	3.939e-17	4.584e-18	-16.405	-17.339	-0.934	(0)
FeCl2+	9.754e-21	5.607e-21	-20.011	-20.251	-0.240	(0)
FeCl4-	9.799e-26	5.633e-26	-25.009	-25.249	-0.240	(0)
Cl(1)	4.298e-29					
HClO	4.281e-29	4.281e-29	-28.368	-28.368	0.000	(0)
ClO-	1.695e-31	9.743e-32	-30.771	-31.011	-0.240	(0)
Cl(3)	0.000e+00					
ClO2-	0.000e+00	0.000e+00	-54.294	-54.534	-0.240	(0)
HClO2	0.000e+00	0.000e+00	-56.291	-56.291	0.000	(0)
Cl(5)	0.000e+00					
ClO3-	0.000e+00	0.000e+00	-69.879	-70.132	-0.253	(0)
Cl(7)	0.000e+00					
ClO4-	0.000e+00	0.000e+00	-88.934	-89.187	-0.253	(0)
F	1.021e-04					
HF	4.023e-05	4.023e-05	-4.395	-4.395	0.000	(0)
MgF+	2.935e-05	1.687e-05	-4.532	-4.773	-0.240	(0)
F-	2.095e-05	1.170e-05	-4.679	-4.932	-0.253	(0)
CaF+	9.179e-06	5.276e-06	-5.037	-5.278	-0.240	(0)

NaF	2.415e-06	2.415e-06	-5.617	-5.617	0.000	(0)
BF2(OH) 2-	2.633e-10	1.514e-10	-9.579	-9.820	-0.240	(0)
HF2-	2.473e-10	1.422e-10	-9.607	-9.847	-0.240	(0)
FeF+	2.401e-10	1.380e-10	-9.620	-9.860	-0.240	(0)
AlF+2	3.280e-13	3.817e-14	-12.484	-13.418	-0.934	(0)
AlF2+	3.093e-13	1.778e-13	-12.510	-12.750	-0.240	(0)
H2F2	1.127e-13	1.127e-13	-12.948	-12.948	0.000	(0)
AlF3	2.619e-14	2.619e-14	-13.582	-13.582	0.000	(0)
BF4-	1.143e-15	6.568e-16	-14.942	-15.183	-0.240	(0)
AlF4-	1.339e-16	7.699e-17	-15.873	-16.114	-0.240	(0)
FeF2+	5.080e-17	2.920e-17	-16.294	-16.535	-0.240	(0)
FeF+2	1.250e-17	1.454e-18	-16.903	-17.837	-0.934	(0)
SiF6-2	2.228e-25	2.334e-26	-24.652	-25.632	-0.980	(0)
BF3OH-	3.508e-37	2.016e-37	-36.455	-36.695	-0.240	(0)
Fe (2)	8.199e-06					
FeCl+	4.263e-06	2.450e-06	-5.370	-5.611	-0.240	(0)
Fe+2	3.401e-06	5.149e-07	-5.468	-6.288	-0.820	(0)
FeCl4-2	4.307e-07	4.514e-08	-6.366	-7.345	-0.980	(0)
FeHCO3+	6.250e-08	3.593e-08	-7.204	-7.445	-0.240	(0)
FeCl2	4.153e-08	4.153e-08	-7.382	-7.382	0.000	(0)
FeF+	2.401e-10	1.380e-10	-9.620	-9.860	-0.240	(0)
FeOH+	2.565e-11	1.474e-11	-10.591	-10.831	-0.240	(0)
FeCO3	1.456e-11	1.456e-11	-10.837	-10.837	0.000	(0)
FeSO4	5.881e-12	5.881e-12	-11.231	-11.231	0.000	(0)
Fe (OH) 2	1.060e-17	1.060e-17	-16.975	-16.975	0.000	(0)
Fe (OH) 3-	6.648e-23	3.822e-23	-22.177	-22.418	-0.240	(0)
Fe (OH) 4-2	3.302e-32	3.460e-33	-31.481	-32.461	-0.980	(0)
Fe (3)	2.832e-16					
Fe (OH) 2+	1.516e-16	8.718e-17	-15.819	-16.060	-0.240	(0)
FeF2+	5.080e-17	2.920e-17	-16.294	-16.535	-0.240	(0)
FeCl+2	3.939e-17	4.584e-18	-16.405	-17.339	-0.934	(0)
FeOH+2	2.499e-17	2.908e-18	-16.602	-17.536	-0.934	(0)
FeF+2	1.250e-17	1.454e-18	-16.903	-17.837	-0.934	(0)
Fe (OH) 3	3.692e-18	3.692e-18	-17.433	-17.433	0.000	(0)
Fe+3	1.533e-19	4.974e-21	-18.815	-20.303	-1.489	(0)
FeSO4+	4.558e-20	2.620e-20	-19.341	-19.582	-0.240	(0)
FeCl2+	9.754e-21	5.607e-21	-20.011	-20.251	-0.240	(0)
FeCO3+	9.030e-21	5.191e-21	-20.044	-20.285	-0.240	(0)
Fe (OH) 4-	1.460e-22	8.396e-23	-21.836	-22.076	-0.240	(0)
FeCl4-	9.799e-26	5.633e-26	-25.009	-25.249	-0.240	(0)
Fe2 (OH) 2+4	6.224e-31	2.276e-34	-30.206	-33.643	-3.437	(0)
Fe (SO4) 2-	7.350e-32	4.226e-32	-31.134	-31.374	-0.240	(0)
Fe3 (OH) 4+5	0.000e+00	0.000e+00	-42.227	-47.382	-5.156	(0)
H (0)	8.943e-06					
H2	4.472e-06	4.851e-06	-5.350	-5.314	0.035	(0)
K	1.115e-02					
K+	1.029e-02	5.568e-03	-1.988	-2.254	-0.267	(0)
KCl	8.598e-04	8.598e-04	-3.066	-3.066	0.000	(0)
KSO4-	1.974e-07	1.135e-07	-6.705	-6.945	-0.240	(0)
KHSO4	2.227e-09	2.227e-09	-8.652	-8.652	0.000	(0)
KOH	1.748e-12	1.748e-12	-11.757	-11.757	0.000	(0)
Li	2.074e-03					
Li+	1.959e-03	1.235e-03	-2.708	-2.908	-0.200	(0)
LiCl	1.144e-04	1.144e-04	-3.942	-3.942	0.000	(0)
LiSO4-	9.115e-10	5.240e-10	-9.040	-9.281	-0.240	(0)
LiOH	2.561e-12	2.561e-12	-11.592	-11.592	0.000	(0)
Mg	1.019e-02					
MgCl+	6.697e-03	3.850e-03	-2.174	-2.415	-0.240	(0)
Mg+2	3.243e-03	6.401e-04	-2.489	-3.194	-0.705	(0)
MgHCO3+	1.792e-04	1.030e-04	-3.747	-3.987	-0.240	(0)
MgSO4	4.180e-05	4.180e-05	-4.379	-4.379	0.000	(0)
MgF+	2.935e-05	1.687e-05	-4.532	-4.773	-0.240	(0)
MgB (OH) 4+	1.096e-07	6.301e-08	-6.960	-7.201	-0.240	(0)
MgCO3	2.507e-08	2.507e-08	-7.601	-7.601	0.000	(0)
Mg4 (OH) 4+4	5.486e-30	2.006e-33	-29.261	-32.698	-3.437	(0)
Na	1.565e-01					
Na+	1.337e-01	7.688e-02	-0.874	-1.114	-0.240	(0)
NaCl	2.272e-02	2.272e-02	-1.644	-1.644	0.000	(0)
NaAlO2	4.462e-06	4.462e-06	-5.351	-5.351	0.000	(0)
NaF	2.415e-06	2.415e-06	-5.617	-5.617	0.000	(0)
NaHSiO3	8.638e-07	8.638e-07	-6.064	-6.064	0.000	(0)
NaHCO3	2.138e-07	2.138e-07	-6.670	-6.670	0.000	(0)
NaOH	2.033e-07	2.033e-07	-6.692	-6.692	0.000	(0)
NaB (OH) 4	1.785e-07	1.785e-07	-6.748	-6.748	0.000	(0)
NaSO4-	6.368e-08	3.661e-08	-7.196	-7.436	-0.240	(0)
NaCO3-	2.528e-14	1.453e-14	-13.597	-13.838	-0.240	(0)
O (0)	4.404e-38					
O2	2.202e-38	2.389e-38	-37.657	-37.622	0.035	(0)
S (-2)	2.183e-04					
H2S	2.154e-04	2.154e-04	-3.667	-3.667	0.000	(0)
HS-	2.884e-06	1.611e-06	-5.540	-5.793	-0.253	(0)
S-2	4.184e-09	5.357e-10	-8.378	-9.271	-0.893	(0)
S2-2	6.256e-14	6.556e-15	-13.204	-14.183	-0.980	(0)
S3-2	7.866e-17	8.244e-18	-16.104	-17.084	-0.980	(0)
S4-2	7.208e-20	7.554e-21	-19.142	-20.122	-0.980	(0)
S5-2	4.961e-23	5.199e-24	-22.304	-23.284	-0.980	(0)
S (2)	3.516e-12					
S2O3-2	1.758e-12	1.842e-13	-11.755	-12.735	-0.980	(0)
HS2O3-	3.921e-17	2.254e-17	-16.407	-16.647	-0.240	(0)
S (3)	8.111e-24					
S2O4-2	4.056e-24	5.192e-25	-23.392	-24.285	-0.893	(0)
S (4)	9.604e-10					
HSO3-	6.124e-10	3.521e-10	-9.213	-9.453	-0.240	(0)
SO2	3.480e-10	3.480e-10	-9.458	-9.458	0.000	(0)
SO3-2	3.262e-14	3.796e-15	-13.487	-14.421	-0.934	(0)
H2SO3	8.706e-16	8.706e-16	-15.060	-15.060	0.000	(0)
S4O6-2	2.436e-24	2.552e-25	-23.613	-24.593	-0.980	(0)
S2O6-2	2.783e-26	2.916e-27	-25.556	-26.535	-0.980	(0)
S3O6-2	2.748e-31	2.880e-32	-30.561	-31.541	-0.980	(0)
S5O6-2	1.645e-39	1.724e-40	-38.784	-39.763	-0.980	(0)
S (5)	3.395e-24					
S2O5-2	1.697e-24	1.779e-25	-23.770	-24.750	-0.980	(0)
S (6)	4.370e-05					
MgSO4	4.180e-05	4.180e-05	-4.379	-4.379	0.000	(0)
SO4-2	4.876e-07	7.207e-08	-6.163	-7.142	-0.980	(0)
CaSO4	6.506e-07	6.506e-07	-6.187	-6.187	0.000	(0)
HSO4-	2.928e-07	1.683e-07	-6.533	-6.774	-0.240	(0)
KSO4-	1.974e-07	1.135e-07	-6.705	-6.945	-0.240	(0)

