THE ELM GROUP

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-- Patricia Murray

RCAP RECEIVED
JAN 18 2011

February 15, 2010

-- Via E-Mail (curt.gardner@basf.com) and Federal Express --

Mr. Curt Gardner, P.E.
Senior EHS Specialist, Central Hub
BASF Corporation
3150 Highway JJ
Palmyra, MO 63461-2611

RE: BASF Corporation – Hannibal, MO
Evaluation of September 2009 Sodium Hydroxide Release

Dear Mr. Gardner:

On behalf of BASF, The ELM Group, Inc. (ELM) has reviewed available information and completed a detailed data analysis related to a sodium hydroxide (NaOH) release at the above-referenced facility. The objectives of this analysis were to: 1) evaluate potential environmental impacts related to the release; 2) to correlate available empirical evidence to the predicted behavior of NaOH in the environment; and 3) provide conclusions regarding further actions that may be needed to address the release.

The results of ELM's analysis strongly support the conclusion that the NaOH released to the environment has been attenuated to near neutral conditions via natural geochemical processes in soil and groundwater within a short time and distance from the release location. Further, it is probable that additional buffering of the release will continue until equilibrium is achieved. These conclusions are consistent with the results of soil and groundwater pH measurements collected at the site by AECOM shortly following the release, and have been further corroborated by geochemical modeling of the release. Based on all available lines of evidence, it is concluded that the NaOH release will not represent any long term detrimental effect to the environment, and it will not affect the ground water treatment system being operated at the site by Wyeth. The analyses and findings that support this conclusion are described below.

Project Background

The release of approximately 2,400 gallons of 50% NaOH occurred into a secondary containment trench adjacent to the East Utility Building on September 23, 2009. Due to a lack of structural integrity in the secondary containment trench and rainfall following the release, NaOH exited the trench and contacted the underlying soil. During the rain storm,

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BASF recovered approximately 5,000 gallons of elevated-pH water from containment trench and sump. BASF was directed by the Missouri Department of Natural Resources (MDNR) to prepare a report documenting the response to and environmental effects of the spill. Concerns were also expressed regarding potential effects on the groundwater treatment program being operated at the site by the previous owner (Wyeth). AECOM subsequently conducted a limited soil and groundwater investigation of the release area on behalf of BASF.

AECOM Limited Soil and Groundwater Investigation (AECOM, 2009)

On November 9-10, 2009, AECOM conducted a limited investigation in the release area to evaluate potential impacts to soil and groundwater. The investigation included installation of 14 soil borings in the release area, using either a hand auger (6 locations) or direct push (8 locations; Attachment A, Figure A1). Hand auger borings were advanced to a maximum depth of 4 feet below ground surface (bgs) or refusal. Direct push borings were advanced to a maximum depth of 9 feet bgs or refusal. Temporary groundwater monitoring wells (1", schedule 40 PVC riser and screen) were installed in 7 of 8 direct push locations (Attachment A, Figure A1). No well was installed at boring location SB-1 due to refusal at 2.5 feet bgs. Soils were logged by an AECOM geologist for all boring locations (Attachment A, Appendix A1).

Soil samples were collected and composited in 2 foot intervals for all hand auger locations and one direct push location (SB-2). Soil pH measurements were collected using a Hannah Model 99121 meter. All temporary monitoring wells were purged after installation and groundwater samples were collected using disposable bailers. Groundwater pH was screened using a Hannah Model 9025C meter. Soil and groundwater pH measurements are presented in Table A1 and Figures A2 and A3 (Attachment A).

The limited soil investigation found an average soil pH of 7.69 in shallow soil (0-2 feet bgs) and 7.52 in deeper soil (2-4 feet bgs) in the release area. Soil pH ranged between 7.46 and 8.57 in shallow soil, and 7.41 and 7.59 in deeper soil. Average groundwater pH was 8.22. Groundwater pH measurement ranged between 7.18 and 7.93, except one location (SB-2) where pH was 12.21. Excluding the reading at SB-2, the average groundwater pH measured by AECOM was 7.56. The findings of the AECOM investigation therefore support a conclusion that soil and groundwater pHs are generally near neutral, with the exception of an isolated reading at location SB-2.

SCOPE OF WORK

ELM conducted several types of analyses to evaluate potential impacts due to the NaOH release at the site, including:

1) Available soil, geology, and groundwater data were reviewed and analyzed to develop basic physical and chemical conceptual site models for the site. Information reviewed included:

    a. USDA Soil Survey for Marion County, MO (1984);

    b. USGS Bedrock Geology Map for Missouri (2005)

    c. Boring logs and pH measurements for the release area (AECOM, 2009)

    d. "Additional Groundwater Delineation and Capture Zone Modeling Documentation Report" (Arcadis, 2009)

2) Relevant scientific literature regarding the fate and transport of alkaline plumes in the environment was reviewed to identify, document and quantify the primary physical and chemical mechanisms that would affect the NaOH once in the environment

3) Geochemical modeling using PHREEQ-C software was conducted to simulate the effects of physical and chemical processes on the equilibrium pH of the NaOH in groundwater

The results of these analyses provide multiple lines of evidence to support a conclusion that the potential impacts of the NaOH release are short-term and limited. The development of the conceptual site model and the results of geochemical modeling are individually discussed in the following sections. The results of the literature review are incorporated throughout, as appropriate.

SUMMARY OF FINDINGS

Conceptual Site Models

The physical and chemical characteristics of soil and groundwater exert significant control on the fate and transport of contaminants in the environment. ELM has therefore developed basic physical and chemical conceptual site models (CSMs) to aide in the evaluation of NaOH behavior in the subsurface environment, and to predict potential impacts.

Physical CSM

The Hannibal, MO facility is situated along the southwestern bank of the Mississippi River. Native surficial soils at the site are mapped by the USDA (1984) as Carlow silty clay, a nearly level, poorly drained flood plain soil. Carlow series soils are characterized by a minimum of 80% clay content, 2 to 4% organic matter content, and slightly acidic soil pH

(USDA, 1984). The surficial USDA mapping is corroborated by subsurface soil characterizations completed by AECOM (2009) for the spill area (see boring logs in Attachment A), and general soil descriptions presented by Arcadis (2009) for the entire site. In the NaOH release area, 6 inches to 2.5 feet of crushed limestone fill was identified overlying the native materials (AECOM, 2009). The silty clays extend to a depth of approximately 14 to 21 feet across the site (Arcadis, 2009).

Deeper subsurface materials consist of a fining-upward series typical of floodplain deposits (Arcadis, 2009), in four additional hydrostratigraphic units. Bedrock underlying the BASF site consists of Quaternary alluvial deposits (USGS, 2005), consistent with the observations presented in Arcadis (2009), and is found approximately 125 – 145 feet below ground surface. The adjacent bedrock formation to the west/southwest is the Osagean Series limestone (USGS, 2005).

The USDA soil survey (1984) states that the high water table in Carlow Series soils is typically 0 to 1 foot below ground surface between November and March. AECOM (2009) identified depths to groundwater in early November ranging between 2 and 4 feet below surface grade, which is generally consistent with USDA predictions considering the additional fill material present atop native soils.

The Carlow silty clays possess low permeability and transmissivity (Arcadis, 2009), and exhibit slow percolation (USDA, 1984). Because of the low permeability of the soil, no monitoring wells have been installed, and no hydraulic data have been collected. Precipitation or materials released to the ground surface, such as the NaOH released in September, would be predicted to rapidly infiltrate the crushed limestone fill material at the surface, but infiltration to the deeper, higher permeability hydrostratigraphic units would be slower and limited by the low permeability silty clays.

Groundwater flow in the hydrologic units at the site is influenced by Mississippi River stage, and is typically (~75% of the time) from north to south under a very low to flat gradient (Arcadis, 2009). The groundwater flow direction can reverse and flow from south to north, resulting in groundwater discharge to the river. Extensive groundwater monitoring at the site indicates that these flow reversals are rare and transitory (Arcadis, 2009). At times of elevated flow in the Mississippi River, the hydraulic gradient can increase substantially, but remains away from the river.

Groundwater flow at the site will be further influenced by extraction wells present as part of the treatment system operated by Wyeth. Based on particle tracking analysis completed by Wyeth in support of the design of the ground water extraction system, transport time from the release area to the nearest extraction well (RW-2, approximately 600 feet to the southwest) in the lower, higher permeability hydrostratigraphic units would be approximately 6 months to 1 year depending on river stage conditions (Arcadis, 2009). However, this time frame underestimates the time needed for transport from the point of

the release to the nearest extraction well because it does not account for vertical transport through the 14 to 21 feet of low permeability silty clay. Because of the buffering effect of several natural chemical processes (discussed below) and the transport time required before groundwater affected by the NaOH release could potentially reach the extraction wells, there is no realistic potential for the NaOH released at the site to affect the groundwater treatment system.

Chemical CSM

The resistance to pH changes in soil in response to acid or base addition (i.e., buffering) is controlled by several chemical mechanisms, which, to some extent, are a function of soil pH. For example, at a low soil pH (< 4.5), aluminum compounds are primarily responsible for soil buffering (Brady & Weil, 2002). However, at intermediate pH (4.5-7.5), cation exchange by clay and organic matter is the primary mechanism responsible for moderating changes in response to the addition of acid or base (Brady & Weil, 2002) in soil. At high pH (> 7.5), carbonate equilibria is the primary mechanism responsible for pH buffering in soils (Brady & Weil, 2002).

It can be predicted that both mechanisms would have acted to buffer the NaOH released at the site. Buffering of the NaOH release by carbonate equilibria and cation exchange would begin during initial infiltration of the spill and continue as the spill moved through the soil and mixed with vadose zone moisture, ground water and rainfall, until equilibrium was reached. The high alkalinity associated with the NaOH release would also cause mineral dissolution and precipitation reactions that would have further moderated the pH. The following summarizes the chemical mechanisms responsible for buffering the NaOH release.

Carbonate Equilibria (pH > 7.5): Upon release from the containment trench, the concentrated NaOH would have contacted the crushed limestone ($CaCO_3$) fill present throughout the release area. The increased pH, in conjunction with exposure to CO_2 in the atmosphere and dissolved calcium (Ca^{2+}) and magnesium (Mg^{2+}) ions in vadose zone water (unsaturated and capillary zones), would result in the precipitation of calcium and magnesium carbonates by the reaction

$$Ca^{2+} + Mg^{2+} + H_2O + CO_2 \rightarrow CaCO_3\ (MgCO_3) + 2H^+ \text{ (Denham, 1998).}$$

The hydrogen ions released during the precipitation of carbonate minerals would provide an immediate and dramatic reduction in groundwater pH, as documented in the literature (Wan, 2004b). Additionally, the NaOH would have affected the carbonate equilibrium reaction in the crushed limestone, which is governed by the equality (Langmuir, 1997):

$$H^+ + H_2CO_3 = CO_3^{2-} + OH^-$$

The addition of hydroxide ions from the NaOH would have forced the equilibrium reaction to the left, creating more hydrogen ions and further decreasing the alkalinity of soil water and groundwater. Initiation of the two carbonate equilibrium reactions involving dissolved phase constituents are nearly instantaneous (Langmiur, 1997), and it can be concluded that buffering of the high pH resulting from NaOH release began to occur immediately on contact with the limestone and ground water.

Cation Exchange (ph 4.5 – 7.5): Although it is likely that the carbonate equilibria reactions discussed previously would have rapidly buffered the NaOH release, any residual NaOH would have been buffered via cation exchange with the native underlying soil. Montmorillonite is the predominant clay mineral in the Carlow series soils (USDA, 1984). This phyllosilicate, smectitic clay is characterized by an abundance of exchangeable sodium, calcium, aluminum, and magnesium, resulting in a high cation exchange capacity (CEC; Brady & Weil, 2002). The CEC for site soils can be estimated based on soil texture and organic matter content, using the following formula:

$$\text{CEC (meq/100g)} = (\%\ \text{organic matter} * 200) + (\%\ \text{clay} * 50)$$

Based on this formula and using the lower end clay and organic matter content percentages described in USDA (1984), the estimated minimum CEC for Carlow series soils is 44 meq/100 g soil. This estimated value is consistent with the range of CECs for clay, and is considered a conservative estimate. Measured CEC for pure montmorillonite is reported to be in the range of 80 to 150 meq/100 g, and is not pH dependent (Langmuir, 1997).

Due to the high CEC of site soils, the release of NaOH to the environment is predicted to result in significant exchange of sodium (Na^+) from the NaOH for calcium (Ca^{2+}) and/or magnesium (Mg^{2+}) from the clay, via the reaction:

$$Na^+ + \tfrac{1}{2}\ Ca\text{-}X \rightarrow Na\text{-}X + \tfrac{1}{2}\ Ca^{2+}$$

where X is the clay complex (Wan, 2004b).

The release of exchangeable Ca and Mg would have provided additional reactant for the precipitation of calcium and magnesium carbonates as described above, reducing the elevated pH of the NaOH release. As is the case with the carbonate equilibria reactions discussed previously, cation exchange reactions are also nearly instantaneous (Brady & Weil, 2002), so the montmorillonite would have begun to take up sodium and release calcium and magnesium immediately upon contact with the NaOH release. Given the high sodium concentrations, cation exchange is expected to be complete (Wan, 2004).

An approximate soil volume required to completely exchange the sodium from the NaOH release can be estimated using the CEC for site soils (discussed above). Fifty percent (50 %) NaOH contains approximately 19 Mol/L, or 19 Equivalents (eq)/L of sodium. If it is

assumed that the entire spill volume of 2,400 gal is retained in the surface soils – without any effect of the carbonate equilibria reactions - then approximately 180,000 eq of sodium (from NaOH) would need to be accommodated to achieve complete cation exchange. Using the minimum soil CEC of 44 meq/100g for Carlow series soil and a bulk density of 1.35 g/cm^3 (USDA, 1984), a CEC of approximately 594 eq/m^3 soil is obtained. Based on this calculation, the entire spill would be completely buffered by the soil within an area of approximately 20 meters by 15 meters (60' x 45'), assuming a one meter penetration into the underlying soil. This calculation overstates the volume of soil needed to fully exchange the sodium by ignoring the buffering effects of the carbonate equilibria reactions and using the minimum CEC for the Carlow series soil.