NaSO4-	6.368e-08	3.661e-08	-7.196	-7.436	-0.240	(0)
KHSO4	2.227e-09	2.227e-09	-8.652	-8.652	0.000	(0)
LiSO4-	9.115e-10	5.240e-10	-9.040	-9.281	-0.240	(0)
FeSO4	5.881e-12	5.881e-12	-11.231	-11.231	0.000	(0)
H2SO4	9.642e-19	9.642e-19	-18.016	-18.016	0.000	(0)
FeSO4+	4.558e-20	2.620e-20	-19.341	-19.582	-0.240	(0)
AlSO4+	4.184e-20	2.405e-20	-19.378	-19.619	-0.240	(0)
Al(SO4)2-	2.341e-25	1.346e-25	-24.631	-24.871	-0.240	(0)
Fe(SO4)2-	7.350e-32	4.226e-32	-31.134	-31.374	-0.240	(0)
S(7)	0.000e+00					
S2O8-2	0.000e+00	0.000e+00	-47.338	-48.318	-0.980	(0)
S(8)	1.863e-36					
HSO5-	1.863e-36	1.071e-36	-35.730	-35.970	-0.240	(0)
Si	5.989e-03					
SiO2	5.987e-03	5.987e-03	-2.223	-2.223	0.000	(0)
HSiO3-	8.662e-07	4.980e-07	-6.062	-6.303	-0.240	(0)
NaHSiO3	8.638e-07	8.638e-07	-6.064	-6.064	0.000	(0)
H6(H2SiO4)4-2	3.509e-12	3.677e-13	-11.455	-12.435	-0.980	(0)
H2SiO4-2	5.135e-15	5.381e-16	-14.289	-15.269	-0.980	(0)
H4(H2SiO4)4-4	1.134e-21	1.313e-25	-20.945	-24.882	-3.936	(0)
SiF6-2	2.228e-25	2.334e-26	-24.652	-25.632	-0.980	(0)
Ti	2.348e-03					
Ti(OH)4	2.348e-03	2.348e-03	-2.629	-2.629	0.000	(0)

-----Saturation indices-----						
Phase	SI**	log IAP	log K (523 K, 155 atm)			
Afwillite	-19.66	15.30	34.96	Ca3Si2O4(OH) 6		
Akermanite	-6.53	15.38	21.92	Ca2MgSi2O7		
Al	-48.70	27.50	76.20	Al		
Al(g)	-74.79	27.50	102.29	Al		
Al2(SO4)3	-34.12	-52.40	-18.28	Al2(SO4) 3		
Al2(SO4)3:6H2O	-30.38	-52.42	-22.04	Al2(SO4) 3:6H2O		
Albite	0.00	-3.57	-3.57	NaAlSi3O8		
Albite_high	-0.49	-3.57	-3.08	NaAlSi3O8		
Albite_low	-0.00	-3.57	-3.57	NaAlSi3O8		
AlF3	-6.36	-30.28	-23.92	AlF3		
Alum-K	-23.06	-32.07	-9.01	KAl(SO4)2:12H2O		
Alunite	-8.82	-33.46	-24.65	KAl3(OH) 6(SO4) 2		
Amesite-14A	7.18	19.30	12.13	Mg4Al4Si2O10(OH) 8		
Analcime	-0.39	-1.57	-1.17	Na.96Al.96Si2.04O6:H2O		
Analcime-dehy	-3.51	-1.56	1.95	Na.96Al.96Si2.04O6		
Anatase	5.87	-2.62	-8.49	TiO2		
Andalusite	0.12	-3.65	-3.77	Al2SiO5		
Andradite	-4.69	2.03	6.73	Ca3Fe2(SiO4) 3		
Anhydrite	-1.88	-10.40	-8.52	CaSO4		
Ankerite	-1.38	-6.52	-5.14	CaMg0.3Fe0.7(CO3) 2		
Annite	-1.00	5.96	6.97	KFe3AlSi3O10(OH) 2		
Anorthite	-0.19	0.71	0.90	CaAl2(SiO4) 2		
Antarcticite	-9.25	-5.36	3.89	CaCl2:6H2O		
Anthophyllite	3.62	28.80	25.18	Mg7Si8O22(OH) 2		
Antigorite	36.47	243.73	207.27	Mg48Si34O85(OH) 62		
Aphthitalite	-18.27	-22.16	-3.89	NaK3(SO4) 2		
Aragonite	-1.01	-2.21	-1.20	CaCO3		
Arcanite	-9.06	-11.65	-2.59	K2SO4		
Artinite	-4.95	4.49	9.45	Mg2CO3(OH) 2:3H2O		
B	-33.52	26.61	60.13	B		
B(g)	-82.35	26.61	108.96	B		
B2O3	-6.26	-3.22	3.03	B2O3		
Bassanite	-2.57	-10.41	-7.83	CaSO4:0.5H2O		
Beidellite-Ca	1.85	-8.74	-10.59	Ca.165Al2.33Si3.67O10(OH) 2		
Beidellite-H	1.08	-9.83	-10.91	H.33Al2.33Si3.67O10(OH) 2		
Beidellite-K	1.02	-8.94	-9.97	K.33Al2.33Si3.67O10(OH) 2		
Beidellite-Mg	2.10	-8.73	-10.83	Mg.165Al2.33Si3.67O10(OH) 2		
Beidellite-Na	1.35	-8.57	-9.92	Na.33Al2.33Si3.67O10(OH) 2		
BF3(g)	-18.30	-31.18	-12.88	BF3		
Bischofite	-9.48	-5.30	4.18	MgCl2:6H2O		
Bloedite	-17.11	-19.72	-2.62	Na2Mg(SO4) 2:4H2O		
Boehmite	0.84	-0.72	-1.55	Al2O2H		
Borax	-17.42	1.14	18.55	Na2(B4O5(OH) 4):8H2O		
Boric_acid	-2.83	-1.62	1.22	B(OH) 3		
Brucite	-1.46	6.65	8.11	Mg(OH) 2		
Burkeite	-29.41	-19.92	9.49	Na6CO3(SO4) 2		
C	-3.54	28.82	32.36	C		
C(g)	-67.33	28.82	96.15	C		
Ca	-51.75	25.40	77.15	Ca		
Ca(g)	-63.80	25.40	89.20	Ca		
Ca-Al Pyroxene	-3.66	2.94	6.59	CaAl2SiO6		
Ca2Al2O5:8H2O	-47.40	11.71	59.12	Ca2Al2O5:8H2O		
Ca2Cl2(OH) 2:H2O	-24.95	1.24	26.19	Ca2Cl2(OH) 2:H2O		
Ca3Al2O6	-31.98	18.33	50.31	Ca3Al2O6		
Ca4Al2Fe2O10	-40.54	13.86	54.40	Ca4Al2Fe2O10		
Ca4Al2O7:13H2O	-81.69	24.87	106.56	Ca4Al2O7:13H2O		
Ca4Al2O7:19H2O	-77.94	24.84	102.78	Ca4Al2O7:19H2O		
Ca4Cl2(OH) 6:13H2O	-53.31	14.36	67.67	Ca4Cl2(OH) 6:13H2O		
CaAl2O4	-7.32	5.16	12.48	CaAl2O4		
CaAl2O4:10H2O	-32.39	5.12	37.51	CaAl2O4:10H2O		
CaAl4O7	-9.86	3.73	13.59	CaAl4O7		
Calcite	-0.85	-2.21	-1.36	CaCO3		
Carnallite	-12.65	-8.59	4.06	KMgCl3:6H2O		
CaSO4:0.5H2O(beta)	-2.57	-10.41	-7.84	CaSO4:0.5H2O		
Celadonite	0.67	-0.28	-0.95	KMgAlSi4O10(OH) 2		
CH4(g)	-5.82	-8.43	-2.60	CH4		
Chalcedony	-0.15	-2.22	-2.07	SiO2		
Chamosite-7A	-0.00	3.46	3.46	Fe2Al2SiO5(OH) 4		
Chloromagnesite	-12.62	-5.27	7.35	MgCl2		
Chrysotile	1.74	15.51	13.77	Mg3Si2O5(OH) 4		
Cl2(g)	-28.12	-30.74	-2.62	Cl2		
Clinocllore-14A	6.68	25.16	18.48	Mg5Al2Si3O10(OH) 8		
Clinocllore-7A	4.22	25.16	20.94	Mg5Al2Si3O10(OH) 8		
Clinoptilolite-Ca	2.07	-23.49	-25.56	Cal.7335Al3.45Fe.017Si14.533O36:10.922H2O		
Clinoptilolite-dehy-Ca	-14.35	-23.44	-9.09	Cal.7335Al3.45Fe.017Si14.533O36		
Clinoptilolite-dehy-K	-23.31	-25.60	-2.29	K3.467Al3.45Fe.017Si14.533O36		
Clinoptilolite-dehy-Na	-19.41	-21.65	-2.24	Na3.467Al3.45Fe.017Si14.533O36		
Clinoptilolite-hy-Ca	1.36	-23.49	-24.85	Cal.7335Al3.45Fe.017Si14.533O36:11.645H2O		
Clinoptilolite-hy-K	-4.26	-25.63	-21.37	K3.467Al3.45Fe.017Si14.533O36:7.499H2O		
Clinoptilolite-hy-Na	-3.07	-21.69	-18.62	Na3.467Al3.45Fe.017Si14.533O36:10.877H2O		
Clinoptilolite-K	-7.21	-25.65	-18.44	K3.467Al3.45Fe.017Si14.533O36:10.922H2O		

Clinoptilolite-Na	-3.11	-21.69	-18.58	Na ₃ .467Al ₃ .45Fe.017Si ₁₄ .533O ₃₆ :10.922H ₂ O
Clinzoisite	-0.20	4.36	4.56	Ca ₂ Al ₃ Si ₃ O ₁₂ (OH)
CO(g)	-5.31	-7.81	-2.51	CO
CO ₂ (g)	1.29	-0.78	-2.08	CO ₂
Coesite	-0.49	-2.22	-1.73	SiO ₂
Colemanite	-18.10	3.49	21.58	Ca ₂ B ₆ O ₁₁ :5H ₂ O
Cordierite_anhyd	0.25	-0.66	-0.91	Mg ₂ Al ₄ Si ₅ O ₁₈
Cordierite_hydr	1.26	-0.66	-1.92	Mg ₂ Al ₄ Si ₅ O ₁₈ :H ₂ O
Corundum	4.28	-1.43	-5.71	Al ₂ O ₃
Cristobalite(alpha)	-0.27	-2.22	-1.96	SiO ₂
Cristobalite(beta)	-0.44	-2.22	-1.78	SiO ₂
Cronstedtite-7A	-1.80	-6.17	-4.38	Fe ₂ Fe ₂ Si ₅ O ₅ (OH) ₄
Daphnite-14A	-0.02	9.69	9.71	Fe ₅ Al ₁ Al ₃ Si ₃ O ₁₀ (OH) ₈
Daphnite-7A	-2.39	9.69	12.08	Fe ₅ Al ₁ Al ₃ Si ₃ O ₁₀ (OH) ₈
Dawsonite	-4.33	-5.71	-1.38	NaAlCO ₃ (OH) ₂
Diaspore	0.98	-0.72	-1.70	AlHO ₂
Dicalcium_silicate	-8.85	10.95	19.80	Ca ₂ SiO ₄
Diopside	-0.59	8.80	9.39	CaMgSi ₂ O ₆
Dolomite	-0.00	-4.36	-4.36	CaMg(CO ₃) ₂
Dolomite-dis	-0.61	-4.36	-3.74	CaMg(CO ₃) ₂
Dolomite-ord	0.01	-4.36	-4.37	CaMg(CO ₃) ₂
Enstatite	-0.00	4.43	4.43	MgSiO ₃
Epidote	0.00	-0.45	-0.46	Ca ₂ FeAl ₂ Si ₃ O ₁₂ OH
Epidote-ord	-0.04	-0.45	-0.42	FeCa ₂ Al ₂ (OH)(SiO ₄) ₃
Epsomite	-8.16	-10.36	-2.20	MgSO ₄ :7H ₂ O
Ettringite	-56.36	-13.01	43.35	Ca ₆ Al ₂ (SO ₄) ₃ (OH) ₁₂ :26H ₂ O
Eucryptite	-2.85	-0.92	1.93	LiAlSiO ₄
F ₂ (g)	-63.45	-38.52	24.93	F ₂
Fayalite	-1.78	4.90	6.68	Fe ₂ SiO ₄
Fe	-7.96	22.37	30.33	Fe
Fe(OH) ₂	-3.16	3.56	6.71	Fe(OH) ₂
Fe(OH) ₃	-4.51	-5.54	-1.03	Fe(OH) ₃
Fe ₂ (SO ₄) ₃	-36.55	-62.03	-25.49	Fe ₂ (SO ₄) ₃
FeF ₂	-7.45	-16.15	-8.71	FeF ₂
FeF ₃	-11.57	-35.10	-23.52	FeF ₃
FeO	-1.83	3.56	5.39	FeO
Ferrite-Ca	-4.52	-4.47	0.04	CaFe ₂ O ₄
Ferrite-Dicalcium	-17.21	2.11	19.33	Ca ₂ Fe ₂ O ₅
Ferrite-Mg	-2.82	-4.41	-1.59	MgFe ₂ O ₄
Ferrosilite	-0.91	1.34	2.25	FeSiO ₃
FesO ₄	-7.82	-13.43	-5.61	FeSO ₄
Fluorite	-1.52	-13.12	-11.60	CaF ₂
Forsterite	-0.64	11.09	11.72	Mg ₂ SiO ₄
Foshagite	-16.79	19.67	36.46	Ca ₄ Si ₃ O ₉ (OH) ₂ :0.5H ₂ O
Gaylussite	-14.40	-3.41	10.99	CaNa ₂ (CO ₃) ₂ :5H ₂ O
Gehlenite	-7.61	9.52	17.14	Ca ₂ Al ₂ SiO ₇
Gibbsite	0.46	-0.72	-1.17	Al(OH) ₃
Gismondine	-39.74	1.39	41.13	Ca ₂ Al ₄ Si ₄ O ₁₆ :9H ₂ O
Glauberite	-14.31	-19.77	-5.47	Na ₂ Ca(SO ₄) ₂
Goethite	-1.41	-5.53	-4.13	FeOOH
Greenalite	-2.49	6.23	8.72	Fe ₃ Si ₂ O ₅ (OH) ₄
Grossular	-3.91	11.67	15.57	Ca ₃ Al ₂ (SiO ₄) ₃
Gypsum	-3.24	-10.41	-7.17	CaSO ₄ :2H ₂ O
Gyrolite	-8.36	6.50	14.85	Ca ₂ Si ₃ O ₇ (OH) ₂ :1.5H ₂ O
H ₂ (g)	-2.71	-5.31	-2.61	H ₂
H ₂ O(g)	1.55	-0.00	-1.56	H ₂ O
H ₂ S(g)	-2.13	-10.72	-8.59	H ₂ S
Halite	-3.06	-2.15	0.91	NaCl
Hatrurite	-21.95	17.54	39.49	Ca ₃ SiO ₅
HCl(g)	-5.78	-5.97	-0.18	HCl
Hedenbergite	-2.85	5.70	8.55	CaFe(SiO ₃) ₂
Hematite	-0.02	-11.06	-11.04	Fe ₂ O ₃
Hercynite	0.67	2.13	1.46	FeAl ₂ O ₄
Hexahydrite	-8.43	-10.36	-1.93	MgSO ₄ :6H ₂ O
Hillebrandite	-9.86	10.95	20.80	Ca ₂ SiO ₃ (OH) ₂ :0.17H ₂ O
Huntite	-1.53	-8.64	-7.11	CaMg ₃ (CO ₃) ₄
Hydroboracite	-16.85	3.55	20.40	MgCaB ₆ O ₁₁ :6H ₂ O
Hydromagnesite	-6.62	-1.94	4.68	Mg ₅ (CO ₃) ₄ (OH) ₂ :4H ₂ O
Hydrophilite	-8.29	-5.34	2.95	CaCl ₂
Ice	-1.14	-0.00	1.14	H ₂ O
Illite	1.57	-6.16	-7.73	K _{0.6} Mg _{0.25} Al _{1.8} Al _{0.5} Si _{3.5} O ₁₀ (OH) ₂
Ilmenite	0.00	0.94	0.94	FeTiO ₃
Jadeite	-1.64	-1.35	0.29	NaAl(SiO ₃) ₂
Jarosite	-21.00	-47.92	-26.91	KFe ₃ (SO ₄) ₂ (OH) ₆
Jarosite-Na	-41.12	-46.77	-5.66	NaFe ₃ (SO ₄) ₂ (OH) ₆
K	-29.15	12.08	41.23	K
K(g)	-33.26	12.08	45.34	K
K-Feldspar	0.00	-4.71	-4.71	KAlSi ₃ O ₈
K ₂ CO ₃ :1.5H ₂ O	-16.79	-3.46	13.33	K ₂ CO ₃ :1.5H ₂ O
K ₂ O	-46.62	5.34	51.96	K ₂ O
K ₃ H(SO ₄) ₂	-22.35	-25.97	-3.62	K ₃ H(SO ₄) ₂
K ₈ H ₄ (CO ₃) ₆ :3H ₂ O	-59.06	-31.45	27.61	K ₈ H ₄ (CO ₃) ₆ :3H ₂ O
Kainite	-13.23	-13.64	-0.42	KMgClSO ₄ :3H ₂ O
KAl(SO ₄) ₂	-18.80	-32.03	-13.22	KAl(SO ₄) ₂
Kalicinite	-6.41	-6.13	0.28	KHCO ₃
Kalsilite	-1.73	-0.27	1.46	KAlSiO ₄
Kaolinite	1.07	-5.88	-6.95	Al ₂ Si ₂ O ₅ (OH) ₄
Katoite	-60.22	18.31	78.53	Ca ₃ Al ₂ H ₂ Si ₂ O ₁₂
Kieserite	-10.04	-10.34	-0.30	MgSO ₄ :H ₂ O
KMgCl ₃	-17.22	-8.57	8.65	KMgCl ₃
KMgCl ₃ :2H ₂ O	-15.12	-8.57	6.54	KMgCl ₃ :2H ₂ O
KNaCO ₃ :6H ₂ O	-12.39	-2.34	10.05	KNaCO ₃ :6H ₂ O
Kyanite	0.07	-3.65	-3.72	Al ₂ SiO ₅
Lansfordite	-6.83	-2.16	4.67	MgCO ₃ :5H ₂ O
Larnite	-9.41	10.95	20.36	Ca ₂ SiO ₄
Laumontite	0.11	-3.75	-3.86	CaAl ₂ Si ₄ O ₁₂ :4H ₂ O
Lawrencite	-8.38	-8.37	0.02	FeCl ₂
Lawsonite	-0.59	0.71	1.30	CaAl ₂ Si ₂ O ₇ (OH) ₂ :H ₂ O
Leonite	-17.75	-22.00	-4.25	K ₂ Mg(SO ₄) ₂ :4H ₂ O
Li	-29.88	11.42	41.30	Li
Li(g)	-40.26	11.42	51.68	Li
Lime	-11.25	6.59	17.83	CaO
Magnesite	0.00	-2.14	-2.14	MgCO ₃
Magnetite	-0.10	-7.50	-7.40	Fe ₃ O ₄
Margarite	1.44	-0.72	-2.15	CaAl ₄ Si ₂ O ₁₀ (OH) ₂
Maximum Microcline	0.02	-4.71	-4.73	KAlSi ₃ O ₈
Mayenite	-118.12	69.06	187.18	Ca ₁₂ Al ₁₄ O ₃₃
Melanterite	-10.61	-13.46	-2.85	FeSO ₄ :7H ₂ O