Mineral Dissolution and Precipitation: The reaction of NaOH with site soils is also predicted to result in the dissolution and precipitation of silicate minerals at pH > 10, and further contribute to the neutralization of alkalinity (Wan, 2004b; He et al, 2005). Dissolution of quartz at high pH results in the generation of protons by the reaction

$$SiO_2 + H_2O = H_2SiO_4^{2-} + 2H^+ \text{ (Wan, 2004b).}$$

When this reaction occurs in the presence of high sodium concentrations, as is the case with the NaOH release at the BASF site, re-precipitation of sodium silicate minerals occurs,

$$H_4SiO_4 + Na^{2+} = Na_2SiO_{3(\text{cancrinite})} + H_2O + 2H^+$$

enhancing silicate dissolution (Wan, 2004b; Deng, 2006) and further lowering the pH by the production of protons.

Laboratory studies by Wan and others (2004) demonstrated that the reactions discussed in the chemical CSM can collectively neutralize alkaline plumes from a pH of 14 to 6.3 in less than 2 meters of vertical transport through the soil column. It is therefore predicted that the effects of the NaOH spill were naturally abated by soil chemical reactions within a short distance from the release location.

Geochemical Modeling

ELM conducted basic geochemical modeling using PHREEQ-C software (Parkhust and Appelo, 1999). The modeling simulation of the chemical mechanisms acting upon the spill provided further perspective on the extent to which the natural processes discussed previously were capable of buffering the effects of the NaOH release, and assists in explaining the near-neutral pH levels observed by AECOM in the majority of the sampling locations.

Based on the physical and chemical CSMs described above, the modeling simulated the following mechanisms that would have acted on the NaOH spill when the NaOH was released:

- mixing of the 50% NaOH released from the containment sump (Solution 1 at a pH of 14) with calcite-equilibrated shallow groundwater in the limestone fill (Solution 2 at a pH of 7.3). The mixing of the two solutions results in a diluted NaOH solution (Solution 3) with a pH lower than the original NaOH release but higher than the calcite-equilibrated ground water.

- re-equilibration of Solution 3 with calcite, which is appropriate given the ubiquitous presence of limestone fill in the release area, and the predicted slow infiltration rate to underlying silty clay. The model predicts that the resulting NaOH and ground water solution (Solution 4) would have possessed a pH that was substantially lower than that resulting only from dilution, and with the addition of rain water, approached neutral.

- cation exchange of Solution 4 with montmorillonite to simulate infiltration into native site soils resulting in a final Solution 5.

For modeling purposes, the following variables were used:

- The area of the release was assumed to be the entire loading area adjacent to the East Utilities Building, an area of 200 m^2 (Figure 1).

- The average depth of the limestone was assumed to be 0.5' (0.163 m).

- The chemical composition of rainwater at the site was approximated using average annual precipitation chemistry as measured approximately 75 miles southwest of the BASF facility in Boone County, MO (Table 2; NADN, 2006-2008). As noted, the average pH of the rainwater is approximately 5.3.

- Estimates of dilution by rainfall were made using precipitation amounts for Quincy, IL (approx. 7 mi. north of the BASF facility) between September 23 and September 27, 2009 (1.2 in. total; Weather Underground, 2010).

A sensitivity analysis was also conducted to test the effect of input parameters on model outcome. Specifically, the effect of the following two variables was tested:

a) the pH of the release (i.e. varying the composition of the initial NaOH release (Solution 1) to account for potential dilution by rainwater). This analysis is considered the most representative of actual site conditions given the rainfall that occurred on the day of the release.

b) the relative proportions of NaOH mixed with site groundwater. Although this simulation does not account for the effects of mixing the release with rain water, it does provide an indication of the worst-case volume of water that would be needed to buffer the effects of the release.

The model input scenarios and results are summarized in Table 1. Model output is provided in Attachment B.

Discussion of Results

The geochemical modeling provides insight into the effectiveness of the natural mechanisms in buffering the elevated pH resulting from the NaOH release and supplements the understanding of the soil and ground water pH levels observed by AECOM during the October 2009 investigation. In particular, the modeling results provide a basis to conclude that dilution alone would not have been sufficient to moderate the pH from the spill, and that the carbonate equilibria reactions were most likely the primary mechanism responsible for mitigating the effects of the NaOH release.

Key observations from the modeling, as presented in Table 1, include:

- Mixing with the lower-pH rain water likely provided a significant initial reduction in the pH of the release. As a result of the lower pH in the rain water (average of 5.24) and the presence of calcium and magnesium, it is predicted that the pH of the solution actually discharged to the subsurface was closer to 10 than the pH of 14 of the 50% NaOH. It is to be noted that the majority of the geochemical benefits from the rain water are obtained with the initial mixing, and additional precipitation provides only dilution benefits.

- Equilibration of the NaOH/rain water mixture with the underlying carbonate material buffered the pH of the release to near-neutral conditions, as observed by AECOM.

- The spill does not represent a threat to the underlying, higher-permeability hydrostratigraphic units. When the solution buffered by the carbonate equilibria reactions is subjected to cation exchange, as would occur as ground water is transported vertically through the underlying Carlow silty clay, a pH slightly less than neutral is predicted.

- The effects of cation exchange, which would be predicted to reduce the pH to less than 7, are likely ongoing. As discussed in the physical CSM, infiltration into and through the Carlow series soil is predicted to be slow, and as the equilibrated ground water moves through the soil, additional buffering will occur.

- Even without the benefit of the rain water mixing or cation exchange, the pH of the spill would have been reduced to approximately 8.5 by carbonate equilibria reactions and dilution in approximately 50,000 gallons of ground water. Assuming a two-foot saturated thickness and a 0.3 porosity, the pH reduction would have been accomplished within an area of approximately 10,000 square feet. This calculation obviously overstates the potential area of impact but provides a basis to conclude that, even under worst-case conditions, the NaOH release woiuld have been attenuated within a relatively small area.

Comparison of model results to observed pH measurements within the release area supports the conclusion that the model satisfactorily predicted the fate of the NaOH spill as a result of dilution and equilibration with naturally occurring mineral phases at the site. As presented in Table 1, the model simulation predicted a pH of approximately 7.3 in Solution 4 when the effects of rain water mixing and carbonate equilibria reactions are considered. This model-simulated pH compares favorably with the average soil (7.52 – 7.69) and ground water pH (7.56 outside of the SB-2 location) pH measurements reported by AECOM.

Based on the model results, the released NaOH is predicted to be neutralized to pHs at or near natural site conditions without further treatment or recovery. Spill area pH measurements collected in November indicate that soil and groundwater had already largely neutralized the released material, and, as discussed above, it is probable that ongoing neutralization via both equilibria reactions and cation exchange is ongoing. These findings are consistent with the physical CSM of slow infiltration into the underlying Carlow series soil, where the cation exchange will occur, and the understanding that reaction half-lives for equilibrium processes involving solid mineral phases are on the order of weeks to a year (Langmiur, 1997).

CONCLUSIONS

The potential impact of a release of approximately 2,400 gallons of NaOH adjacent to the East Utilities Building was conducted to predict the environmental fate of the release and develop conclusions regarding the need for additional actions to address the release. The site-specific geology and hydrogeology were evaluated, and scientific literature documenting the mechanisms affecting the fate of alkaline materials in the environment was reviewed.

Based on the information obtained, physical and chemical conceptual site models were developed based on this data review. Based on the physical CSM, both horizontal and vertical transport of ground water is slow. Vertical transport is limited by the low permeability silty clays present in the shallow subsurface, and horizontal transport is limited by the very flat horizontal gradient (0.0004 – 0.003 ft/ft) documented at the site as well as the low permeability material. Based on the geology and hydrogeology documented

in the physical CSM, there is no realistic mechanism for the NaOH/elevated pH material to affect any receptor, including the river or the Wyeth ground water extraction and treatment system:

- The ground water flow direction is typically north to south, away from the river, and the spill was approximately 1,800 feet away from the river.

- The Wyeth extraction wells will be installed in the lower hydrostratigraphic units in order to achieve the projected 150 gpm extraction rate. This, in order for any of the HaOH to reach the nearest extraction well, it would need to be transported vertically through approximately 20 feet of the silty Carlow clay and travel several hundred feet horizontally. Even if the ground water within the release area were to be transported vertically and horizontally, the pH effects of the spill would be fully attenuated by cation exchange in the clay, as predicted by the modeling.

NaOH

As discussed in the chemical CSM, carbonate equilibrium reactions, cation exchange, and mineral dissolution/precipitation are the primary mechanisms that will affect the NaOH release. As documented in the scientific literature, these mechanisms are predicted to contribute sufficient acidity to neutralize the alkalinity introduced as a result of the spill. As presented previously, relatively small volumes of soil (approximately 300 m^3) and ground water (50,000 gallons) would individually be adequate to attenuate the effects of the release. The combined effects of the physical and chemical attenuation mechanisms would have reduced the pH to near neutral conditions within a short distance from the location of the release.

The predictions based on the CSMs are corroborated by geochemical modeling using PHREEQ-C geochemical software. The results of the model simulations support a conclusion that the mixing with rain water and subsequent carbonate equilibria reactions would have reduced the ground water pH to near-neutral (7.3) conditions, which is consistent with the average pH in ground water, outside of the SB-2 location, measured by AECOM.

The physical and chemical CSMs and modeling results also support a conclusion that further buffering of the NaOH release is occurring. The crushed limestone fill material will provide an ongoing source of carbonate, and, as the spill/rain water/ground water slowly infiltrates into the underlying silty clay, additional buffering via cation exchange will occur.

Based on these findings, no further action is recommended in response to the NaOH release at the site. The alkalinity associated with the spill is predicted to be neutralized rapidly and within a short distance from the release location via natural processes, and this prediction has been corroborated by pH measurements in the spill area. Furthermore, the spill is not anticipated to result in detrimental effects to either the onsite groundwater treatment system or local ecological receptors (i.e., surface water).

If you have any questions regarding the information presented in this report please feel free to contact our office.

Sincerely,

THE ELM GROUP, INC.

Jennifer Wollenberg, Ph.D.
Project Manager

for
Hank Martin, P.E.
Principal

c: Mr. Vernon Burrows, BASF

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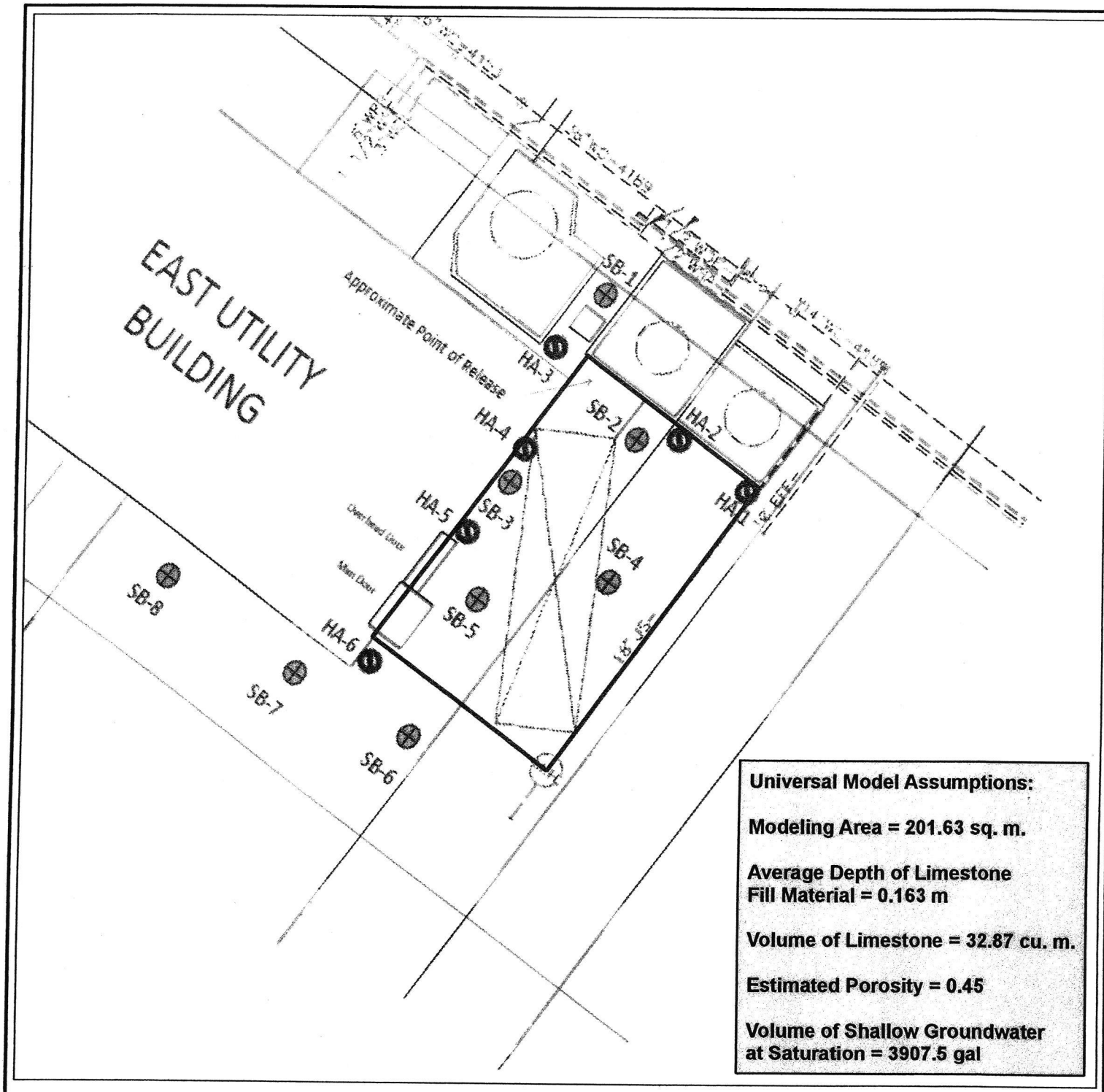

Universal Model Assumptions:

Modeling Area = 201.63 sq. m.

Average Depth of Limestone Fill Material = 0.163 m

Volume of Limestone = 32.87 cu. m.

Estimated Porosity = 0.45

Volume of Shallow Groundwater at Saturation = 3907.5 gal

LEGEND

- Extent of Modeling Area
- Soil Boring Location
- Hand Auger Location

SOURCE:
1. Basemap and sample locations from AECOM, 2009.

0 25 50

SCALE: 1" = 25'

TITLE:
FIGURE 1
Location of NaOH Release, Soil/Groundwater Sample Locations, and Extent of Modeling Area

LOCATION:
BASF
Hannibal, MO

DATE: 01/07/10

FILENAME: Fig1 010710 EastUtilBldg.mxd

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Table 1
Summary of PHREEQC Geochemical Model Results and Sensitivity Analysis

Run	Description	Solution pH				
		Solution 1	Solution 2	Solution 3	Solution 4	Solution 5
		NaOH	Calcite Groundwater	Solution 1 + Solution 2	Solution 3 Eqb. With Calcite and CO2	Solution 4 Eqb. With Monmorillonite
Effect of Dilution of NaOH by Precipitation [1]						
1	0% rainwater + 100% NaOH	14	7.3	13.73	9.35	9.1
2	1% rainwater + 99% NaOH	10.144	7.3	9.875	7.31	6.62
3	10% rainwater + 90% NaOH	10.088	7.3	9.84	7.31	6.62
4	25% rainwater + 75% NaOH	9.99	7.3	9.79	7.31	6.62
5	40% rainwater + 60% NaOH	9.9	7.3	9.75	7.31	6.62
Effect of Groundwater to NaOH Ratio [2]						
1	40% groundwater + 60% NaOH	14	7.3	13.73	9.35	9.1
6	50% groundwater + 50% NaOH	14	7.3	13.65	9.17	8.75
7	75% groundwater + 25% NaOH	14	7.3	13.43	8.99	8.33
8	90% groundwater + 10% NaOH	14	7.3	13.17	8.76	7.84
9	95% groundwater + 5% NaOH	14	7.3	12.98	8.58	7.57
10	99% groundwater + 1% NaOH	14	7.3	12.45	8.07	7.03

[1] All runs conducted with 40:60 Groundwater to NaOH Ratio; description percentages indicate mixing proportions, not concentration

[2] All runs conducted with undiluted 50% NaOH as released; description percentages indicate mixing proportions, not concentration

Table 2
Chemical Composition of Precipitation[1]
Boone County, MO

Constituent	2008	2007	2006	Average
Calcium	0.28	0.256	0.837	0.458
Magnesium	0.028	0.035	0.038	0.034
Potassium	0.03	0.052	0.048	0.043
Sodium	0.078	0.097	0.07	0.082
Ammonium	0.33	0.335	0.414	0.360
Nitrate	0.87	0.978	1.163	1.004
Chloride	0.12	0.136	0.111	0.122
Sulfate	1.03	1.036	1.328	1.131
pH	5.6	5.17	4.95	5.24

[1] NADN, 2006-2008

ATTACHMENTS

Attachment A: Initial Site Investigation Findings (AECOM, 2009)

Attachment B: Model Run Output

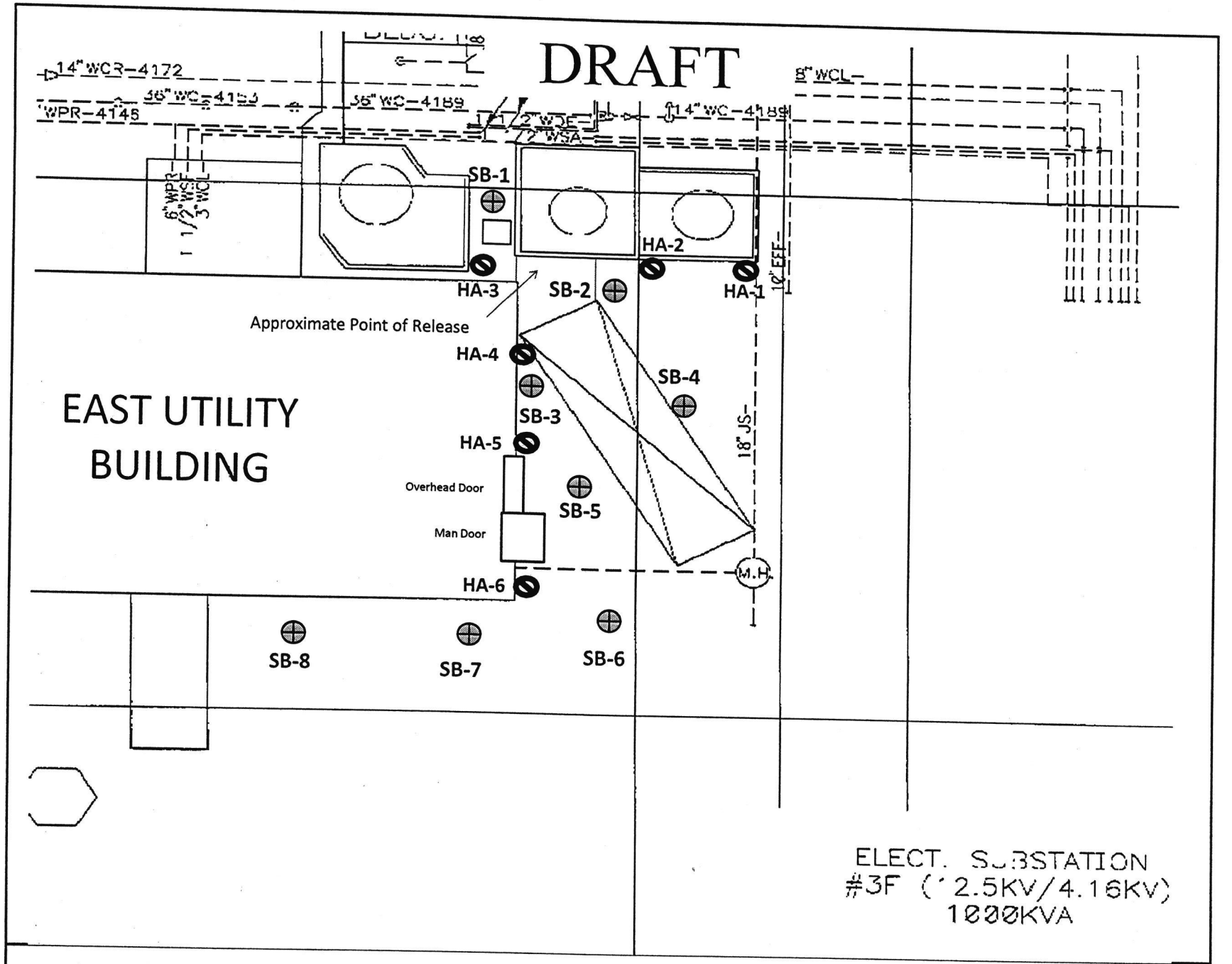
Attachment A

Initial Site Investigation Findings (AECOM, 2009)

Table A1
Soil and Groundwater pH Results
BASF Corporation - Hannibal, MO
Source: AECOM Initial Site Investigation (November, 2009)

Boring Location	Date	Total Depth (ft bgs)	Soil pH 0-2 ft bgs	Soil pH 2-4 ft bgs	Depth to Groundwater (ft bgs)	Groundwater pH
Hand Auger Borings						
HA-1	11/9/2009	4	8.57	nt	n/a	n/a
HA-2	11/9/2009	4	7.62	7.59	n/a	n/a
HA-3	11/9/2009	4	7.49	nt	n/a	n/a
HA-4	11/9/2009	4	7.46	7.58	n/a	n/a
HA-5	11/9/2009	4	7.53	7.51	n/a	n/a
HA-6	11/9/2009	4	7.37	7.41	n/a	n/a
Direct Push Borings						
SB-1	11/10/2009	2.5	n/a	refusal @ 2.5	refusal @ 2.5	n/a
SB-2	11/10/2009	8	7.77	nt	4	12.21
SB-3	11/10/2009	9	nt	nt	4	7.93
SB-4	11/10/2009	8	nt	nt	4	7.18
SB-5	11/10/2009	9	nt	nt	5	7.3
SB-6	11/10/2009	9	nt	nt	5.5	7.36
SB-7	11/10/2009	9	nt	nt	3.5	7.88
SB-8	11/10/2009	9	nt	nt	0	7.71

bgs below ground surface
n/a not available
nt not taken



BASF - Hannibal, Missouri Facility
Initial Site Investigation - Sodium Hydroxide Release
Approximate Soil Boring / Temporary Well Locations
Approximate Hand Auger Locations

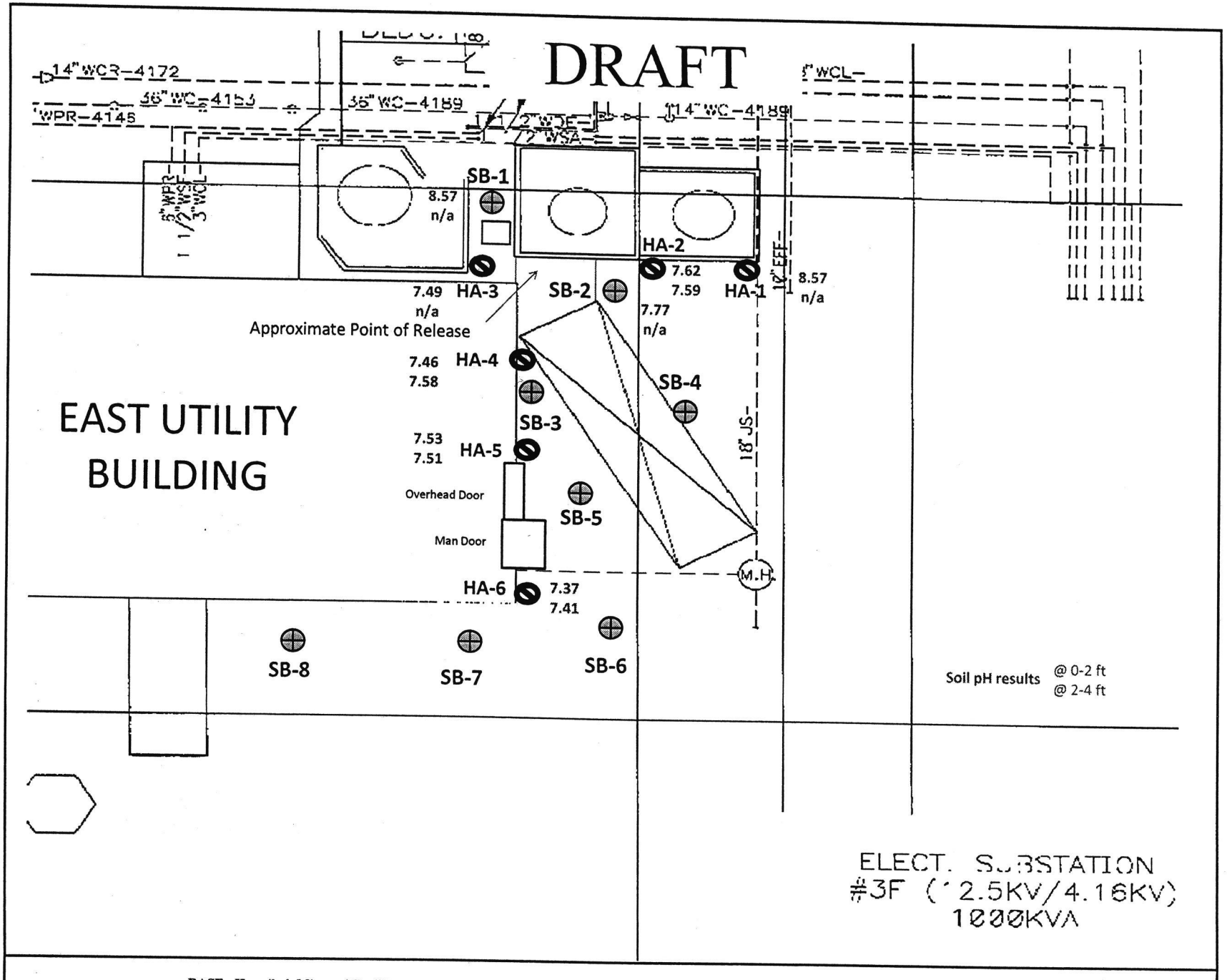
FIGURE 1

Not to scale

N

Source of Figure : BASF Corporation Drawing No. 77-2-029, Rev No. 01, Date 01/96

Figure A1



BASF - Hannibal, Missouri Facility
Initial Site Investigation - Sodium Hydroxide Release
Approximate Soil Boring / Temporary Well Locations
Approximate Hand Auger Locations

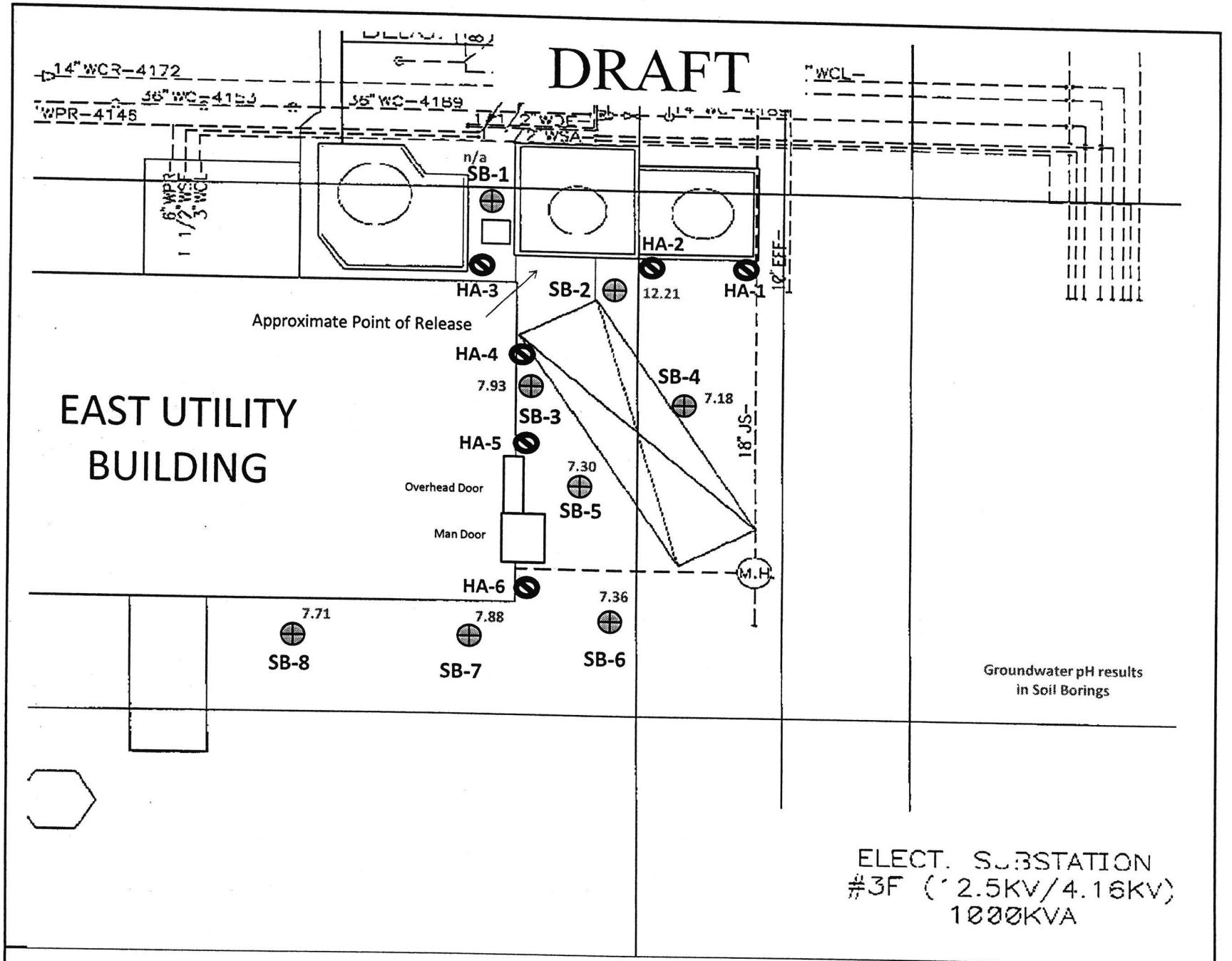
FIGURE 2
Soil pH Results

Not to scale

N

Source of Figure : BASF Corporation Drawing No. 77-2-029, Rev No. 01, Date 01/96

Figure A2



BASF - Hannibal, Missouri Facility
Initial Site Investigation - Sodium Hydroxide Release
Approximate Soil Boring / Temporary Well Locations
Approximate Hand Auger Locations