Mercallite	-12.88	-14.32	-1.44	KHSO4
Merwinite	-12.35	21.97	34.32	MgCa3(SiO4)2
Mesolite	1.23	-1.22	-2.45	Na.676Ca.657Al1.99Si3.01O10:2.647H2O
Mg	-40.33	25.47	65.79	Mg
Mg(g)	-49.19	25.47	74.66	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-4.09	-8.68	-4.59	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-4.21	-7.01	-2.80	Mg1.5SO4(OH)
MgCl2:2H2O	-8.95	-5.28	3.67	MgCl2:2H2O
MgCl2:4H2O	-7.51	-5.29	2.22	MgCl2:4H2O
MgCl2:H2O	-10.05	-5.28	4.78	MgCl2:H2O
MgOHC1	-5.12	0.69	5.81	MgOHC1
MgSO4	-5.69	-10.34	-4.64	MgSO4
Minnesotaite	-1.17	1.79	2.96	Fe3Si4O10(OH)2
Mirabilite	-18.17	-9.41	8.76	Na2SO4:10H2O
Misenite	-86.51	-97.59	-11.08	K8H6(SO4)7
Molysite	-20.86	-23.42	-2.56	FeCl3
Monohydrocalcite	-3.27	-2.22	1.06	CaCO3:H2O
Monticellite	-3.01	11.02	14.03	CaMgSiO4
Montmor-Ca	2.04	-6.80	-8.84	Ca.165Mg.33Al1.67Si4O10(OH)2
Montmor-K	1.34	-7.01	-8.35	K.33Mg.33Al1.67Si4O10(OH)2
Montmor-Mg	2.32	-6.79	-9.11	Mg.495Al1.67Si4O10(OH)2
Montmor-Na	1.58	-6.63	-8.21	Na.33Mg.33Al1.67Si4O10(OH)2
Mordenite	-0.92	-8.65	-7.73	Ca.2895Na.361Al.94Si5.06O12:3.468H2O
Mordenite-dehy	-7.83	-8.64	-0.81	Ca.2895Na.361Al.94Si5.06O12
Muscovite	2.35	-6.14	-8.50	KAl3Si3O10(OH)2
Na	-25.53	13.22	38.75	Na
Na(g)	-31.14	13.22	44.35	Na
Na2CO3	-8.75	-1.18	7.58	Na2CO3
Na2CO3:7H2O	-17.06	-1.21	15.85	Na2CO3:7H2O
Na2O	-33.92	7.62	41.54	Na2O
Na2SiO3	-10.52	5.40	15.92	Na2SiO3
Na3H(SO4)2	-21.66	-22.55	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-23.19	-29.15	-5.96	Na4Ca(SO4)3:2H2O
Na4SiO4	-33.47	13.02	46.49	Na4SiO4
Na6Si2O7	-48.00	18.42	66.42	Na6Si2O7
NaFeO2	-9.64	-1.72	7.92	NaFeO2
Nahcolite	-5.41	-4.99	0.42	NaHCO3
Natrolite	-2.50	-0.48	2.01	Na2Al2Si3O10:2H2O
Natron	-16.02	-1.22	14.80	Na2CO3:10H2O
Natrosilite	-10.24	3.17	13.41	Na2Si2O5
Nepheline	-1.69	0.87	2.56	NaAlSiO4
Nesquehonite	-6.13	-2.16	3.97	MgCO3:3H2O
Nontronite-Ca	0.13	-18.37	-18.50	Ca.165Fe2Al.33Si3.67H2O12
Nontronite-H	-0.58	-19.46	-18.88	H.33Fe2Al.33Si3.67H2O12
Nontronite-K	-0.70	-18.58	-17.88	K.33Fe2Al.33Si3.67H2O12
Nontronite-Mg	0.38	-18.36	-18.74	Mg.165Fe2Al.33Si3.67H2O12
Nontronite-Na	-0.37	-18.20	-17.83	Na.33Fe2Al.33Si3.67H2O12
O2(g)	-34.99	-37.62	-2.64	O2
Okenite	-6.88	2.13	9.02	CaSi2O4(OH)2:2H2O
Oxychloride-Mg	-18.27	7.32	25.59	Mg2Cl(OH)3:4H2O
Paragonite	1.71	-5.00	-6.71	NaAl3Si3O10(OH)2
Parasite	-1.80	28.12	29.92	NaCa2Al3Mg4Si6O22(OH)2
Pentahydrate	-8.80	-10.36	-1.56	MgSO4:5H2O
Periclase	-3.40	6.65	10.06	MgO
Petalite	0.31	-7.59	-7.90	LiAlSi4O10
Phlogopite	3.56	15.25	11.69	KAlMg3Si3O10(OH)2
Picromerite	-17.36	-22.01	-4.65	K2Mg(SO4)2:6H2O
Pirssonite	-14.65	-3.40	11.25	Na2Ca(CO3)2:2H2O
Polyhalite	-28.42	-42.80	-14.38	K2MgCa2(SO4)4:2H2O
Portlandite	-6.28	6.58	12.86	Ca(OH)2
Prehnite	-0.85	5.07	5.92	Ca2Al2Si3O10(OH)2
Pseudowollastonite	-2.80	4.36	7.16	CaSiO3
Pyrite	-0.13	-19.44	-19.31	FeS2
Pyrophyllite	0.86	-10.32	-11.18	Al2Si4O10(OH)2
Pyrrhotite	-1.36	-7.15	-5.79	FeS
Quartz	0.00	-2.22	-2.22	SiO2
Rankinite	-11.98	15.32	27.30	Ca3Si2O7
Ripidolite-14A	4.16	18.97	14.81	Mg3Fe2Al2Si3O10(OH)8
Ripidolite-7A	1.73	18.97	17.25	Mg3Fe2Al2Si3O10(OH)8
Rutile	6.95	-2.62	-9.58	TiO2
S	-3.63	-29.53	-25.89	S
S2(g)	-11.58	-24.57	-12.99	S2
Sanidine_high	-0.35	-4.71	-4.36	KAlSi3O8
Saponite-Ca	4.58	12.65	8.07	Ca.165Mg3Al.33Si3.67O10(OH)2
Saponite-H	3.81	11.57	7.75	H.33Mg3Al.33Si3.67O10(OH)2
Saponite-K	3.76	12.45	8.69	K.33Mg3Al.33Si3.67O10(OH)2
Saponite-Mg	4.82	12.67	7.84	Mg3.165Al.33Si3.67O10(OH)2
Saponite-Na	4.08	12.82	8.75	Na.33Mg3Al.33Si3.67O10(OH)2
Scolecite	1.20	-1.52	-2.72	CaAl2Si3O10:3H2O
Sellaite	-0.41	-13.06	-12.65	MgF2
Sepiolite	-2.62	13.25	15.88	Mg4Si6O15(OH)2:6H2O
Si	-46.41	35.40	81.81	Si
Si(g)	-83.86	35.40	119.26	Si
Siderite	-1.38	-5.24	-3.86	FeCO3
SiF4(g)	-19.74	-41.65	-21.90	SiF4
Sillimanite	-0.00	-3.65	-3.65	Al2SiO5
SiO2(am)	-0.51	-2.22	-1.71	SiO2
Smectite-high-Fe-Mg	1.61	0.73	-0.88	Ca.025Na.1K.2Fe.5Fe.2Mg1.15Al1.25Si3.5H2O12
Smectite-low-Fe-Mg	1.36	-1.86	-3.22	Ca.02Na.15K.2Fe.29Fe.16Mg.9Al1.25Si3.75H2O12
SO2(g)	-8.47	-9.46	-0.99	SO2
Spinel	-1.17	5.23	6.40	Al2MgO4
Spodumene	-1.73	-3.14	-1.41	LiAlSi2O6
Starkeyite	-9.21	-10.35	-1.14	MgSO4:4H2O
Stilbite	1.19	-9.50	-10.69	Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O
Sylvite	-4.28	-3.29	0.99	KCl
Syngenite	-14.42	-22.06	-7.63	K2Ca(SO4)2:2H2O
Tachyhydrite	-32.66	-15.93	16.73	Mg2CaCl6:12H2O
Talc	3.67	11.07	7.40	Mg3Si4O10(OH)2
Thenardite	-6.83	-9.37	-2.54	Na2SO4
Thermonatrite	-9.85	-1.18	8.67	Na2CO3:H2O
Ti	-114.37	35.00	149.37	Ti
Ti(g)	-189.42	35.00	224.42	Ti
Ti2O3	-29.56	13.57	43.12	Ti2O3
Ti3O5	-23.92	10.95	34.86	Ti3O5
TiB2	-224.38	88.21	312.59	TiB2
TiC	-118.09	63.82	181.92	TiC
TiCl2	-66.78	4.26	71.04	TiCl2
TiCl3	-50.54	-11.11	39.43	TiCl3

TiCl4(g)	-54.66	-26.47	28.19	TiCl4
TiF4(am)	-29.74	-42.05	-12.30	TiF4
TiO(alpha)	-45.01	16.19	61.20	TiO
TiO(g)	-129.45	16.19	145.64	TiO
Titanite	-717.88	1.74	719.62	CaTiSiO5
Tobermorite-11A	-20.56	19.58	40.14	Ca5Si6H11O22.5
Tobermorite-14A	-24.90	19.56	44.46	Ca5Si6H21O27.5
Tobermorite-9A	-20.22	19.59	39.80	Ca5Si6H6O20
Tremolite	3.56	28.66	25.10	Ca2Mg5Si8O22(OH)2
Tridymite	-0.52	-2.22	-1.70	SiO2
Troilite	-1.29	-7.15	-5.86	FeS
Trona-K	-19.98	-8.46	11.52	K2NaH(CO3)2·2H2O
Wairakite	0.03	-3.74	-3.77	CaAl2Si4O10(OH)4
Wollastonite	-2.78	4.36	7.14	CaSiO3
Mustite	-2.08	2.41	4.48	Fe.9470
Xonotlite	-28.64	26.18	54.82	Ca6Si6O17(OH)2
Zoisite	-0.22	4.36	4.58	Ca2Al3(SiO4)3OH

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

TIME STEP 1 YEAR

Reaction step 10.

Using solution 1. AWI 1-2
 Using pure phase assemblage 1. Reservoir
 Using kinetics 1.

Kinetics 1.

Time step: 3e+09 seconds (Incremented time: 3.33333e+09 seconds)

Rate name	Delta Moles	Total Moles	Reactant	Coefficient
Quartz	-8.606e-05	4.876e+01	SiO2	1
Anorthite	2.459e-05	1.085e+01	CaAl2(SiO4)2	1
Albite	-2.926e-05	3.101e+01	NaAlSi3O8	1
K-Feldspar	-2.123e-06	7.877e+00	KAlSi3O8	1
Diopside	-0.000e+00	0.000e+00	CaMgSi2O6	1
Enstatite	1.559e-04	2.173e+00	MgSiO3	1
Ilmenite	6.205e-02	4.456e-01	FeTiO3	1
Titanite	-6.205e-02	1.921e+00	CaTiSiO5	1
Hematite	-1.551e-02	2.063e+00	Fe2O3	1
Epidote	3.102e-02	1.015e+01	Ca2FeAl2Si3O12OH	1
Chamosite-7A	-3.103e-02	1.170e+01	Fe2Al2SiO5(OH)4	1
Calcite	-0.000e+00	0.000e+00	CaCO3	1
Dolomite	-0.000e+00	0.000e+00	CaMg(CO3)2	1
Magnesite	-1.440e-04	8.649e+00	MgCO3	1

Phase assemblage

Phase	SI	log IAP	log K(T, P)	Initial	Final	Delta
CO2(g)	1.29	-0.78	-2.08	0.000e+00	0	0.000e+00

Solution composition

Elements	Molality	Moies
Al	2.552e-05	2.357e-05
B	2.484e-02	2.294e-02
C	1.657e-01	1.530e-01
Ca	6.794e-03	6.274e-03
Cl	2.072e-01	1.913e-01
F	1.050e-04	9.697e-05
Fe	1.039e-05	9.598e-06
K	1.004e-02	9.271e-03
Li	2.132e-03	1.969e-03
Mg	2.030e-02	1.875e-02
Na	1.407e-01	1.299e-01
S	2.694e-04	2.487e-04
Si	5.988e-03	5.530e-03
Ti	3.686e-03	3.404e-03

Description of solution

pH = 4.778 Charge balance
 pe = -1.651 Adjusted to redox equilibrium
 Density (g/cm³) = 0.82047
 Volume (L) = 1.14964
 Activity of water = 0.991
 Ionic strength (mol/kgw) = 1.806e-01
 Mass of water (kg) = 9.235e-01
 Total alkalinity (eq/kg) = 5.801e-04
 Total CO2 (mol/kg) = 1.657e-01
 Temperature (°C) = 250.00
 Pressure (atm) = 155.00
 Electrical balance (eq) = -1.101e-03
 Percent error, 100*(Cat-[An])/(Cat+[An]) = -0.35
 Iterations = 85
 Total H = 1.026357e+02
 Total O = 5.167734e+01

Distribution of species

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	2.413e-05	1.666e-05	-4.618	-4.778	-0.161	0.00
OH-	7.379e-07	4.101e-07	-6.132	-6.387	-0.255	(0)
H2O	5.553e+01	9.907e-01	1.744	-0.004	0.000	22.19
Al	2.552e-05					
HALO2	1.191e-05	1.191e-05	-4.924	-4.924	0.000	(0)
ALO2-	9.086e-06	5.199e-06	-5.042	-5.284	-0.242	(0)
NALO2	4.462e-06	4.462e-06	-5.351	-5.351	0.000	(0)
Al(OH)2+	6.582e-08	3.766e-08	-7.182	-7.424	-0.242	(0)
AlOH+2	3.481e-10	3.980e-11	-9.458	-10.400	-0.942	(0)
AlF+2	1.023e-12	1.169e-13	-11.990	-12.932	-0.942	(0)
AlF2+	6.685e-13	3.826e-13	-12.175	-12.417	-0.242	(0)
Al+3	4.470e-14	1.422e-15	-13.350	-14.847	-1.497	(0)
AlF3	3.959e-14	3.959e-14	-13.402	-13.402	0.000	(0)
AlF4-	1.428e-16	8.174e-17	-15.845	-16.088	-0.242	(0)