FIGURE 3
Groundwater pH Results

Not to scale

Source of Figure : BASF Corporation Drawing No. 77-2-029, Rev No. 01, Date 01/96

Figure A3

DRAFT

AECOM	Client: BASF - Hannibal		BORING ID: HA-1
	Project Number: #60142705		
	Site Location: 3150 Highway JJ, Palmyra, MO		
	Coordinates:	Elevation:	Sheet: 1 of 1
	Drilling Method: Hand Auger		Monitoring Well Installed:
	Sample Type(s): Soil	Boring Diameter: 4 in	Screened Interval:
Weather: Clear, 60 °F	Logged By: Matt Lewis	Date/Time Started: 11-9-09	Depth of Boring: 2 ft
Drilling Contractor: Harriss Drilling	Ground Elevation:	Date/Time Finished: 11-9-09	Water Level: n/a

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Blows per 6"	Recovery (inches)	Headspace (ppm)	U.S.C.S	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
1							Crushed limestone backfill, damp to moist, refusal at 2.5 ft.	pH	
2								8.75	
3									
4									
5									
6									
7									
8									
9									
10									
11									
12									
13									
14									
15									
16									
17									
18									
19									
20									

NOTES: refusal at 2 locations

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

DRAFT

AECOM	Client: BASF - Hannibal		BORING ID: HA-2
	Project Number: #60142705		
	Site Location: 3150 Highway JJ, Palmyra, MO		
	Coordinates:	Elevation:	Sheet: 1 of 1
	Drilling Method: Hand Auger		Monitoring Well Installed:
	Sample Type(s): Soil	Boring Diameter: 4 in	Screened Interval:
Weather: Clear, 60 °F	Logged By: Matt Lewis	Date/Time Started: 11-9-09	Depth of Boring: 3.5 ft
Drilling Contractor: Harriss Drilling	Ground Elevation:	Date/Time Finished: 11-9-09	Water Level: 2 ft

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Blows per 6"	Recovery (inches)	Headspace (ppm)	U.S.C.S	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
1							Crushed limestone backfill, moist to wet at 2 ft.	pH	
2							V - wet	7.62	
3							Black, SILTY CLAY, wet, organic odor.	7.59	
4							3.5 ft End of boring - Gravel cave in		
5									
6									
7									
8									
9									
10									
11									
12									
13									
14									
15									
16									
17									
18									
19									
20									

NOTES: near source area

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

DRAFT

AECOM	Client: BASF - Hannibal		BORING ID: HA-3
	Project Number: #60142705		
	Site Location: 3150 Highway JJ, Palmyra, MO		
	Coordinates:	Elevation:	Sheet: 1 of 1
	Drilling Method: Hand Auger		Monitoring Well Installed:
	Sample Type(s): Soil	Boring Diameter: 4 in	Screened Interval:
Weather: Clear, 60 °F	Logged By: Matt Lewis	Date/Time Started: 11-9-09	Depth of Boring: 2 ft
Drilling Contractor: Harriss Drilling	Ground Elevation:	Date/Time Finished: 11-9-09	Water Level: n/a

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Blows per 6"	Recovery (inches)	Headspace (ppm)	U.S.C.S	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
1							Crushed limestone backfill, damp to moist, concrete refusal at 2 ft.	pH	
2								7.49	
3							End of boring at 2 ft		
4									
5									
6									
7									
8									
9									
10									
11									
12									
13									
14									
15									
16									
17									
18									
19									
20									

NOTES: refusal at 2 locations (concrete pad) between containments

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

DRAFT

AECOM

Client: BASF - Hannibal		BORING ID: HA-4
Project Number: #60142705		
Site Location: 3150 Highway JJ, Palmyra, MO		
Coordinates:	Elevation:	Sheet: 1 of 1
Drilling Method: Hand Auger		Monitoring Well Installed:
Sample Type(s): Soil	Boring Diameter: 4 in	Screened Interval:
Weather: Clear, 60 °F	Logged By: Matt Lewis / Date/Time Started: 11-9-09	Depth of Boring: 4 ft
Drilling Contractor: Harriss Drilling	Ground Elevation: / Date/Time Finished: 11-9-09	Water Level: 2.5 ft

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Blows per 6"	Recovery (inches)	Headspace (ppm)	U.S.C.S	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
							Crushed limestone backfill	pH	
1							Dark Brown, SILTY CLAY, damp to wet at 2.5 ft, no odor		
2								7.46	
3							V Wet		
4								7.58	
5							End of boring at 4 ft		
6									
7									
8									
9									
10									
11									
12									
13									
14									
15									
16									
17									
18									
19									
20									

NOTES:

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

DRAFT

AECOM	Client: BASF - Hannibal		BORING ID: HA-5
	Project Number: #60142705		
	Site Location: 3150 Highway JJ, Palmyra, MO		
	Coordinates:	Elevation:	Sheet: 1 of 1
	Drilling Method: Hand Auger		Monitoring Well Installed:
	Sample Type(s): Soil	Boring Diameter: 4 in	Screened Interval:
Weather: Clear, 60 °F	Logged By: Matt Lewis	Date/Time Started: 11-9-09	Depth of Boring: 3.5 ft
Drilling Contractor: Harriss Drilling	Ground Elevation:	Date/Time Finished: 11-9-09	Water Level: n/a

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Blows per 6"	Recovery (inches)	Headspace (ppm)	U.S.C.S	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
							Crushed limestone backfill	pH	
1							Dark Brown, SILTY CLAY, damp to moist, no odor, refusal at 3.5 ft		
								7.53	
2									
3									
								7.51	
4							End of boring at 3.5 ft		
5									
6									
7									
8									
9									
10									
11									
12									
13									
14									
15									
16									
17									
18									
19									
20									

NOTES:

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

DRAFT

AECOM	Client: BASF - Hannibal		BORING ID: HA-6
	Project Number: #60142705		
	Site Location: 3150 Highway JJ, Palmyra, MO		
	Coordinates:	Elevation:	Sheet: 1 of 1
	Drilling Method: Hand Auger		Monitoring Well Installed:
	Sample Type(s): Soil	Boring Diameter: 4 in	Screened Interval:
Weather: Clear, 60 °F	Logged By: Matt Lewis	Date/Time Started: 11-9-09	Depth of Boring: 2.5 ft
Drilling Contractor: Harriss Drilling	Ground Elevation:	Date/Time Finished: 11-9-09	Water Level: n/a

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Blows per 6"	Recovery (inches)	Headspace (ppm)	U.S.C.S	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
1							Crushed limestone backfill, damp to moist, cave in at 2.5 ft.	pH	
2								7.37	
3								7..41	
4									
5									
6									
7									
8									
9									
10									
11									
12									
13									
14									
15									
16									
17									
18									
19									
20									

NOTES:

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

DRAFT

AECOM	Client: **BASF - Hannibal**		**BORING ID: SB-1**
	Project Number: #60142705		
	Site Location: 3150 Highway JJ, Palmyra, MO		
	Coordinates:	Elevation:	Sheet: 1 of 1
	Drilling Method: Hand Auger		Monitoring Well Installed:
	Sample Type(s): Soil	Boring Diameter: 4 in	Screened Interval:
Weather: Rain, 45-50 °F	Logged By: Matt Lewis	Date/Time Started: 11-10-09	Depth of Boring: 2.5 ft
Drilling Contractor: Harriss Drilling	Ground Elevation:	Date/Time Finished: 11-10-09	Water Level: n/a

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Blows per 6"	Recovery (inches)	Headspace (ppm)	U.S.C.S	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
1							Crushed limestone backfill, damp to moist, concrete pad at 2.5 ft.		
2									
3									
4									
5									
6									
7									
8									
9									
10									
11									
12									
13									
14									
15									
16									
17									
18									
19									
20									

NOTES:

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

DRAFT

AECOM

Client: BASF - Hannibal		BORING ID: SB-2
Project Number: #60142705		
Site Location: 3150 Highway JJ, Palmyra, MO		
Coordinates:	Elevation:	Sheet: 1 of 1
Drilling Method: Hand Auger		Monitoring Well Installed:
Sample Type(s): Soil	Boring Diameter: 4 in	Screened Interval:
Weather: Rain, 45-50 °F	Logged By: Matt Lewis / Date/Time Started: 11-10-09	Depth of Boring: 8 ft
Drilling Contractor: Harriss Drilling	Ground Elevation: / Date/Time Finished: 11-10-09	Water Level: 4 ft

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Hand Auger	Recovery (inches)	Headspace (ppm)	Temp Const.	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
1							Crushed limestone backfill, damp to moist	pH	
2							Black, SILTY CLAY, moist to wet, organic odor	7.77	
3									
4							V - wet		
5									
6									
7									
8		8	HA						
9							End of boring 8 ft		
10									
11									
12									
13									
14									
15									
16									
17									
18									
19									
20									

NOTES: Temporary piezometer set at total depth of 8 ft with 5 ft of screen.

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

DRAFT

AECOM	Client: BASF - Hannibal	BORING ID: SB-3
	Project Number: #60142705	
	Site Location: 3150 Highway JJ, Palmyra, MO	
	Coordinates: Elevation:	Sheet: 1 of 1
	Drilling Method: Hand Auger / Direct Push Geoprobe	Monitoring Well Installed:
	Sample Type(s): Soil Boring Diameter: 4 in	Screened Interval:
Weather: Rain, 45-50 °F	Logged By: Matt Lewis / Date/Time Started: 11-10-09	Depth of Boring: 9 ft
Drilling Contractor: Harriss Drilling	Ground Elevation: / Date/Time Finished: 11-10-09	Water Level: 4 ft

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Hand Auger	Geoprobe	Recovery (inches)	Headspace (ppm)	Temp Const.	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
1								Crushed limestone backfill, damp to moist		
2								Dark Brown to Black, SILTY CLAY, moist to wet, no odor		
3										
4		4	HA					V - wet		
5										
6										
7		7		GP	75%					
8										
9		9		GP	75%					
10								End of boring 9 ft		
11										
12										
13										
14										
15										
16										
17										
18										
19										
20										

NOTES: Temporary piezometer set at total depth of 9 ft with 5 ft of screen.

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

DRAFT

AECOM	Client: **BASF - Hannibal**		BORING ID: SB-4
	Project Number: #60142705		
	Site Location: 3150 Highway JJ, Palmyra, MO		
	Coordinates:	Elevation:	Sheet: 1 of 1
	Drilling Method: Hand Auger		Monitoring Well Installed:
	Sample Type(s): Soil	Boring Diameter: 4 in	Screened Interval:
Weather: Rain, 45-50 °F	Logged By: Matt Lewis	Date/Time Started: 11-10-09	Depth of Boring: 8 ft
Drilling Contractor: Harriss Drilling	Ground Elevation:	Date/Time Finished: 11-10-09	Water Level: 4 ft

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Hand Auger	Recovery (inches)	Headspace (ppm)	U.S.C.S	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
1							Crushed limestone backfill, damp to moist		
2							Dark Brown to Black, SILTY CLAY, moist to wet, no odor		
3									
4							V - wet		
5									
6									
7									
8		8	HA						
9							End of boring 8 ft		
10									
11									
12									
13									
14									
15									
16									
17									
18									
19									
20									

NOTES: Temporary piezometer set at total depth of 8 ft with 5 ft of screen.

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

DRAFT

AECOM

Client: **BASF - Hannibal**	***BORING ID: SB-5***
Project Number: #60142705	
Site Location: 3150 Highway JJ, Palmyra, MO	
Coordinates: *Elevation:*	*Sheet: 1 of 1*
Drilling Method: Hand Auger / Direct Push Geoprobe	*Monitoring Well Installed:*
Sample Type(s): Soil *Boring Diameter: 4 in*	*Screened Interval:*
Weather: Rain, 45-50 ° F *Logged By: Matt Lewis* *Date/Time Started: 11-10-09*	*Depth of Boring: 9 ft*
Drilling Contractor: Harriss Drilling *Ground Elevation:* *Date/Time Finished: 11-10-09*	*Water Level: 5 ft*

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Hand Auger	Geoprobe	Recovery (%)	Headspace (ppm)	Temp Const.	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
1								Crushed limestone backfill, damp to moist		
2								Dark Brown to Black, SILTY CLAY, moist to wet, no odor		
3										
4		4	HA					V - wet		
5										
6										
7		7		GP	75%					
8										
9		9		GP	75%					
10								End of boring 9 ft		
11										
12										
13										
14										
15										
16										
17										
18										
19										
20										

NOTES: Temporary piezometer set at total depth of 9 ft with 5 ft of screen.

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

DRAFT

AECOM

Client: BASF - Hannibal		BORING ID: SB-6
Project Number: #60142705		
Site Location: 3150 Highway JJ, Palmyra, MO		
Coordinates:	Elevation:	Sheet: 1 of 1
Drilling Method: Hand Auger / Direct Push Geoprobe		Monitoring Well Installed:
Sample Type(s): Soil	Boring Diameter: 4 in	Screened Interval:
Weather: Rain, 45-50 °F	Logged By: Matt Lewis / Date/Time Started: 11-10-09	Depth of Boring: 9 ft
Drilling Contractor: Harriss Drilling	Ground Elevation: / Date/Time Finished: 11-10-09	Water Level: 5.5 ft

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Hand Auger	Geoprobe	Recovery (inches)	Headspace (ppm)	Temp Const.	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
1								Crushed limestone backfill, damp to moist		
2								Dark Brown to Black, SILTY CLAY, moist to wet, no odor		
3										
4		4	HA							
5								V - wet		
6										
7		7		GP	80%					
8										
9		9		GP	80%					
10								End of boring 9 ft		
11										
12										
13										
14										
15										
16										
17										
18										
19										
20										

NOTES: Temporary piezometer set at total depth of 9 ft with 5 ft of screen.

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

DRAFT

AECOM	Client: **BASF - Hannibal**		**BORING ID: SB-7**
	Project Number: #60142705		
	Site Location: 3150 Highway JJ, Palmyra, MO		
	Coordinates:	Elevation:	Sheet: 1 of 1
	Drilling Method: Hand Auger / Direct Push Geoprobe		Monitoring Well Installed:
	Sample Type(s): Soil	Boring Diameter: 4 in	Screened Interval:
Weather: Rain, 45-50 °F	Logged By: Matt Lewis	Date/Time Started: 11-10-09	Depth of Boring: 9 ft
Drilling Contractor: Harriss Drilling	Ground Elevation:	Date/Time Finished: 11-10-09	Water Level: 3.5 ft

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Hand Auger	Geoprobe	Recovery (inches)	Headspace (ppm)	U.S.C.S	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
1								Crushed limestone backfill, damp to moist		
2										
3								Dark Brown to Black, SILTY CLAY, moist to wet, no odor		
4		4	HA					V - wet		
5										
6										
7		7		GP	80%					
8										
9		9		GP	80%					
10								End of boring 9 ft		
11										
12										
13										
14										
15										
16										
17										
18										
19										
20										

NOTES: Temporary piezometer set at total depth of 9 ft with 5 ft of screen.

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

DRAFT

AECOM

Client: BASF - Hannibal	BORING ID: SB-8
Project Number: #60142705	
Site Location: 3150 Highway JJ, Palmyra, MO	
Coordinates: Elevation:	Sheet: 1 of 1
Drilling Method: Hand Auger / Direct Push Geoprobe	Monitoring Well Installed:
Sample Type(s): Soil Boring Diameter: 4 in	Screened Interval:
Weather: Rain, 45-50 °F Logged By: Matt Lewis Date/Time Started: 11-10-09	Depth of Boring: 9 ft
Drilling Contractor: Harriss Drilling Ground Elevation: Date/Time Finished: 11-10-09	Water Level: surface

Depth (ft)	Geologic sample ID	Sample Depth (ft)	Hand Auger	Geoprobe	Recovery (inches)	Headspace (ppm)	U.S.C.S	MATERIALS: Color, size, range, MAIN COMPONENT, minor component(s), moisture content, structure, angularity, maximum grain size, odor, and Geologic Unit (If Known)	Lab Sample ID	Lab Sample Depth (Ft.)
1								Crushed limestone backfill, wet at surface		
2										
3								Dark Brown to Black, SILTY CLAY, wet, no odor		
4		4	HA							
5										
6										
7		7		GP	80%					
8										
9		9		GP	80%					
10								End of boring 9 ft		
11										
12										
13										
14										
15										
16										
17										
18										
19										
20										

NOTES: Temporary piezometer set at total depth of 9 ft with 5 ft of screen.

Date	Time	Depth to groundwater while drilling

Checked by _____ Date: _____

Attachment B

Model Run Output

Run 1 - 40% Groundwater:60% NaOH

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\40-60\mix NaOH and calcite GW.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\40-60\mix NaOH and calcite GW.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 2 NaOH
          temp      20
          pH        14
          pe        4
          redox     pe
          units     mmol/kgw
          density   1
          Na        24.9 Mol/kgw
          water    1 # kg
      SOLUTION 1 GW @ eqb w/ Calcite
          temp      20
          pH        7.301
          pe        -1.841
          redox     pe
          units     mmol/kgw
          density   1
          Ca        0.001789
          C         0.003961
          water    1 # kg
      SAVE solution 1-2
      MIX 1 Mix NaOH and GW @ equ w/ calcite
          1    0.4
          2    0.6
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.     GW @ eqb w/ Calcite

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

      Elements           Molality       Moles

      C                3.961e-006  3.961e-006
      Ca               1.789e-006  1.789e-006

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

                                     pH  =   7.301
                                     pe  =  -1.841
                        Activity of water  =   1.000
                           Ionic strength  =  5.444e-006
                       Mass of water (kg)  =  1.000e+000
```

```
                 Total alkalinity (eq/kg)  =  3.626e-006
                       Total CO2 (mol/kg)  =  3.961e-006
                     Temperature (deg C)   =  20.000
                  Electrical balance (eq)  = -4.751e-008
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.65
                              Iterations  =   3
                                 Total H  = 1.110124e+002
                                 Total O  = 5.550623e+001

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

                                                  Log       Log        Log
   Species                 Molality    Activity  Molality  Activity    Gamma

   OH-                   1.361e-007  1.358e-007    -6.866    -6.867   -0.001
   H+                    5.014e-008  5.000e-008    -7.300    -7.301   -0.001
   H2O                   5.551e+001  1.000e+000     1.744    -0.000    0.000
C(-4)            1.058e-025
   CH4                   1.058e-025  1.058e-025   -24.975   -24.975    0.000
C(4)             3.961e-006
   HCO3-                 3.533e-006  3.524e-006    -5.452    -5.453   -0.001
   CO2                   4.245e-007  4.245e-007    -6.372    -6.372    0.000
   CO3-2                 3.000e-009  2.968e-009    -8.523    -8.528   -0.005
   CaHCO3+               7.328e-011  7.309e-011   -10.135   -10.136   -0.001
   CaCO3                 8.056e-012  8.056e-012   -11.094   -11.094    0.000
Ca               1.789e-006
   Ca+2                  1.789e-006  1.770e-006    -5.747    -5.752   -0.005
   CaHCO3+               7.328e-011  7.309e-011   -10.135   -10.136   -0.001
   CaCO3                 8.056e-012  8.056e-012   -11.094   -11.094    0.000
   CaOH+                 5.889e-012  5.873e-012   -11.230   -11.231   -0.001
H(0)             1.791e-014
   H2                    8.953e-015  8.953e-015   -14.048   -14.048    0.000
O(0)             0.000e+000
   O2                    0.000e+000  0.000e+000   -65.925   -65.925    0.000

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

      Phase               SI log IAP  log KT

      Aragonite        -5.97  -14.28   -8.31  CaCO3
      Calcite          -5.83  -14.28   -8.45  CaCO3
      CH4(g)          -22.16  -24.98   -2.82  CH4
      CO2(g)           -4.97   -6.37   -1.41  CO2
      H2(g)           -10.92  -14.05   -3.13  H2
      H2O(g)           -1.64   -0.00    1.64  H2O
      O2(g)           -63.07  -65.93   -2.85  O2

Initial solution 2.     NaOH

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

      Elements           Molality       Moles

      Na               2.490e+001  2.490e+001

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

                                     pH  =  14.000
                                     pe  =   4.000
                       Activity of water  =   0.562
                          Ionic strength  =  1.184e+001
                     Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg) =  2.931e+000
                    Total carbon (mol/kg) =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                    Temperature (deg C)   =  20.000
                  Electrical balance (eq) =  2.197e+001
```

```
  Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  92.76
                                Iterations  =   6
                                   Total H  = 1.139431e+002
                                   Total O  = 5.843693e+001

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

                                                   Log       Log        Log
   Species                 Molality    Activity  Molality  Activity    Gamma

   OH-                   8.574e-001  3.816e-001    -0.067    -0.418    -0.352
   H+                    1.432e-014  1.000e-014   -13.844   -14.000    -0.156
   H2O                   5.551e+001  5.621e-001     1.744    -0.250     0.000
H(0)             0.000e+000
   H2                    0.000e+000  7.447e-040   -40.312   -39.128     1.184
Na               2.490e+001
   Na+                   2.283e+001  8.532e+001     1.358     1.931     0.573
   NaOH                  2.073e+000  3.169e+001     0.317     1.501     1.184
O(0)             7.102e-018
   O2                    3.551e-018  5.427e-017   -17.450   -16.265     1.184

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

      Phase               SI log IAP  log KT

      H2(g)           -36.00  -39.13   -3.13  H2
      H2O(g)           -1.89   -0.25    1.64  H2O
      O2(g)           -13.41  -16.27   -2.85  O2

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

Reaction step 1.

Using mix 1.      Mix NaOH and GW @ equ w/ calcite

Mixture 1.  Mix NaOH and GW @ equ w/ calcite

       4.000e-001 Solution 1  GW @ eqb w/ Calcite
       6.000e-001 Solution 2  NaOH

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

      Elements           Molality       Moles

      C                1.584e-006  1.584e-006
      Ca               7.156e-007  7.156e-007
      Na               1.494e+001  1.494e+001

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

                                     pH  =  13.727      Charge balance
                                     pe  =   4.804      Adjusted to redox equilibrium
                       Activity of water  =   0.736
                          Ionic strength  =  7.164e+000
                     Mass of water (kg)   =  1.000e+000
                Total alkalinity (eq/kg)  =  1.758e+000
                     Total CO2 (mol/kg)   =  1.584e-006
                   Temperature (deg C)    =  20.000
                 Electrical balance (eq)  =  1.318e+001
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  92.00
                                Iterations  =  11
                                   Total H  = 1.127709e+002
                                   Total O  = 5.726465e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	5.734e-001	2.668e-001	-0.242	-0.574	-0.332
H+	2.659e-014	1.874e-014	-13.575	-13.727	-0.152
H2O	5.551e+001	7.363e-001	1.744	-0.133	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-141.862	-141.145	0.716
C(4)	1.584e-006				
NaCO3-	1.397e-006	7.298e-006	-5.855	-5.137	0.718
CO3-2	1.870e-007	2.132e-008	-6.728	-7.671	-0.943
NaHCO3	2.434e-011	1.267e-010	-10.614	-9.897	0.716
HCO3-	1.632e-011	9.485e-012	-10.787	-11.023	-0.236
CaCO3	2.350e-012	1.223e-011	-11.629	-10.913	0.716
CaHCO3+	7.156e-017	4.158e-017	-16.145	-16.381	-0.236
CO2	1.117e-019	5.815e-019	-18.952	-18.235	0.716
Ca	7.156e-007				
CaOH+	4.671e-007	2.439e-006	-6.331	-5.613	0.718
Ca+2	2.485e-007	3.740e-007	-6.605	-6.427	0.178
CaCO3	2.350e-012	1.223e-011	-11.629	-10.913	0.716
CaHCO3+	7.156e-017	4.158e-017	-16.145	-16.381	-0.236
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.908	-40.191	0.716
Na	1.494e+001				
Na+	1.376e+001	2.376e+001	1.138	1.376	0.237
NaOH	1.185e+000	6.168e+000	0.074	0.790	0.716
NaCO3-	1.397e-006	7.298e-006	-5.855	-5.137	0.718
NaHCO3	2.434e-011	1.267e-010	-10.614	-9.897	0.716
O(0)	4.784e-015				
O2	2.392e-015	1.245e-014	-14.621	-13.905	0.716

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

Phase	SI	log IAP	log KT	
Aragonite	-5.79	-14.10	-8.31	CaCO3
Calcite	-5.65	-14.10	-8.45	CaCO3
CH4(g)	-138.33	-141.15	-2.82	CH4
CO2(g)	-16.83	-18.24	-1.41	CO2
H2(g)	-37.06	-40.19	-3.13	H2
H2O(g)	-1.77	-0.13	1.64	H2O
O2(g)	-11.05	-13.90	-2.85	O2

End of simulation.

Reading input data for simulation 2.

End of run.

Run 1 Continued...