AlSO4+	5.243e-19	3.001e-19	-18.280	-18.523	-0.242	(0)
Al(SO4)2-	8.392e-24	4.802e-24	-23.076	-23.319	-0.242	(0)
Al2(OH)2+4	4.974e-25	1.713e-28	-24.303	-27.766	-3.463	(0)
Al3(OH)4+5	1.018e-34	6.522e-40	-33.992	-39.186	-5.193	(0)
Al13O4(OH)24+7	0.000e+00	0.000e+00	-127.792	-137.977	-10.185	(0)
B(-5)	0.000e+00					
BH4-	0.000e+00	0.000e+00	-54.802	-55.044	-0.242	(0)
B(3)	2.484e-02					
B(OH)3	2.484e-02	2.484e-02	-1.605	-1.605	0.000	(0)
BO2-	2.583e-06	1.478e-06	-5.588	-5.830	-0.242	(0)
MgB(OH)4+	1.592e-07	9.109e-08	-6.798	-7.041	-0.242	(0)
NaB(OH)4	1.169e-07	1.169e-07	-6.932	-6.932	0.000	(0)
CaB(OH)4+	7.182e-08	4.110e-08	-7.144	-7.386	-0.242	(0)
BF2(OH)2-	1.887e-10	1.080e-10	-9.724	-9.967	-0.242	(0)
BF4-	7.981e-16	4.567e-16	-15.098	-15.340	-0.242	(0)
B2O(OH)5-	1.337e-17	7.648e-18	-16.874	-17.116	-0.242	(0)
BF3OH-	2.482e-37	1.420e-37	-36.605	-36.848	-0.242	(0)
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-40.126	-40.126	0.000	(0)
C(-3)	1.432e-07					
C2H6	7.159e-08	7.159e-08	-7.145	-7.145	0.000	(0)
C(-4)	8.172e-11					
CH4	8.172e-11	8.172e-11	-10.088	-10.088	0.000	(0)
C(2)	5.892e-09					
CO	5.892e-09	5.892e-09	-8.230	-8.230	0.000	(0)
C(4)	1.657e-01					
CO2	1.585e-01	1.652e-01	-0.800	-0.782	0.018	79.97
(CO2)2	3.337e-03	3.479e-03	-2.477	-2.459	0.018	159.93
MgHCO3+	2.531e-04	1.448e-04	-3.597	-3.839	-0.242	(0)
HCO3-	1.653e-04	9.458e-05	-3.782	-4.024	-0.242	(0)
CaHCO3+	1.366e-04	7.814e-05	-3.865	-4.107	-0.242	(0)
NaHCO3	1.362e-07	1.362e-07	-6.866	-6.866	0.000	(0)
CaCO3	1.196e-07	1.196e-07	-6.922	-6.922	0.000	(0)
FeHCO3+	5.622e-08	3.217e-08	-7.250	-7.493	-0.242	(0)
MgCO3	2.507e-08	2.507e-08	-7.601	-7.601	0.000	(0)
CO3-2	6.224e-10	7.115e-11	-9.206	-10.148	-0.942	(0)
FeCO3	9.270e-12	9.270e-12	-11.033	-11.033	0.000	(0)
NaCO3-	1.151e-14	6.584e-15	-13.939	-14.181	-0.242	(0)
FeCO3+	1.310e-20	7.496e-21	-19.883	-20.125	-0.242	(0)
Ca	6.794e-03					
Ca+2	4.547e-03	6.792e-04	-2.342	-3.168	-0.826	(0)
CaCl+	1.590e-03	9.096e-04	-2.799	-3.041	-0.242	(0)
CaCl2	5.106e-04	5.106e-04	-3.292	-3.292	0.000	(0)
CaHCO3+	1.366e-04	7.814e-05	-3.865	-4.107	-0.242	(0)
CaF+	8.031e-06	4.596e-06	-5.095	-5.338	-0.242	(0)
CaSO4	2.308e-06	2.308e-06	-5.637	-5.637	0.000	(0)
CaCO3	1.196e-07	1.196e-07	-6.922	-6.922	0.000	(0)
CaB(OH)4+	7.182e-08	4.110e-08	-7.144	-7.386	-0.242	(0)
CaOH+	1.080e-11	6.179e-12	-10.967	-11.209	-0.242	(0)
Cl(-1)	2.072e-01					
Cl-	1.700e-01	9.144e-02	-0.770	-1.039	-0.269	(0)
NaCl	2.035e-02	2.035e-02	-1.691	-1.691	0.000	(0)
MgCl+	1.330e-02	7.610e-03	-1.876	-2.119	-0.242	(0)
CaCl+	1.590e-03	9.096e-04	-2.799	-3.041	-0.242	(0)
KCl	7.701e-04	7.701e-04	-3.113	-3.113	0.000	(0)
CaCl2	5.106e-04	5.106e-04	-3.292	-3.292	0.000	(0)
LiCl	1.173e-04	1.173e-04	-3.931	-3.931	0.000	(0)
HCl	5.537e-06	5.537e-06	-5.257	-5.257	0.000	(0)
FeCl+	5.391e-06	3.085e-06	-5.268	-5.511	-0.242	(0)
FeCl4-2	5.534e-07	5.688e-08	-6.257	-7.245	-0.988	(0)
FeCl2	5.230e-08	5.230e-08	-7.282	-7.282	0.000	(0)
FeCl4+2	1.145e-16	1.309e-17	-15.941	-16.883	-0.942	(0)
FeCl2+	2.798e-20	1.601e-20	-19.553	-19.796	-0.242	(0)
FeCl4-	2.812e-25	1.609e-25	-24.551	-24.793	-0.242	(0)
Cl(1)	1.571e-28					
HClO	1.566e-28	1.566e-28	-27.805	-27.805	0.000	(0)
ClO-	4.431e-31	2.535e-31	-30.354	-30.596	-0.242	(0)
Cl(3)	0.000e+00					
ClO2-	0.000e+00	0.000e+00	-53.461	-53.704	-0.242	(0)
HClO2	0.000e+00	0.000e+00	-55.312	-55.312	0.000	(0)
Cl(5)	0.000e+00					
ClO3-	0.000e+00	0.000e+00	-68.631	-68.886	-0.255	(0)
Cl(7)	0.000e+00					
ClO4-	0.000e+00	0.000e+00	-87.271	-87.526	-0.255	(0)
F	1.050e-04					
MgF+	4.094e-05	2.342e-05	-4.388	-4.630	-0.242	(0)
HF	3.973e-05	3.973e-05	-4.401	-4.401	0.000	(0)
F-	1.479e-05	8.220e-06	-4.830	-5.085	-0.255	(0)
CaF+	8.031e-06	4.596e-06	-5.095	-5.338	-0.242	(0)
NaF	1.519e-06	1.519e-06	-5.818	-5.818	0.000	(0)
FeF+	2.133e-10	1.220e-10	-9.671	-9.913	-0.242	(0)
BF2(OH)2-	1.887e-10	1.080e-10	-9.724	-9.967	-0.242	(0)
HF2-	1.723e-10	9.861e-11	-9.764	-10.006	-0.242	(0)
AlF+2	1.023e-12	1.169e-13	-11.990	-12.932	-0.942	(0)
AlF2+	6.685e-13	3.826e-13	-12.175	-12.417	-0.242	(0)
H2F2	1.099e-13	1.099e-13	-12.959	-12.959	0.000	(0)
AlF3	3.959e-14	3.959e-14	-13.402	-13.402	0.000	(0)
BF4-	7.981e-16	4.567e-16	-15.098	-15.340	-0.242	(0)
AlF4-	1.428e-16	8.174e-17	-15.845	-16.088	-0.242	(0)
FeF2+	7.186e-17	4.112e-17	-16.144	-16.386	-0.242	(0)
FeF+2	2.550e-17	2.915e-18	-16.593	-17.535	-0.942	(0)
SiF6-2	1.066e-25	1.095e-26	-24.972	-25.961	-0.988	(0)
BF3OH-	2.482e-37	1.420e-37	-36.605	-36.848	-0.242	(0)
Fe(2)	1.039e-05					
FeCl+	5.391e-06	3.085e-06	-5.268	-5.511	-0.242	(0)
Fe+2	4.339e-06	6.481e-07	-5.363	-6.188	-0.826	(0)
FeCl4-2	5.534e-07	5.688e-08	-6.257	-7.245	-0.988	(0)
FeHCO3+	5.622e-08	3.217e-08	-7.250	-7.493	-0.242	(0)
FeCl2	5.230e-08	5.230e-08	-7.282	-7.282	0.000	(0)
FeF+	2.133e-10	1.220e-10	-9.671	-9.913	-0.242	(0)
FeOH+	2.307e-11	1.320e-11	-10.637	-10.879	-0.242	(0)
FeSO4	2.116e-11	2.116e-11	-10.674	-10.674	0.000	(0)
FeCO3	9.270e-12	9.270e-12	-11.033	-11.033	0.000	(0)
Fe(OH)2	6.754e-18	6.754e-18	-17.170	-17.170	0.000	(0)
Fe(OH)3-	3.027e-23	1.732e-23	-22.519	-22.761	-0.242	(0)
Fe(OH)4-2	1.085e-32	1.116e-33	-31.964	-32.953	-0.988	(0)
Fe(3)	4.881e-16					
Fe(OH)2+	2.200e-16	1.259e-16	-15.658	-15.900	-0.242	(0)