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\40-60\mix 1 eqb calcite and CO2.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\40-60\mix 1 eqb calcite and CO2.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 1 mix 1 eqb with calcite and CO2
          temp      25
          pH        13.727
          pe        4.804
          redox     pe
          units     mmol/kgw
          density   1
          C         1.584e-006
          Ca        7.156e-007
          Na        14.94
          water    1 # kg
      EQUILIBRIUM_PHASES 1
          Calcite   0 10
          CO2(g)    -2 10
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.     mix 1 eqb with calcite and CO2

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

      Elements           Molality       Moles

      C                1.584e-009  1.584e-009
      Ca               7.156e-010  7.156e-010
      Na               1.494e-002  1.494e-002

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

                                       pH  =  13.727
                                       pe  =   4.804
                          Activity of water  =   0.986
                             Ionic strength  =  4.120e-001
                        Mass of water (kg)   =  1.000e+000
                  Total alkalinity (eq/kg)   =  8.146e-001
                        Total CO2 (mol/kg)   =  1.584e-009
                      Temperature (deg C)    =  25.000
                   Electrical balance (eq)   = -7.996e-001
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   = -97.04
                                 Iterations  =   5
                                    Total H  = 1.118270e+002
                                    Total O  = 5.632080e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	8.118e-001	5.264e-001	-0.091	-0.279	-0.188
H+	2.431e-014	1.875e-014	-13.614	-13.727	-0.113
H2O	5.551e+001	9.859e-001	1.744	-0.006	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-144.089	-144.047	0.041
C(4)	1.584e-009				
CO3-2	1.502e-009	3.674e-010	-8.823	-9.435	-0.612
NaCO3-	8.144e-011	5.952e-011	-10.089	-10.225	-0.136
HCO3-	2.089e-013	1.469e-013	-12.680	-12.833	-0.153
NaHCO3	6.536e-016	7.187e-016	-15.185	-15.143	0.041
CaCO3	2.568e-017	2.823e-017	-16.590	-16.549	0.041
CO2	5.712e-021	6.281e-021	-20.243	-20.202	0.041
CaHCO3+	1.219e-022	8.572e-023	-21.914	-22.067	-0.153
Ca	7.156e-010				
CaOH+	5.461e-010	3.992e-010	-9.263	-9.399	-0.136
Ca+2	1.695e-010	4.574e-011	-9.771	-10.340	-0.569
CaCO3	2.568e-017	2.823e-017	-16.590	-16.549	0.041
CaHCO3+	1.219e-022	8.572e-023	-21.914	-22.067	-0.153
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.253	-40.212	0.041
Na	1.494e-002				
Na+	1.219e-002	8.701e-003	-1.914	-2.060	-0.146
NaOH	2.749e-003	3.023e-003	-2.561	-2.520	0.041
NaCO3-	8.144e-011	5.952e-011	-10.089	-10.225	-0.136
NaHCO3	6.536e-016	7.187e-016	-15.185	-15.143	0.041
O(0)	1.957e-012				
O2	9.784e-013	1.076e-012	-12.009	-11.968	0.041

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

Phase	SI	log IAP	log KT	
Aragonite	-11.44	-19.77	-8.34	CaCO3
Calcite	-11.29	-19.77	-8.48	CaCO3
CH4(g)	-141.19	-144.05	-2.86	CH4
CO2(g)	-18.73	-20.20	-1.47	CO2
H2(g)	-37.06	-40.21	-3.15	H2
H2O(g)	-1.52	-0.01	1.51	H2O
O2(g)	-9.08	-11.97	-2.89	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. mix 1 eqb with calcite and CO2
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Calcite	0.00	-8.48	-8.48	1.000e+001	1.000e+001	-5.868e-006
CO2(g)	-2.00	-3.47	-1.47	1.000e+001	9.348e+000	-6.517e-001

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

Elements	Molality	Moles

C	6.498e-001	6.517e-001
Ca	5.851e-006	5.868e-006
Na	1.490e-002	1.494e-002

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

pH	=	9.347	Charge balance
pe	=	9.186	Adjusted to redox equilibrium
Activity of water	=	0.989	
Ionic strength	=	5.646e-001	
Mass of water (kg)	=	1.003e+000	
Total alkalinity (eq/kg)	=	8.122e-001	
Total CO2 (mol/kg)	=	6.498e-001	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-7.996e-001	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-97.89	
Iterations	=	15	
Total H	=	1.118270e+002	
Total O	=	5.762417e+001	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	3.532e-005	2.201e-005	-4.452	-4.657	-0.205
H+	5.913e-010	4.497e-010	-9.228	-9.347	-0.119
H2O	5.551e+001	9.888e-001	1.744	-0.005	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-127.392	-127.336	0.056
C(4)	6.498e-001				
HCO3-	4.858e-001	3.329e-001	-0.314	-0.478	-0.164
CO3-2	1.574e-001	3.472e-002	-0.803	-1.459	-0.656
NaCO3-	5.320e-003	3.923e-003	-2.274	-2.406	-0.132
NaHCO3	9.978e-004	1.136e-003	-3.001	-2.945	0.056
CO2	2.990e-004	3.405e-004	-3.524	-3.468	0.056
CaCO3	4.886e-006	5.565e-006	-5.311	-5.255	0.056
CaHCO3+	5.914e-007	4.053e-007	-6.228	-6.392	-0.164
Ca	5.851e-006				
CaCO3	4.886e-006	5.565e-006	-5.311	-5.255	0.056
CaHCO3+	5.914e-007	4.053e-007	-6.228	-6.392	-0.164
Ca+2	3.731e-007	9.542e-008	-6.428	-7.020	-0.592
CaOH+	4.721e-011	3.482e-011	-10.326	-10.458	-0.132
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.273	-40.217	0.056
Na	1.490e-002				
Na+	8.578e-003	6.069e-003	-2.067	-2.217	-0.150
NaCO3-	5.320e-003	3.923e-003	-2.274	-2.406	-0.132
NaHCO3	9.978e-004	1.136e-003	-3.001	-2.945	0.056
NaOH	7.742e-008	8.816e-008	-7.111	-7.055	0.056
O(0)	1.945e-012				
O2	9.723e-013	1.107e-012	-12.012	-11.956	0.056

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

Phase	SI	log IAP	log KT	
Aragonite	-0.14	-8.48	-8.34	CaCO3
Calcite	0.00	-8.48	-8.48	CaCO3
CH4(g)	-124.48	-127.34	-2.86	CH4
CO2(g)	-2.00	-3.47	-1.47	CO2
H2(g)	-37.07	-40.22	-3.15	H2
H2O(g)	-1.51	-0.00	1.51	H2O
O2(g)	-9.06	-11.96	-2.89	O2

End of simulation.

```
------------------

-----------------------------------
Reading input data for simulation 2.
-----------------------------------

-----------
End of run.
-----------
```

Run 1 Continued...

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\40-60\mix 2 eqb montmorillonite.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\40-60\mix 2 eqb montmorillonite.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 1 mix 2 eqb montmorillonite
          temp      20
          pH        9.347
          pe        9.186
          redox     pe
          units     mmol/kgw
          density   1
          C         0.6498
          Ca        5.851e-006
          Na        0.0149
          water    1 # kg
      EQUILIBRIUM_PHASES 1
          Ca-Montmorillonite 0 10
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     mix 2 eqb montmorillonite

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

      Elements           Molality       Moles

      C                 6.498e-004  6.498e-004
      Ca                5.851e-009  5.851e-009
      Na                1.490e-005  1.490e-005

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

                                       pH  =   9.347
                                       pe  =   9.186
                         Activity of water  =   1.000
                            Ionic strength  =  4.286e-004
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  7.239e-004
                       Total CO2 (mol/kg)   =  6.498e-004
                      Temperature (deg C)   =  20.000
                  Electrical balance (eq)   = -7.090e-004
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   = -95.97
                                Iterations  =   4
                                   Total H  = 1.110130e+002
                                   Total O  = 5.550818e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.545e-005	1.509e-005	-4.811	-4.821	-0.010
H+	4.601e-010	4.498e-010	-9.337	-9.347	-0.010
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-129.392	-129.392	0.000
C(4)	6.498e-004				
HCO3-	5.899e-004	5.764e-004	-3.229	-3.239	-0.010
CO3-2	5.922e-005	5.397e-005	-4.228	-4.268	-0.040
CO2	6.245e-007	6.246e-007	-6.204	-6.204	0.000
NaCO3-	1.157e-008	1.131e-008	-7.937	-7.947	-0.010
NaHCO3	4.712e-009	4.713e-009	-8.327	-8.327	0.000
CaCO3	4.078e-010	4.078e-010	-9.390	-9.390	0.000
CaHCO3+	3.407e-011	3.328e-011	-10.468	-10.478	-0.010
Ca	5.851e-009				
Ca+2	5.407e-009	4.927e-009	-8.267	-8.307	-0.040
CaCO3	4.078e-010	4.078e-010	-9.390	-9.390	0.000
CaHCO3+	3.407e-011	3.328e-011	-10.468	-10.478	-0.010
CaOH+	1.861e-012	1.818e-012	-11.730	-11.740	-0.010
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.194	-40.194	0.000
Na	1.490e-005				
Na+	1.488e-005	1.454e-005	-4.827	-4.837	-0.010
NaCO3-	1.157e-008	1.131e-008	-7.937	-7.947	-0.010
NaHCO3	4.712e-009	4.713e-009	-8.327	-8.327	0.000
NaOH	2.136e-010	2.136e-010	-9.670	-9.670	0.000
O(0)	4.654e-014				
O2	2.327e-014	2.327e-014	-13.633	-13.633	0.000

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

Phase	SI	log IAP	log KT	
Aragonite	-4.27	-12.58	-8.31	CaCO3
Calcite	-4.12	-12.58	-8.45	CaCO3
CH4(g)	-126.57	-129.39	-2.82	CH4
CO2(g)	-4.80	-6.20	-1.41	CO2
H2(g)	-37.07	-40.19	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-10.78	-13.63	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. mix 2 eqb montmorillonite
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca-Montmorillonite	0.00	-45.76	-45.76	1.000e+001	1.000e+001	-1.305e-005

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

Elements	Molality	Moles
Al	3.040e-005	3.040e-005
C	6.498e-004	6.498e-004

Ca	2.159e-006	2.159e-006
Na	1.490e-005	1.490e-005
Si	4.789e-005	4.789e-005

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

pH	=	9.090	Charge balance
pe	=	9.461	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	4.096e-004	
Mass of water (kg)	=	1.000e+000	
Total alkalinity (eq/kg)	=	8.194e-004	
Total CO2 (mol/kg)	=	6.498e-004	
Temperature (deg C)	=	20.000	
Electrical balance (eq)	=	-7.090e-004	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-94.91	
Iterations	=	10	
Total H	=	1.110131e+002	
Total O	=	5.550834e+001	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	8.548e-006	8.353e-006	-5.068	-5.078	-0.010
H+	8.310e-010	8.127e-010	-9.080	-9.090	-0.010
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Al	3.040e-005				
Al(OH)4-	3.039e-005	2.970e-005	-4.517	-4.527	-0.010
Al(OH)3	1.361e-008	1.361e-008	-7.866	-7.866	0.000
Al(OH)2+	1.124e-010	1.098e-010	-9.949	-9.959	-0.010
AlOH+2	1.957e-014	1.786e-014	-13.708	-13.748	-0.040
Al+3	2.479e-018	2.030e-018	-17.606	-17.693	-0.087
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-129.263	-129.263	0.000
C(4)	6.498e-004				
HCO3-	6.144e-004	6.006e-004	-3.212	-3.221	-0.010
CO3-2	3.408e-005	3.112e-005	-4.467	-4.507	-0.039
CO2	1.176e-006	1.176e-006	-5.930	-5.930	0.000
CaCO3	8.957e-008	8.958e-008	-7.048	-7.048	0.000
CaHCO3+	1.351e-008	1.321e-008	-7.869	-7.879	-0.010
NaCO3-	6.677e-009	6.525e-009	-8.175	-8.185	-0.010
NaHCO3	4.914e-009	4.915e-009	-8.309	-8.308	0.000
Ca	2.159e-006				
Ca+2	2.055e-006	1.877e-006	-5.687	-5.727	-0.040
CaCO3	8.957e-008	8.958e-008	-7.048	-7.048	0.000
CaHCO3+	1.351e-008	1.321e-008	-7.869	-7.879	-0.010
CaOH+	3.921e-010	3.832e-010	-9.407	-9.417	-0.010
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.230	-40.230	0.000
Na	1.490e-005				
Na+	1.489e-005	1.455e-005	-4.827	-4.837	-0.010
NaCO3-	6.677e-009	6.525e-009	-8.175	-8.185	-0.010
NaHCO3	4.914e-009	4.915e-009	-8.309	-8.308	0.000
NaOH	1.183e-010	1.183e-010	-9.927	-9.927	0.000
O(0)	5.504e-014				
O2	2.752e-014	2.752e-014	-13.560	-13.560	0.000
Si	4.789e-005				
H4SiO4	4.146e-005	4.146e-005	-4.382	-4.382	0.000
H3SiO4-	6.430e-006	6.284e-006	-5.192	-5.202	-0.010
H2SiO4-2	4.122e-010	3.761e-010	-9.385	-9.425	-0.040

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

Phase	SI	log IAP	log KT

Al(OH)3(a)	-1.55	9.58	11.13	Al(OH)3
Albite	-4.19	-22.51	-18.33	NaAlSi3O8
Anorthite	-3.69	-23.55	-19.86	CaAl2Si2O8
Aragonite	-1.93	-10.23	-8.31	CaCO3
Ca-Montmorillonite	0.00	-45.76	-45.76	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-1.78	-10.23	-8.45	CaCO3
CH4(g)	-126.44	-129.26	-2.82	CH4
Chalcedony	-0.77	-4.38	-3.61	SiO2
CO2(g)	-4.52	-5.93	-1.41	CO2
Gibbsite	1.18	9.58	8.40	Al(OH)3
H2(g)	-37.10	-40.23	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
Kaolinite	2.51	10.39	7.88	Al2Si2O5(OH)4
O2(g)	-10.71	-13.56	-2.85	O2
Quartz	-0.33	-4.38	-4.06	SiO2
SiO2(a)	-1.63	-4.38	-2.75	SiO2

End of simulation.

Reading input data for simulation 2.

End of run.

Run 2

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\1-99\1%rainwater+99%NaOH.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\1-99\1%rainwater+99%NaOH.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          CO2(g)     -3.5 10
      SOLUTION 1 rainwater
          temp       25
          pH         5.24
          pe         4
          redox      pe
          units      mg/l
          density    1
          Ca         0.458
          Mg         0.034
          Na         0.082
          K          0.043
          Cl         0.122
          S(6)       1.131
          N(5)       1.004
          N(-3)      0.36
          water     1 # kg
      SOLUTION 2 NaOH
          temp       20
          pH         14
          pe         4
          redox      pe
          units      mmol/kgw
          density    1
          Na         24.9 mol/kgw
          water     1 # kg
      MIX 1
          1     0.01
          2     0.99
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.     rainwater

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

      Elements           Molality       Moles

      Ca                1.143e-005  1.143e-005
      Cl                3.441e-006  3.441e-006
      K                 1.100e-006  1.100e-006
```

Mg	1.398e-006	1.398e-006
N(-3)	2.570e-005	2.570e-005
N(5)	7.168e-005	7.168e-005
Na	3.567e-006	3.567e-006
S(6)	1.177e-005	1.177e-005

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

```
                                    pH  =   5.240
                                    pe  =   4.000
                     Activity of water  =   1.000
                        Ionic strength  =  1.047e-004
                    Mass of water (kg)  =  1.000e+000
              Total alkalinity (eq/kg)  = -5.824e-006
                 Total carbon (mol/kg)  =  0.000e+000
                    Total CO2 (mol/kg)  =  0.000e+000
                   Temperature (deg C)  =  25.000
             Electrical balance (eq)    = -3.682e-005
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -22.96
                            Iterations  =   3
                               Total H  = 1.110125e+002
                               Total O  = 5.550648e+001
```

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

Redox couple	pe	Eh (volts)
N(-3)/N(5)	8.3903	0.4963

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	5.822e-006	5.754e-006	-5.235	-5.240	-0.005
OH-	1.760e-009	1.740e-009	-8.754	-8.760	-0.005
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Ca	1.143e-005				
Ca+2	1.140e-005	1.088e-005	-4.943	-4.963	-0.020
CaSO4	2.429e-008	2.429e-008	-7.614	-7.614	0.000
CaHSO4+	8.288e-013	8.190e-013	-12.082	-12.087	-0.005
CaOH+	3.174e-013	3.137e-013	-12.498	-12.503	-0.005
Cl	3.441e-006				
Cl-	3.441e-006	3.401e-006	-5.463	-5.468	-0.005
H(0)	4.688e-022				
H2	2.344e-022	2.344e-022	-21.630	-21.630	0.000
K	1.100e-006				
K+	1.100e-006	1.087e-006	-5.959	-5.964	-0.005
KSO4-	8.649e-011	8.547e-011	-10.063	-10.068	-0.005
KOH	6.547e-016	6.548e-016	-15.184	-15.184	0.000
Mg	1.398e-006				
Mg+2	1.395e-006	1.331e-006	-5.855	-5.876	-0.020
MgSO4	3.492e-009	3.492e-009	-8.457	-8.457	0.000
MgOH+	8.497e-013	8.397e-013	-12.071	-12.076	-0.005
N(-3)	2.570e-005				
NH4+	2.570e-005	2.539e-005	-4.590	-4.595	-0.005
NH4SO4-	3.705e-009	3.662e-009	-8.431	-8.436	-0.005
NH3	2.515e-009	2.515e-009	-8.600	-8.600	0.000
N(5)	7.168e-005				
NO3-	7.168e-005	7.083e-005	-4.145	-4.150	-0.005
Na	3.567e-006				
Na+	3.567e-006	3.525e-006	-5.448	-5.453	-0.005
NaSO4-	2.001e-010	1.977e-010	-9.699	-9.704	-0.005
NaOH	4.047e-015	4.047e-015	-14.393	-14.393	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-49.120	-49.120	0.000
S(6)	1.177e-005				

SO4-2	1.174e-005	1.119e-005	-4.931	-4.951	-0.021
CaSO4	2.429e-008	2.429e-008	-7.614	-7.614	0.000
HSO4-	6.337e-009	6.263e-009	-8.198	-8.203	-0.005
NH4SO4-	3.705e-009	3.662e-009	-8.431	-8.436	-0.005
MgSO4	3.492e-009	3.492e-009	-8.457	-8.457	0.000
NaSO4-	2.001e-010	1.977e-010	-9.699	-9.704	-0.005
KSO4-	8.649e-011	8.547e-011	-10.063	-10.068	-0.005
CaHSO4+	8.288e-013	8.190e-013	-12.082	-12.087	-0.005

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

Phase	SI	log IAP	log KT	
Anhydrite	-5.55	-9.91	-4.36	CaSO4
Gypsum	-5.33	-9.91	-4.58	CaSO4:2H2O
H2(g)	-18.48	-21.63	-3.15	H2
H2O(g)	-1.51	-0.00	1.51	H2O
Halite	-12.50	-10.92	1.58	NaCl
NH3(g)	-10.37	-8.60	1.77	NH3
O2(g)	-46.23	-49.12	-2.89	O2

Initial solution 2. NaOH

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

Elements	Molality	Moles
Na	2.490e+001	2.490e+001

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

pH	=	14.000
pe	=	4.000
Activity of water	=	0.562
Ionic strength	=	1.184e+001
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	2.931e+000
Total carbon (mol/kg)	=	0.000e+000
Total CO2 (mol/kg)	=	0.000e+000
Temperature (deg C)	=	20.000
Electrical balance (eq)	=	2.197e+001
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	92.76
Iterations	=	6
Total H	=	1.139431e+002
Total O	=	5.843693e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	8.574e-001	3.816e-001	-0.067	-0.418	-0.352
H+	1.432e-014	1.000e-014	-13.844	-14.000	-0.156
H2O	5.551e+001	5.621e-001	1.744	-0.250	0.000
H(0)	0.000e+000				
H2	0.000e+000	7.447e-040	-40.312	-39.128	1.184
Na	2.490e+001				
Na+	2.283e+001	8.532e+001	1.358	1.931	0.573
NaOH	2.073e+000	3.169e+001	0.317	1.501	1.184
O(0)	7.102e-018				
O2	3.551e-018	5.427e-017	-17.450	-16.265	1.184

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

Phase	SI	log IAP	log KT	
H2(g)	-36.00	-39.13	-3.13	H2

```
      H2O(g)            -1.89   -0.25    1.64  H2O
      O2(g)            -13.41  -16.27   -2.85  O2

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

Reaction step 1.

Using mix 1.
Using pure phase assemblage 1.

Mixture 1.

       1.000e-002 Solution 1  rainwater
       9.900e-001 Solution 2  NaOH

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

                                                      Moles in assemblage
Phase                  SI log IAP  log KT      Initial       Final       Delta

CO2(g)               -3.50   -4.91   -1.41   1.000e+001  8.447e+000 -1.553e+000

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

      Elements           Molality       Moles

      C                1.516e+000  1.553e+000
      Ca               1.116e-007  1.143e-007
      Cl               3.360e-008  3.441e-008
      K                1.074e-008  1.100e-008
      Mg               1.365e-008  1.398e-008
      N                9.507e-007  9.738e-007
      Na               2.407e+001  2.465e+001
      S                1.149e-007  1.177e-007

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

                                     pH  =  10.144      Charge balance
                                     pe  =   8.273      Adjusted to redox equilibrium
                       Activity of water  =   0.586
                          Ionic strength  =  1.248e+001
                     Mass of water (kg)   =  1.024e+000
                Total alkalinity (eq/kg)  =  2.833e+000
                     Total CO2 (mol/kg)   =  1.516e+000
                   Temperature (deg C)    =  20.050
                Electrical balance (eq)   =  2.175e+001
 Percent error, 100*(Cat-|An|)/(Cat+|An|) =  86.70
                            Iterations    =  21
                               Total H    = 1.139138e+002
                               Total O    = 6.151422e+001

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

                                                   Log       Log        Log
   Species                Molality    Activity  Molality  Activity    Gamma

   OH-                  1.256e-004  5.567e-005   -3.901    -4.254    -0.353
   H+                   1.028e-010  7.170e-011   -9.988   -10.144    -0.156
   H2O                  5.551e+001  5.856e-001    1.744    -0.232     0.000
C(-4)           0.000e+000
   CH4                  0.000e+000  0.000e+000 -127.964  -126.716     1.248
C(4)            1.516e+000
   NaCO3-               1.077e+000  3.392e+001    0.032     1.530     1.498
   CO3-2                2.384e-001  2.468e-002   -0.623    -1.608    -0.985
   NaHCO3               1.268e-001  2.246e+000   -0.897     0.351     1.248
```

HCO3-	7.400e-002	4.198e-002	-1.131	-1.377	-0.246
CO2	6.985e-007	1.237e-005	-6.156	-4.908	1.248
CaCO3	7.684e-008	1.361e-006	-7.114	-5.866	1.248
CaHCO3+	3.119e-008	1.769e-008	-7.506	-7.752	-0.246
MgCO3	1.317e-008	2.333e-007	-7.881	-6.632	1.248
MgHCO3+	1.635e-010	5.147e-009	-9.787	-8.288	1.498
Ca	1.116e-007				
CaCO3	7.684e-008	1.361e-006	-7.114	-5.866	1.248
CaHCO3+	3.119e-008	1.769e-008	-7.506	-7.752	-0.246
Ca+2	3.529e-009	3.593e-008	-8.452	-7.445	1.008
CaOH+	1.547e-012	4.870e-011	-11.811	-10.312	1.498
CaSO4	8.830e-016	1.564e-014	-15.054	-13.806	1.248
CaHSO4+	1.968e-025	6.196e-024	-24.706	-23.208	1.498
Cl	3.360e-008				
Cl-	3.360e-008	2.292e-008	-7.474	-7.640	-0.166
H(0)	0.000e+000				
H2	0.000e+000	1.087e-040	-41.212	-39.964	1.248
K	1.074e-008				
K+	1.074e-008	7.323e-009	-7.969	-8.135	-0.166
KOH	1.171e-014	2.074e-013	-13.932	-12.683	1.248
KSO4-	3.424e-018	1.078e-016	-17.466	-15.967	1.498
Mg	1.365e-008				
MgCO3	1.317e-008	2.333e-007	-7.881	-6.632	1.248
Mg+2	3.173e-010	1.069e-008	-9.499	-7.971	1.527
MgHCO3+	1.635e-010	5.147e-009	-9.787	-8.288	1.498
MgOH+	6.387e-012	2.011e-010	-11.195	-9.697	1.498
MgSO4	2.840e-016	5.032e-015	-15.547	-14.298	1.248
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-51.744	-52.202	-0.458
NH3	0.000e+000	0.000e+000	-52.705	-51.456	1.248
NH4SO4-	0.000e+000	0.000e+000	-61.231	-59.733	1.498
N(0)	4.015e-007				
N2	2.007e-007	3.556e-006	-6.697	-5.449	1.248
N(3)	1.770e-014				
NO2-	1.770e-014	7.062e-015	-13.752	-14.151	-0.399
N(5)	5.493e-007				
NO3-	5.493e-007	2.191e-007	-6.260	-6.659	-0.399
Na	2.407e+001				
Na+	2.286e+001	9.513e+001	1.359	1.978	0.619
NaCO3-	1.077e+000	3.392e+001	0.032	1.530	1.498
NaHCO3	1.268e-001	2.246e+000	-0.897	0.351	1.248
NaOH	2.897e-004	5.133e-003	-3.538	-2.290	1.248
NaSO4-	3.355e-008	1.056e-006	-7.474	-5.976	1.498
O(0)	3.245e-016				
O2	1.622e-016	2.874e-015	-15.790	-14.541	1.248
S(-2)	0.000e+000				
HS-	0.000e+000	0.000e+000	-130.451	-130.804	-0.353
S-2	0.000e+000	0.000e+000	-132.675	-133.727	-1.052
H2S	0.000e+000	0.000e+000	-135.188	-133.939	1.248
S(6)	1.149e-007				
SO4-2	8.140e-008	2.287e-009	-7.089	-8.641	-1.551
NaSO4-	3.355e-008	1.056e-006	-7.474	-5.976	1.498
CaSO4	8.830e-016	1.564e-014	-15.054	-13.806	1.248
MgSO4	2.840e-016	5.032e-015	-15.547	-14.298	1.248
KSO4-	3.424e-018	1.078e-016	-17.466	-15.967	1.498
HSO4-	4.555e-019	1.434e-017	-18.341	-16.843	1.498
CaHSO4+	1.968e-025	6.196e-024	-24.706	-23.208	1.498
NH4SO4-	0.000e+000	0.000e+000	-61.231	-59.733	1.498

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

Phase	SI	log IAP	log KT	
Anhydrite	-11.74	-16.09	-4.34	CaSO4
Aragonite	-0.75	-9.05	-8.31	CaCO3
Calcite	-0.60	-9.05	-8.45	CaCO3
CH4(g)	-123.90	-126.72	-2.82	CH4

```
CO2(g)          -3.50   -4.91   -1.41  CO2
Dolomite        -1.66  -18.63  -16.97  CaMg(CO3)2
Gypsum         -11.97  -16.55   -4.58  CaSO4:2H2O
H2(g)          -36.84  -39.96   -3.13  H2
H2O(g)          -1.87   -0.23    1.64  H2O
H2S(g)        -133.00 -133.94   -0.94  H2S
Halite          -7.23   -5.66    1.57  NaCl
N2(g)           -2.21   -5.45   -3.24  N2
NH3(g)         -53.33  -51.46    1.87  NH3
O2(g)          -11.69  -14.54   -2.85  O2
Sulfur        -102.10  -97.10    5.00  S

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 2.
-----------------------------------

-----------
End of run.
-----------
```

Run 2 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\1-99\mix rain NaOH and calcite GW.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\1-99\mix rain NaOH and calcite GW.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 2 NaOH
          temp      20
          pH        10.144
          pe        8.273
          redox     pe
          units     mmol/kgw
          density   1
          Na        24.07 Mol/kgw
          C         1.516
          Ca        1.116e-007
          Cl        3.36e-008
          K         1.074e-008
          Mg        1.365e-008
          N(5)      5.493e-007
          S(6)      1.149e-007
          water    1 # kg
      SOLUTION 1 GW @ eqb w/ Calcite
          temp      20
          pH        7.301
          pe        -1.841
          redox     pe
          units     mmol/kgw
          density   1
          Ca        0.001789
          C         0.003961
          water    1 # kg
      SAVE solution 1-2
      MIX 1 Mix NaOH and GW @ equ w/ calcite
          1    0.4
          2    0.6
------------------------------------------
Beginning of initial solution calculations.
------------------------------------------

Initial solution 1.     GW @ eqb w/ Calcite

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

      Elements           Molality       Moles

      C                 3.961e-006  3.961e-006
      Ca                1.789e-006  1.789e-006
```

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

pH	=	7.301
pe	=	-1.841
Activity of water	=	1.000
Ionic strength	=	5.444e-006
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	3.626e-006
Total CO2 (mol/kg)	=	3.961e-006
Temperature (deg C)	=	20.000
Electrical balance (eq)	=	-4.751e-008
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-0.65
Iterations	=	3
Total H	=	1.110124e+002
Total O	=	5.550623e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.361e-007	1.358e-007	-6.866	-6.867	-0.001
H+	5.014e-008	5.000e-008	-7.300	-7.301	-0.001
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	1.058e-025				
CH4	1.058e-025	1.058e-025	-24.975	-24.975	0.000
C(4)	3.961e-006				
HCO3-	3.533e-006	3.524e-006	-5.452	-5.453	-0.001
CO2	4.245e-007	4.245e-007	-6.372	-6.372	0.000
CO3-2	3.000e-009	2.968e-009	-8.523	-8.528	-0.005
CaHCO3+	7.328e-011	7.309e-011	-10.135	-10.136	-0.001
CaCO3	8.056e-012	8.056e-012	-11.094	-11.094	0.000
Ca	1.789e-006				
Ca+2	1.789e-006	1.770e-006	-5.747	-5.752	-0.005
CaHCO3+	7.328e-011	7.309e-011	-10.135	-10.136	-0.001
CaCO3	8.056e-012	8.056e-012	-11.094	-11.094	0.000
CaOH+	5.889e-012	5.873e-012	-11.230	-11.231	-0.001
H(0)	1.791e-014				
H2	8.953e-015	8.953e-015	-14.048	-14.048	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-65.925	-65.925	0.000