	FeCl+2	1.145e-16	1.309e-17	-15.941	-16.883	-0.942	(0)
	FeF2+	7.186e-17	4.112e-17	-16.144	-16.386	-0.242	(0)
	FeOH+2	5.164e-17	5.903e-18	-16.287	-17.229	-0.942	(0)
	FeF+2	2.550e-17	2.915e-18	-16.593	-17.535	-0.942	(0)
	Fe(OH)3	3.793e-18	3.793e-18	-17.421	-17.421	0.000	(0)
	Fe+3	4.462e-19	1.420e-20	-18.350	-19.848	-1.497	(0)
	FeSO4+	3.738e-19	2.139e-19	-18.427	-18.670	-0.242	(0)
	FeCl2+	2.798e-20	1.601e-20	-19.553	-19.796	-0.242	(0)
	FeCO3+	1.310e-20	7.496e-21	-19.883	-20.125	-0.242	(0)
	Fe(OH)4-	1.072e-22	6.137e-23	-21.970	-22.212	-0.242	(0)
	FeCl4-	2.812e-25	1.609e-25	-24.551	-24.793	-0.242	(0)
	Fe2(OH)2+4	2.725e-30	9.380e-34	-29.565	-33.028	-3.463	(0)
	Fe(SO4)2-	1.725e-30	9.870e-31	-29.763	-30.006	-0.242	(0)
	Fe3(OH)4+5	0.000e+00	0.000e+00	-41.414	-46.608	-5.193	(0)
H(0)	H2	3.430e-06					
	H2	1.715e-06	1.865e-06	-5.766	-5.729	0.036	(0)
K	K+	1.004e-02					
	K+	9.269e-03	4.986e-03	-2.033	-2.302	-0.269	(0)
	KCl	7.701e-04	7.701e-04	-3.113	-3.113	0.000	(0)
	KSO4-	5.081e-07	2.907e-07	-6.294	-6.537	-0.242	(0)
	KHSO4	8.018e-09	8.018e-09	-8.096	-8.096	0.000	(0)
	KOH	1.113e-12	1.113e-12	-11.953	-11.953	0.000	(0)
Li	Li	2.132e-03					
	Li+	2.015e-03	1.266e-03	-2.696	-2.898	-0.202	(0)
	LiCl	1.173e-04	1.173e-04	-3.931	-3.931	0.000	(0)
	LiSO4-	2.685e-09	1.537e-09	-8.571	-8.813	-0.242	(0)
	LiOH	1.868e-12	1.868e-12	-11.729	-11.729	0.000	(0)
Mg	Mg	2.030e-02					
	MgCl+	1.330e-02	7.610e-03	-1.876	-2.119	-0.242	(0)
	Mg+2	6.473e-03	1.265e-03	-2.189	-2.898	-0.709	(0)
	MgHCO3+	2.531e-04	1.448e-04	-3.597	-3.839	-0.242	(0)
	MgSO4	2.363e-04	2.363e-04	-3.626	-3.626	0.000	(0)
	MgF+	4.094e-05	2.342e-05	-4.388	-4.630	-0.242	(0)
	MgB(OH)4+	1.592e-07	9.109e-08	-6.798	-7.041	-0.242	(0)
	MgCO3	2.507e-08	2.507e-08	-7.601	-7.601	0.000	(0)
	Mg4(OH)4+4	2.277e-29	7.839e-33	-28.643	-32.106	-3.463	(0)
Na	Na	1.407e-01					
	Na+	1.203e-01	6.885e-02	-0.920	-1.162	-0.242	(0)
	NaCl	2.035e-02	2.035e-02	-1.691	-1.691	0.000	(0)
	NaAlO2	4.462e-06	4.462e-06	-5.351	-5.351	0.000	(0)
	NaF	1.519e-06	1.519e-06	-5.818	-5.818	0.000	(0)
	NaHSiO3	5.502e-07	5.502e-07	-6.259	-6.259	0.000	(0)
	NaSO4-	1.639e-07	9.378e-08	-6.785	-7.028	-0.242	(0)
	NaHCO3	1.362e-07	1.362e-07	-6.866	-6.866	0.000	(0)
	NaOH	1.295e-07	1.295e-07	-6.888	-6.888	0.000	(0)
	NaB(OH)4	1.169e-07	1.169e-07	-6.932	-6.932	0.000	(0)
	NaCO3-	1.151e-14	6.584e-15	-13.939	-14.181	-0.242	(0)
O(0)	O2	2.975e-37					
	O2	1.487e-37	1.617e-37	-36.828	-36.791	0.036	(0)
S(-2)	S	2.683e-05					
	H2S	2.658e-05	2.658e-05	-4.575	-4.575	0.000	(0)
	HS-	2.544e-07	1.414e-07	-6.594	-6.850	-0.255	(0)
	S-2	2.656e-10	3.345e-11	-9.576	-10.476	-0.900	(0)
	S2-2	1.279e-15	1.314e-16	-14.893	-15.881	-0.988	(0)
	S3-2	5.163e-19	5.306e-20	-18.287	-19.275	-0.988	(0)
	S4-2	1.519e-22	1.561e-23	-21.819	-22.807	-0.988	(0)
	S5-2	3.356e-26	3.449e-27	-25.474	-26.462	-0.988	(0)
S(2)	S	1.266e-12					
	S2O3-2	6.329e-13	6.504e-14	-12.199	-13.187	-0.988	(0)
	HS2O3-	1.955e-17	1.119e-17	-16.709	-16.951	-0.242	(0)
S(3)	S	7.571e-24					
	S2O4-2	3.785e-24	4.769e-25	-23.422	-24.322	-0.900	(0)
S(4)	S	1.707e-09					
	HSO3-	9.510e-10	5.442e-10	-9.022	-9.264	-0.242	(0)
	SO2	7.562e-10	7.562e-10	-9.121	-9.121	0.000	(0)
	SO3-2	3.651e-14	4.174e-15	-13.438	-14.379	-0.942	(0)
	H2SO3	1.892e-15	1.892e-15	-14.723	-14.723	0.000	(0)
	S4O6-2	1.591e-24	1.635e-25	-23.798	-24.786	-0.988	(0)
	S2O6-2	1.764e-25	1.813e-26	-24.754	-25.742	-0.988	(0)
	S3O6-2	5.592e-31	5.747e-32	-30.252	-31.241	-0.988	(0)
	S5O6-2	3.450e-40	0.000e+00	-39.462	-40.450	-0.988	(0)
S(5)	S	8.272e-24					
	S2O5-2	4.136e-24	4.251e-25	-23.383	-24.372	-0.988	(0)
S(6)	S	2.425e-04					
	MgSO4	2.363e-04	2.363e-04	-3.626	-3.626	0.000	(0)
	CaSO4	2.308e-06	2.308e-06	-5.637	-5.637	0.000	(0)
	SO4-2	2.006e-06	2.062e-07	-5.698	-6.686	-0.988	(0)
	HSO4-	1.183e-06	6.769e-07	-5.927	-6.169	-0.242	(0)
	KSO4-	5.081e-07	2.907e-07	-6.294	-6.537	-0.242	(0)
	NaSO4-	1.639e-07	9.378e-08	-6.785	-7.028	-0.242	(0)
	KHSO4	8.018e-09	8.018e-09	-8.096	-8.096	0.000	(0)
	LiSO4-	2.685e-09	1.537e-09	-8.571	-8.813	-0.242	(0)
	FeSO4	2.118e-11	2.118e-11	-10.674	-10.674	0.000	(0)
	H2SO4	5.451e-18	5.451e-18	-17.264	-17.264	0.000	(0)
	AlSO4+	5.243e-19	3.001e-19	-18.280	-18.523	-0.242	(0)
	FeSO4+	3.738e-19	2.139e-19	-18.427	-18.670	-0.242	(0)
	Al(SO4)2-	8.392e-24	4.802e-24	-23.076	-23.319	-0.242	(0)
	Fe(SO4)2-	1.725e-30	9.870e-31	-29.763	-30.006	-0.242	(0)
S(7)	S	0.000e+00					
	S2O8-2	0.000e+00	0.000e+00	-45.706	-46.694	-0.988	(0)
S(8)	S	1.958e-35					
	HSO5-	1.958e-35	1.120e-35	-34.708	-34.951	-0.242	(0)
Si	Si	5.988e-03					
	SiO2	5.987e-03	5.987e-03	-2.223	-2.223	0.000	(0)
	HSiO3-	6.191e-07	3.543e-07	-6.208	-6.451	-0.242	(0)
	NaHSiO3	5.502e-07	5.502e-07	-6.259	-6.259	0.000	(0)
	H6(H2SiO4)4-2	1.811e-12	1.861e-13	-11.742	-12.730	-0.988	(0)
	H2SiO4-2	2.650e-15	2.723e-16	-14.577	-15.565	-0.988	(0)
	H4(H2SiO4)4-4	3.145e-22	3.363e-26	-21.502	-25.473	-3.971	(0)
	SiF6-2	1.066e-25	1.095e-26	-24.972	-25.961	-0.988	(0)
Ti	Ti	3.686e-03					
	Ti(OH)4	3.686e-03	3.686e-03	-2.433	-2.433	0.000	(0)

-----Saturation indices-----				
Phase	SI**	log IAP	log K(523 K, 155 atm)	
Afwillite	-20.27	14.70	34.96	Ca3Si2O4(OH)6
Akermanite	-6.94	14.98	21.92	Ca2MgSi2O7

Al	-49.13	27.08	76.20	Al
Al (g)	-75.22	27.08	102.29	Al
Al2 (SO4)3	-31.47	-49.75	-18.28	Al2 (SO4)3
Al2 (SO4)3:6H2O	-27.73	-49.78	-22.04	Al2 (SO4)3:6H2O
Albite	-0.00	-3.57	-3.57	NaAlSi3O8
Albite_high	-0.49	-3.57	-3.08	NaAlSi3O8
Albite_low	-0.00	-3.57	-3.57	NaAlSi3O8
AlF3	-6.18	-30.10	-23.92	AlF3
Alum-K	-21.56	-30.57	-9.01	KAl (SO4)2:12H2O
Alunite	-6.92	-31.57	-24.65	KAl3 (OH)6 (SO4)2
Amesite-14A	7.96	20.09	12.13	Mg4Al4Si2O10 (OH)8
Analcime	-0.39	-1.57	-1.17	Na.96Al.96Si2.04O6:H2O
Analcime-dehy	-3.51	-1.56	1.95	Na.96Al.96Si2.04O6
Anatase	6.06	-2.43	-8.49	TiO2
Andalusite	0.52	-3.26	-3.77	Al2SiO5
Andradite	-5.28	1.45	6.73	Ca3Fe2 (SiO4)3
Anhydrite	-1.33	-9.85	-8.52	CaSO4
Ankerite	-1.72	-6.86	-5.14	CaMg0.3Fe0.7 (CO3)2
Annite	-1.59	5.38	6.97	KFe3AlSi3O10 (OH)2
Anorthite	-0.00	0.90	0.90	CaAl2 (SiO4)2
Antarcticite	-9.16	-5.27	3.89	CaCl2:6H2O
Anthophyllite	3.62	28.80	25.18	Mg7Si8O22 (OH)2
Antigorite	36.47	243.74	207.27	Mg48Si34O85 (OH)62
Aphthitalite	-17.55	-21.44	-3.89	NaK3 (SO4)2
Aragonite	-1.21	-2.41	-1.20	CaCO3
Arcanite	-8.70	-11.29	-2.59	K2SO4
Artinite	-4.95	4.50	9.45	Mg2CO3 (OH)2:3H2O
B	-34.14	25.99	60.13	B
B (g)	-82.96	25.99	108.96	B
B2O3	-6.23	-3.20	3.03	B2O3
Bassanite	-2.02	-9.86	-7.83	CaSO4:0.5H2O
Beidellite-Ca	2.28	-8.31	-10.59	Ca.165Al2.33Si3.67O10 (OH)2
Beidellite-H	1.54	-9.37	-10.91	H.33Al2.33Si3.67O10 (OH)2
Beidellite-K	1.41	-8.55	-9.97	K.33Al2.33Si3.67O10 (OH)2
Beidellite-Mg	2.56	-8.27	-10.83	Mg.165Al2.33Si3.67O10 (OH)2
Beidellite-Na	1.74	-8.18	-9.92	Na.33Al2.33Si3.67O10 (OH)2
BF3 (g)	-18.30	-31.18	-12.88	BF3
Bischofite	-9.18	-5.00	4.18	MgCl2:6H2O
Bloedite	-15.99	-18.61	-2.62	Na2Mg (SO4)2:4H2O
Boehmite	1.03	-0.52	-1.55	AlO2H
Borax	-17.76	0.79	18.55	Na2 (B4O5 (OH)4) :8H2O
Boric acid	-2.82	-1.60	1.22	B (OH)3
Brucite	-1.46	6.65	8.11	Mg (OH)2
Burkeite	-29.08	-19.59	9.49	Na6CO3 (SO4)2
C	-4.37	27.99	32.36	C
C (g)	-68.16	27.99	96.15	C
Ca	-52.37	24.78	77.15	Ca
Ca (g)	-64.42	24.78	89.20	Ca
Ca-Al Pyroxene	-3.47	3.13	6.59	CaAl2SiO6
Ca2Al2O5:8H2O	-47.42	11.70	59.12	Ca2Al2O5:8H2O
Ca2Cl2 (OH)2:2H2O	-25.06	1.13	26.19	Ca2Cl2 (OH)2:2H2O
Ca3Al2O6	-32.19	18.12	50.31	Ca3Al2O6
Ca4Al2Fe2O10	-40.93	13.47	54.40	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-82.11	24.45	106.56	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-78.36	24.43	102.78	Ca4Al2O7:19H2O
Ca4Cl2 (OH)6:13H2O	-53.83	13.84	67.67	Ca4Cl2 (OH)6:13H2O
CaAl2O4	-7.13	5.35	12.48	CaAl2O4
CaAl2O4:10H2O	-32.20	5.31	37.51	CaAl2O4:10H2O
CaAl4O7	-9.28	4.31	13.59	CaAl4O7
Calcite	-1.05	-2.41	-1.36	CaCO3
Carnallite	-12.41	-8.34	4.06	KMgCl3:6H2O
CaSO4:0.5H2O (beta)	-2.02	-9.86	-7.84	CaSO4:0.5H2O
Celadonite	0.67	-0.28	-0.95	KMgAlSi4O10 (OH)2
CH4 (g)	-7.48	-10.09	-2.60	CH4
Chalcedony	-0.15	-2.22	-2.07	SiO2
Chamosite-7A	-0.00	3.46	3.46	Fe2Al2SiO5 (OH)4
Chloromagnesite	-12.32	-4.98	7.35	MgCl2
Chrysotile	1.74	15.51	13.77	Mg3Si2O5 (OH)4
Cl2 (g)	-27.40	-30.03	-2.62	Cl2
Clinocllore-14A	7.07	25.55	18.48	Mg5Al2Si3O10 (OH)8
Clinocllore-7A	4.61	25.55	20.94	Mg5Al2Si3O10 (OH)8
Clinoptilolite-Ca	2.40	-23.16	-25.56	Ca1.7335Al3.45Fe.017Si14.533036:10.922H2O
Clinoptilolite-dehy-Ca	-14.02	-23.12	-9.09	Ca1.7335Al3.45Fe.017Si14.533036
Clinoptilolite-dehy-K	-23.32	-25.61	-2.29	K3.467Al3.45Fe.017Si14.533036
Clinoptilolite-dehy-Na	-19.42	-21.65	-2.24	Na3.467Al3.45Fe.017Si14.533036
Clinoptilolite-hy-Ca	1.69	-23.16	-24.85	Ca1.7335Al3.45Fe.017Si14.533036:11.645H2O
Clinoptilolite-hy-K	-4.27	-25.64	-21.37	K3.467Al3.45Fe.017Si14.533036:7.499H2O
Clinoptilolite-hy-Na	-3.08	-21.70	-18.62	Na3.467Al3.45Fe.017Si14.533036:10.877H2O
Clinoptilolite-K	-7.21	-25.65	-18.44	K3.467Al3.45Fe.017Si14.533036:10.922H2O
Clinoptilolite-Na	-3.11	-21.70	-18.58	Na3.467Al3.45Fe.017Si14.533036:10.922H2O
Clinozoisite	-0.02	4.55	4.56	Ca2Al3Si3O12 (OH)
CO (g)	-5.72	-8.23	-2.51	CO
CO2 (g)	1.29	-0.78	-2.08	CO2
Coesite	-0.49	-2.22	-1.73	SiO2
Colemanite	-18.43	3.16	21.58	Ca2B6O11:5H2O
Cordierite anhyd	1.04	0.12	-0.91	Mg2Al4Si5O18
Cordierite_hydr	2.04	0.12	-1.92	Mg2Al4Si5O18:H2O
Corundum	4.67	-1.04	-5.71	Al2O3
Cristobalite (alpha)	-0.27	-2.22	-1.96	SiO2
Cristobalite (beta)	-0.44	-2.22	-1.78	SiO2
Cronstedtite-7A	-2.16	-6.54	-4.38	Fe2Fe2SiO5 (OH)4
Daphnite-14A	-0.61	9.10	9.71	Fe5AlAlSi3O10 (OH)8
Daphnite-7A	-2.97	9.10	12.08	Fe5AlAlSi3O10 (OH)8
Dawsonite	-4.33	-5.71	-1.38	NaAlCO3 (OH)2
Diaspore	1.18	-0.52	-1.70	AlHO2
Dicalcium_silicate	-9.26	10.55	19.80	Ca2SiO4
Diopside	-0.80	8.59	9.39	CaMgSi2O6
Dolomite	-0.20	-4.56	-4.36	CaMg (CO3)2
Dolomite-dis	-0.82	-4.56	-3.74	CaMg (CO3)2
Dolomite-ord	-0.19	-4.56	-4.37	CaMg (CO3)2
Enstatite	-0.00	4.43	4.43	MgSiO3
Epidote	-0.00	-0.46	-0.46	Ca2FeAl2Si3O12OH
Epidote-ord	-0.04	-0.46	-0.42	FeCa2Al2 (OH) (SiO4)3
Epsomite	-7.41	-9.61	-2.20	MgSO4:7H2O
Ettringite	-54.92	-11.57	43.35	Ca6Al2 (SO4)3 (OH)12:26H2O
Eucryptite	-2.79	-0.86	1.93	LiAlSiO4
F2 (g)	-63.04	-38.12	24.93	F2
Fayalite	-2.18	4.51	6.68	Fe2SiO4

Fe	-8.57	21.76	30.33	Fe
Fe(OH)2	-3.35	3.36	6.71	Fe(OH)2
Fe(OH)3	-4.49	-5.52	-1.03	Fe(OH)3
Fe2(SO4)3	-34.27	-59.75	-25.49	Fe2(SO4)3
FeF2	-7.65	-16.36	-8.71	FeF2
FeF3	-11.58	-35.10	-23.52	FeF3
FeO	-2.03	3.36	5.39	FeO
Ferrite-Ca	-4.70	-4.65	0.04	CaFe2O4
Ferrite-Dicalcium	-17.59	1.73	19.33	Ca2Fe2O5
Ferrite-Mg	-2.79	-4.38	-1.59	MgFe2O4
Ferrosilite	-1.10	1.14	2.25	FeSiO3
FeSO4	-7.26	-12.87	-5.61	FeSO4
Fluorite	-1.74	-13.34	-11.60	CaF2
Forsterite	-0.64	11.09	11.72	Mg2SiO4
Foshagite	-17.60	18.86	36.46	Ca4Si3O9(OH)2·0.5H2O
Gaylussite	-15.00	-4.00	10.99	CaNa2(CO3)2·5H2O
Gehlenite	-7.62	9.51	17.14	Ca2Al2SiO7
Gibbsite	0.65	-0.52	-1.17	Al(OH)3
Gismondine	-39.36	1.77	41.13	Ca2Al4Si4O16·9H2O
Glauberite	-13.39	-18.86	-5.47	Na2Ca(SO4)2
Goethite	-1.40	-5.52	-4.13	FeOOH
Greenalite	-3.08	5.64	8.72	Fe3Si2O5(OH)4
Grossular	-4.12	11.45	15.57	Ca3Al2(SiO4)3
Gypsum	-2.69	-9.86	-7.17	CaSO4·2H2O
Gyrolite	-8.76	6.09	14.85	Ca2Si3O7(OH)2·1.5H2O
H2(g)	-3.12	-5.73	-2.61	H2
H2O(g)	1.56	-0.00	-1.56	H2O
H2S(g)	-3.04	-11.63	-8.59	H2S
Halite	-3.11	-2.20	0.91	NaCl
Hatrurite	-22.56	16.93	39.49	Ca3SiO5
HCl(g)	-5.63	-5.82	-0.18	HCl
Hedenbergite	-3.25	5.30	8.55	CaFe(SiO3)2
Hematite	-0.00	-11.04	-11.04	Fe2O3
Hercynite	0.86	2.33	1.46	FeAl2O4
Hexahydrite	-7.67	-9.61	-1.93	MgSO4·6H2O
Hillebrandite	-10.26	10.54	20.80	Ca2SiO3(OH)2·0.17H2O
Huntite	-1.73	-8.84	-7.11	CaMg3(CO3)4
Hydroboracite	-16.98	3.42	20.40	MgCaB6O11·6H2O
Hydromagnesite	-6.62	-1.94	4.68	Mg5(CO3)4(OH)2·4H2O
Hydrophilite	-8.20	-5.25	2.95	CaCl2
Ice	-1.14	-0.00	1.14	H2O
Illite	1.90	-5.83	-7.73	K0.6Mg0.25Al1.8Al0.5Si3.5O10(OH)2
Ilmenite	0.00	0.94	0.94	FeTiO3
Jadeite	-1.64	-1.35	0.29	NaAl(SiO3)2
Jarosite	-19.66	-46.57	-26.91	KFe3(SO4)2(OH)6
Jarosite-Na	-39.78	-45.43	-5.66	NaFe3(SO4)2(OH)6
K	-29.56	11.67	41.23	K
K(g)	-33.67	11.67	45.34	K
K-Feldspar	-0.00	-4.71	-4.71	KAlSi3O8
K2CO3·1.5H2O	-17.18	-3.86	13.33	K2CO3·1.5H2O
K2O	-47.01	4.95	51.96	K2O
K3H(SO4)2	-21.43	-25.06	-3.62	K3H(SO4)2
K8H4(CO3)6·3H2O	-60.63	-33.02	27.61	K8H4(CO3)6·3H2O
Kainite	-12.52	-12.94	-0.42	KMgClSO4·3H2O
KAl(SO4)2	-17.30	-30.52	-13.22	KAl(SO4)2
Kalichinite	-6.61	-6.33	0.28	KHCO3
Kalsilite	-1.73	-0.27	1.46	KAlSiO4
Kaolinite	1.46	-5.49	-6.95	Al2Si2O5(OH)4
Katoite	-60.43	18.09	78.53	Ca3Al2H12O12
Kieserite	-9.29	-9.59	-0.30	MgSO4·H2O
KMgCl3	-16.97	-8.32	8.65	KMgCl3
KMgCl3·2H2O	-14.87	-8.32	6.54	KMgCl3·2H2O
KNaCO3·6H2O	-12.79	-2.73	10.05	KNaCO3·6H2O
Kyanite	0.46	-3.26	-3.72	Al2SiO5
Lansfordite	-6.83	-2.16	4.67	MgCO3·5H2O
Larnite	-9.82	10.55	20.36	Ca2SiO4
Laumontite	0.30	-3.56	-3.86	CaAl2Si4O12·4H2O
Lawrencite	-8.28	-8.27	0.02	FeCl2
Lawsonite	-0.40	0.90	1.30	CaAl2Si2O7(OH)2·H2O
Leonite	-16.64	-20.89	-4.25	K2Mg(SO4)2·4H2O
Li	-30.23	11.08	41.30	Li
Li(g)	-40.60	11.08	51.68	Li
Lime	-11.45	6.38	17.83	CaO
Magnesite	-0.00	-2.14	-2.14	MgCO3
Magnetite	-0.28	-7.67	-7.40	Fe3O4
Margarite	2.02	-0.14	-2.15	CaAl4Si2O10(OH)2
Maximum Microcline	0.02	-4.71	-4.73	KAlSi3O8
Mayenite	-117.81	69.37	187.18	Ca12Al14O33
Melanterite	-10.06	-12.90	-2.85	FeSO4·7H2O
Mercallite	-12.33	-13.77	-1.44	KHSO4
Merwinite	-12.95	21.36	34.32	MgCa3(SiO4)2
Mesolite	1.36	-1.09	-2.45	Na.676Ca.657Al1.99Si3.01O10·2.647H2O
Mg	-40.74	25.05	65.79	Mg
Mg(g)	-49.60	25.05	74.66	Mg
Mg1.25SO4(OH)0.5·0.5H2O	-3.33	-7.92	-4.59	Mg1.25SO4(OH)0.5·0.5H2O
Mg1.5SO4(OH)	-3.46	-6.26	-2.80	Mg1.5SO4(OH)
MgCl2·2H2O	-8.65	-4.98	3.67	MgCl2·2H2O
MgCl2·4H2O	-7.21	-4.99	2.22	MgCl2·4H2O
MgCl2·H2O	-9.75	-4.98	4.78	MgCl2·H2O
MgOHCl	-4.97	0.84	5.81	MgOHCl
MgSO4	-4.94	-9.58	-4.64	MgSO4
Minnesotaite	-1.76	1.20	2.96	Fe3Si4O10(OH)2
Mirabilite	-17.81	-9.05	8.76	Na2SO4·10H2O
Misenite	-82.81	-93.89	-11.08	K8H6(SO4)7
Molysite	-20.41	-22.96	-2.56	FeCl3
Monohydrocalcite	-3.48	-2.42	1.06	CaCO3·H2O
Monticellite	-3.21	10.82	14.03	CaMgSiO4
Montmor-Ca	2.33	-6.51	-8.84	Ca.165Mg.33Al1.67Si4O10(OH)2
Montmor-K	1.60	-6.75	-8.35	K.33Mg.33Al1.67Si4O10(OH)2
Montmor-Mg	2.64	-6.47	-9.11	Mg.495Al1.67Si4O10(OH)2
Montmor-Na	1.84	-6.37	-8.21	Na.33Mg.33Al1.67Si4O10(OH)2
Mordenite	-0.86	-8.59	-7.73	Ca.2895Na.361Al.94Si5.06O12·3.468H2O
Mordenite-dehy	-7.77	-8.58	-0.81	Ca.2895Na.361Al.94Si5.06O12
Muscovite	2.74	-5.75	-8.50	KAl3Si3O10(OH)2
Na	-25.93	12.81	38.75	Na
Na(g)	-31.54	12.81	44.35	Na
Na2CO3	-9.15	-1.57	7.58	Na2CO3
Na2CO3·7H2O	-17.45	-1.60	15.85	Na2CO3·7H2O

Na2O	-34.32	7.23	41.54	Na2O
Na2SiO3	-10.91	5.01	15.92	Na2SiO3
Na3H(SO4)2	-20.75	-21.64	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.92	-27.88	-5.96	Na4Ca(SO4)3:2H2O
Na4SiO4	-34.26	12.23	46.49	Na4SiO4
Na6Si2O7	-49.18	17.24	66.42	Na6Si2O7
NaFeO2	-9.83	-1.90	7.92	NaFeO2
Nahcolite	-5.61	-5.19	0.42	NaHCO3
Natrolite	-2.50	-0.48	2.01	Na2Al2Si3O10:2H2O
Natron	-16.41	-1.61	14.80	Na2CO3:10H2O
Natrosilite	-10.63	2.78	13.41	Na2Si2O5
Nepheline	-1.69	0.87	2.56	NaAlSiO4
Nesquehonite	-6.13	-2.16	3.97	MgCO3:3H2O
Nontronite-Ca	0.19	-18.32	-18.50	Ca.165Fe2Al.33Si3.67H2O12
Nontronite-H	-0.49	-19.37	-18.88	H.33Fe2Al.33Si3.67H2O12
Nontronite-K	-0.68	-18.55	-17.88	K.33Fe2Al.33Si3.67H2O12
Nontronite-Mg	0.47	-18.27	-18.74	Mg.165Fe2Al.33Si3.67H2O12
Nontronite-Na	-0.35	-18.18	-17.83	Na.33Fe2Al.33Si3.67H2O12
O2(g)	-34.15	-36.79	-2.64	O2
Okenite	-7.08	1.93	9.02	CaSi2O4(OH)2:H2O
Oxychloride-Mg	-18.12	7.47	25.59	Mg2Cl(OH)3:4H2O
Paragonite	2.10	-4.61	-6.71	NaAl3Si3O10(OH)2
Pargasite	-1.81	28.11	29.92	NaCa2Al3Mg4Si6O22(OH)2
Pentahydrate	-8.04	-9.60	-1.56	MgSO4:5H2O
Periclase	-3.40	6.65	10.06	MgO
Petalite	0.37	-7.53	-7.90	LiAlSi4O10
Phlogopite	3.56	15.25	11.69	KAlMg3Si3O10(OH)2
Picromerite	-16.25	-20.90	-4.65	K2Mg(SO4)2:6H2O
Pirssonite	-15.25	-3.99	11.25	Na2Ca(CO3)2:2H2O
Polyhalite	-26.21	-40.59	-14.38	K2MgCa2(SO4)4:2H2O
Portlandite	-6.48	6.38	12.86	Ca(OH)2
Prehnite	-0.86	5.06	5.92	CaAl2Si3O10(OH)2
Pseudowollastonite	-3.00	4.16	7.16	CaSiO3
Pyrite	-1.73	-21.04	-19.31	FeS2
Pyrophyllite	1.25	-9.93	-11.18	Al2Si4O10(OH)2
Pyrrhotite	-2.47	-8.26	-5.79	FeS
Quartz	0.00	-2.22	-2.22	SiO2
Rankinite	-12.59	14.71	27.30	Ca3Si2O7
Ripidolite-14A	4.16	18.97	14.81	Mg3Fe2Al2Si3O10(OH)8
Ripidolite-7A	1.73	18.97	17.25	Mg3Fe2Al2Si3O10(OH)8
Rutile	7.15	-2.43	-9.58	TiO2
S	-4.13	-30.02	-25.89	S
S2(g)	-12.56	-25.56	-12.99	S2
Sanidine_high	-0.35	-4.71	-4.36	KAlSi3O8
Saponite-Ca	4.62	12.69	8.07	Ca.165Mg3Al.33Si3.67O10(OH)2
Saponite-H	3.88	11.63	7.75	H.33Mg3Al.33Si3.67O10(OH)2
Saponite-K	3.76	12.45	8.69	K.33Mg3Al.33Si3.67O10(OH)2
Saponite-Mg	4.89	12.73	7.84	Mg3.165Al.33Si3.67O10(OH)2
Saponite-Na	4.08	12.82	8.75	Na.33Mg3Al.33Si3.67O10(OH)2
Scolecite	1.39	-1.33	-2.72	CaAl2Si3O10:3H2O
Sellaite	-0.42	-13.07	-12.65	MgF2
Sepiolite	-2.62	13.25	15.88	Mg4Si6O15(OH)2:6H2O
Si	-47.24	34.57	81.81	Si
Si(g)	-84.69	34.57	119.26	Si
Siderite	-1.57	-5.43	-3.86	FeCO3
SiF4(g)	-19.76	-41.67	-21.90	SiF4
Sillimanite	0.39	-3.26	-3.65	Al2SiO5
SiO2(am)	-0.51	-2.22	-1.71	SiO2
Smectite-high-Fe-Mg	1.70	0.82	-0.88	Ca.025Na.1K.2Fe.5Fe.2Mg1.15Al1.25Si3.5H2O12
Smectite-low-Fe-Mg	1.48	-1.74	-3.22	Ca.02Na.15K.2Fe.29Fe.16Mg.9Al1.25Si3.75H2O12
SO2(g)	-8.13	-9.12	-0.99	SO2
Spinel	-0.78	5.62	6.40	Al2MgO4
Spodumene	-1.67	-3.08	-1.41	LiAlSi2O6
Starkeyite	-8.46	-9.60	-1.14	MgSO4:4H2O
Stilbite	1.39	-9.31	-10.69	Ca1.019Na.136K.006Al2.18Si6.82O18:7.33H2O
Sylvite	-4.33	-3.34	0.99	KCl
Syngenite	-13.51	-21.15	-7.63	K2Ca(SO4)2:2H2O
Tachyhydrite	-31.97	-15.25	16.73	Mg2CaCl6:12H2O
Talc	3.67	11.07	7.40	Mg3Si4O10(OH)2
Thenardite	-6.47	-9.01	-2.54	Na2SO4
Thermonatrite	-10.25	-1.57	8.67	Na2CO3:H2O
Ti	-115.00	34.37	149.37	Ti
Ti(g)	-190.05	34.37	224.42	Ti
Ti2O3	-29.58	13.55	43.12	Ti2O3
Ti3O5	-23.74	11.12	34.86	Ti3O5
TiB2	-226.24	86.36	312.59	TiB2
TiC	-119.56	62.36	181.92	TiC
TiCl2	-66.70	4.34	71.04	TiCl2
TiCl3	-50.10	-10.67	39.43	TiCl3
TiCl4(g)	-53.88	-25.69	28.19	TiCl4
TiF4(am)	-29.57	-41.87	-12.30	TiF4
TiO(alpha)	-45.23	15.97	61.20	TiO
TiO(g)	-129.67	15.97	145.64	TiO
Titanite	-717.88	1.74	719.62	CaTiSiO5
Tobermorite-11A	-21.57	18.56	40.14	Ca5Si6H11O22.5
Tobermorite-14A	-25.91	18.54	44.46	Ca5Si6H21O27.5
Tobermorite-9A	-21.23	18.58	39.80	Ca5Si6H6O20
Tremolite	3.16	28.26	25.10	Ca2Mg5Si8O22(OH)2
Tridymite	-0.52	-2.22	-1.70	SiO2
Troilite	-2.40	-8.26	-5.86	FeS
Trona-K	-20.56	-9.04	11.52	K2NaH(CO3)2:2H2O
Wairakite	0.22	-3.55	-3.77	CaAl2Si4O10(OH)4
Wollastonite	-2.98	4.16	7.14	CaSiO3
Wustite	-2.24	2.24	4.48	Fe.947O
Xenotlite	-29.86	24.97	54.82	Ca6Si6O17(OH)2
Zoisite	-0.04	4.55	4.58	Ca2Al3(SiO4)3OH

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

End of simulation.