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

Phase	SI	log IAP	log KT	
Aragonite	-5.97	-14.28	-8.31	CaCO3
Calcite	-5.83	-14.28	-8.45	CaCO3
CH4(g)	-22.16	-24.98	-2.82	CH4
CO2(g)	-4.97	-6.37	-1.41	CO2
H2(g)	-10.92	-14.05	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.07	-65.93	-2.85	O2

Initial solution 2. NaOH

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

Elements	Molality	Moles
C	1.516e-003	1.516e-003
Ca	1.116e-010	1.116e-010
Cl	3.360e-011	3.360e-011
K	1.074e-011	1.074e-011
Mg	1.365e-011	1.365e-011
N(5)	5.493e-010	5.493e-010
Na	2.407e+001	2.407e+001

S(6) 1.149e-010 1.149e-010

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

pH	=	10.144
pe	=	8.273
Activity of water	=	0.591
Ionic strength	=	1.204e+001
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	3.282e-003
Total CO2 (mol/kg)	=	1.516e-003
Temperature (deg C)	=	20.000
Electrical balance (eq)	=	2.407e+001
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	99.99
Iterations	=	12
Total H	=	1.110131e+002
Total O	=	5.551121e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.257e-004	5.588e-005	-3.901	-4.253	-0.352
H+	1.028e-010	7.178e-011	-9.988	-10.144	-0.156
H2O	5.551e+001	5.908e-001	1.744	-0.229	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-130.958	-129.754	1.204
C(4)	1.516e-003				
NaCO3-	1.109e-003	2.997e-002	-2.955	-1.523	1.432
CO3-2	2.149e-004	2.238e-005	-3.668	-4.650	-0.982
NaHCO3	1.248e-004	1.993e-003	-3.904	-2.700	1.204
HCO3-	6.716e-005	3.815e-005	-4.173	-4.418	-0.246
CO2	6.989e-010	1.117e-008	-9.156	-7.952	1.204
CaCO3	2.021e-012	3.229e-011	-11.694	-10.491	1.204
CaHCO3+	7.402e-013	4.205e-013	-12.131	-12.376	-0.246
MgCO3	4.419e-013	7.060e-012	-12.355	-11.151	1.204
MgHCO3+	5.783e-015	1.562e-013	-14.238	-12.806	1.432
Ca	1.116e-010				
Ca+2	1.088e-010	9.404e-010	-9.963	-9.027	0.937
CaCO3	2.021e-012	3.229e-011	-11.694	-10.491	1.204
CaHCO3+	7.402e-013	4.205e-013	-12.131	-12.376	-0.246
CaOH+	4.755e-014	1.285e-012	-13.323	-11.891	1.432
CaSO4	2.542e-020	4.062e-019	-19.595	-18.391	1.204
CaHSO4+	5.958e-030	1.610e-028	-29.225	-27.793	1.432
Cl	3.360e-011				
Cl-	3.360e-011	2.263e-011	-10.474	-10.645	-0.172
H(0)	0.000e+000				
H2	0.000e+000	1.091e-040	-41.166	-39.962	1.204
K	1.074e-011				
K+	1.074e-011	7.235e-012	-10.969	-11.141	-0.172
KOH	1.292e-017	2.065e-016	-16.889	-15.685	1.204
KSO4-	3.909e-024	1.056e-022	-23.408	-21.976	1.432
Mg	1.365e-011				
Mg+2	1.295e-011	3.569e-010	-10.888	-9.447	1.440
MgCO3	4.419e-013	7.060e-012	-12.355	-11.151	1.204
MgOH+	2.494e-013	6.739e-012	-12.603	-11.171	1.432
MgHCO3+	5.783e-015	1.562e-013	-14.238	-12.806	1.432
MgSO4	1.043e-020	1.666e-019	-19.982	-18.778	1.204
N(5)	5.493e-010				
NO3-	5.493e-010	2.200e-010	-9.260	-9.658	-0.397
Na	2.407e+001				
Na+	2.407e+001	9.291e+001	1.381	1.968	0.587
NaCO3-	1.109e-003	2.997e-002	-2.955	-1.523	1.432
NaOH	3.162e-004	5.053e-003	-3.500	-2.296	1.204
NaHCO3	1.248e-004	1.993e-003	-3.904	-2.700	1.204
NaSO4-	3.789e-011	1.024e-009	-10.422	-8.990	1.432

```
O(0)            3.493e-016
   O2                   1.747e-016  2.791e-015   -15.758   -14.554     1.204
S(6)            1.149e-010
   SO4-2                7.701e-011  2.270e-012   -10.113   -11.644    -1.531
   NaSO4-               3.789e-011  1.024e-009   -10.422    -8.990     1.432
   CaSO4                2.542e-020  4.062e-019   -19.595   -18.391     1.204
   MgSO4                1.043e-020  1.666e-019   -19.982   -18.778     1.204
   HSO4-                5.270e-022  1.424e-020   -21.278   -19.847     1.432
   KSO4-                3.909e-024  1.056e-022   -23.408   -21.976     1.432
   CaHSO4+              5.958e-030  1.610e-028   -29.225   -27.793     1.432

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

      Phase               SI log IAP  log KT

      Anhydrite       -16.33  -20.67   -4.34  CaSO4
      Aragonite        -5.37  -13.68   -8.31  CaCO3
      Calcite          -5.22  -13.68   -8.45  CaCO3
      CH4(g)         -126.94 -129.75   -2.82  CH4
      CO2(g)           -6.55   -7.95   -1.41  CO2
      Dolomite        -10.80  -27.77  -16.97  CaMg(CO3)2
      Gypsum          -16.55  -21.13   -4.58  CaSO4:2H2O
      H2(g)           -36.83  -39.96   -3.13  H2
      H2O(g)           -1.87   -0.23    1.64  H2O
      Halite          -10.25   -8.68    1.57  NaCl
      O2(g)           -11.70  -14.55   -2.85  O2

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

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying smaller step size, pe step size 10, 5 ...

WARNING: Maximum iterations exceeded, 200

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying diagonal scaling ...

Using mix 1.      Mix NaOH and GW @ equ w/ calcite

Mixture 1.  Mix NaOH and GW @ equ w/ calcite

       4.000e-001 Solution 1  GW @ eqb w/ Calcite
       6.000e-001 Solution 2  NaOH

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

      Elements           Molality       Moles

      C                9.112e-004  9.112e-004
      Ca               7.157e-007  7.157e-007
      Cl               2.016e-011  2.016e-011
      K                6.444e-012  6.444e-012
      Mg               8.190e-012  8.190e-012
      N                3.296e-010  3.296e-010
      Na               1.444e+001  1.444e+001
      S                6.894e-011  6.894e-011

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

```
                                   pH  =   9.906      Charge balance
                                   pe  =   8.696      Adjusted to redox equilibrium
                   Activity of water  =   0.754
                      Ionic strength  =  7.221e+000
                  Mass of water (kg)  =  1.000e+000
            Total alkalinity (eq/kg)  =  1.971e-003
                  Total CO2 (mol/kg)  =  9.112e-004
                Temperature (deg C)   =  20.000
             Electrical balance (eq)  =  1.444e+001
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  99.99
                          Iterations  =  19
                             Total H  = 1.110128e+002
                             Total O  = 5.550922e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	8.864e-005	4.121e-005	-4.052	-4.385	-0.333
H+	1.765e-010	1.243e-010	-9.753	-9.906	-0.152
H2O	5.551e+001	7.545e-001	1.744	-0.122	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-132.141	-131.419	0.722
C(4)	9.112e-004				
NaCO3-	6.904e-004	3.675e-003	-3.161	-2.435	0.726
CO3-2	8.901e-005	1.013e-005	-4.051	-4.994	-0.944
NaHCO3	8.027e-005	4.233e-004	-4.095	-3.373	0.722
HCO3-	5.149e-005	2.990e-005	-4.288	-4.524	-0.236
CaCO3	3.219e-009	1.698e-008	-8.492	-7.770	0.722
CO2	2.251e-009	1.187e-008	-8.648	-7.926	0.722
CaHCO3+	6.592e-010	3.829e-010	-9.181	-9.417	-0.236
MgCO3	4.484e-014	2.365e-013	-13.348	-12.626	0.722
MgHCO3+	1.703e-015	9.062e-015	-14.769	-14.043	0.726
Ca	7.157e-007				
Ca+2	7.116e-007	1.092e-006	-6.148	-5.962	0.186
CaCO3	3.219e-009	1.698e-008	-8.492	-7.770	0.722
CaHCO3+	6.592e-010	3.829e-010	-9.181	-9.417	-0.236
CaOH+	2.068e-010	1.100e-009	-9.685	-8.958	0.726
CaSO4	6.373e-017	3.361e-016	-16.196	-15.474	0.722
CaHSO4+	4.334e-026	2.307e-025	-25.363	-24.637	0.726
Cl	2.016e-011				
Cl-	2.016e-011	1.203e-011	-10.696	-10.920	-0.224
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-41.054	-40.332	0.722
K	6.444e-012				
K+	6.444e-012	3.844e-012	-11.191	-11.415	-0.224
KOH	1.534e-017	8.091e-017	-16.814	-16.092	0.722
KSO4-	7.509e-024	3.997e-023	-23.124	-22.398	0.726
Mg	8.190e-012				
Mg+2	8.074e-012	2.641e-011	-11.093	-10.578	0.515
MgOH+	6.909e-014	3.677e-013	-13.161	-12.435	0.726
MgCO3	4.484e-014	2.365e-013	-13.348	-12.626	0.722
MgHCO3+	1.703e-015	9.062e-015	-14.769	-14.043	0.726
MgSO4	1.665e-021	8.782e-021	-20.779	-20.056	0.722
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-56.274	-56.698	-0.424
NH3	0.000e+000	0.000e+000	-56.915	-56.193	0.722
NH4SO4-	0.000e+000	0.000e+000	-68.106	-67.380	0.726
N(0)	5.698e-015				
N2	2.849e-015	1.502e-014	-14.545	-13.823	0.722
N(3)	3.578e-018				
NO2-	3.578e-018	1.516e-018	-17.446	-17.819	-0.373
N(5)	3.296e-010				
NO3-	3.296e-010	1.397e-010	-9.482	-9.855	-0.373
Na	1.444e+001				
Na+	1.444e+001	2.517e+001	1.160	1.401	0.241

```
   NaCO3-                 6.904e-004  3.675e-003    -3.161    -2.435     0.726
   NaOH                   1.914e-004  1.009e-003    -3.718    -2.996     0.722
   NaHCO3                 8.027e-005  4.233e-004    -4.095    -3.373     0.722
   NaSO4-                 3.711e-011  1.975e-010   -10.431    -9.704     0.726
O(0)            9.475e-015
   O2                     4.737e-015  2.498e-014   -14.324   -13.602     0.722
S(-2)           0.000e+000
   HS-                    0.000e+000  0.000e+000  -135.288  -135.621    -0.333
   S-2                    0.000e+000  0.000e+000  -137.779  -138.784    -1.005
   H2S                    0.000e+000  0.000e+000  -139.238  -138.516     0.722
S(6)            6.894e-011
   NaSO4-                 3.711e-011  1.975e-010   -10.431    -9.704     0.726
   SO4-2                  3.183e-011  1.617e-012   -10.497   -11.791    -1.294
   CaSO4                  6.373e-017  3.361e-016   -16.196   -15.474     0.722
   HSO4-                  3.299e-021  1.756e-020   -20.482   -19.755     0.726
   MgSO4                  1.665e-021  8.782e-021   -20.779   -20.056     0.722
   KSO4-                  7.509e-024  3.997e-023   -23.124   -22.398     0.726
   CaHSO4+                4.334e-026  2.307e-025   -25.363   -24.637     0.726
   NH4SO4-                0.000e+000  0.000e+000   -68.106   -67.380     0.726

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

      Phase               SI log IAP  log KT

      Anhydrite       -13.41  -17.75   -4.34  CaSO4
      Aragonite        -2.65  -10.96   -8.31  CaCO3
      Calcite          -2.50  -10.96   -8.45  CaCO3
      CH4(g)        -128.60 -131.42   -2.82  CH4
      CO2(g)           -6.52   -7.93   -1.41  CO2
      Dolomite         -9.56  -26.53  -16.97  CaMg(CO3)2
      Gypsum          -13.42  -18.00   -4.58  CaSO4:2H2O
      H2(g)           -37.20  -40.33   -3.13  H2
      H2O(g)           -1.76   -0.12    1.64  H2O
      H2S(g)        -137.58 -138.52   -0.94  H2S
      Halite          -11.09   -9.52    1.57  NaCl
      N2(g)           -10.58  -13.82   -3.24  N2
      NH3(g)          -58.07  -56.19    1.87  NH3
      O2(g)           -10.75  -13.60   -2.85  O2
      Sulfur         -106.31 -101.31    5.00  S

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 2.
-----------------------------------

-----------
End of run.
-----------
```

```
    Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\1-99\eqb mix 1 with calcite and co2.pqi
   Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\1-99\eqb mix 1 with calcite and co2.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          CO2(g)    -2 10
          Calcite   0 10
      SOLUTION 1
          temp      20
          pH        9.906
          pe        8.696
          redox     pe
          units     mmol/kgw
          density   1
          C         0.0009112
          Ca        7.157e-007
          Cl        2.016e-011
          K         6.444e-012
          Mg        8.198e-012
          N(5)      3.296e-010
          Na        14.44
          S(6)      6.894e-011
          water    1 # kg
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.

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

      Elements           Molality       Moles

      C                9.112e-007  9.112e-007
      Ca               7.157e-010  7.157e-010
      Cl               2.016e-014  2.016e-014
      K                6.444e-015  6.444e-015
      Mg               8.198e-015  8.198e-015
      N(5)             3.296e-013  3.296e-013
      Na               1.444e-002  1.444e-002
      S(6)             6.894e-014  6.894e-014

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

                                     pH  =   9.906
                                     pe  =   8.696
                        Activity of water  =   1.000
```

```
                    Ionic strength  =  7.250e-003
                Mass of water (kg)  =  1.000e+000
           Total alkalinity (eq/kg) =  6.174e-005
                 Total CO2 (mol/kg) =  9.112e-007
               Temperature (deg C)  =  20.000
            Electrical balance (eq) =  1.438e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) =  99.16
                         Iterations =   4
                            Total H = 1.110125e+002
                            Total O = 5.550628e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	5.983e-005	5.467e-005	-4.223	-4.262	-0.039
H+	1.344e-010	1.242e-010	-9.872	-9.906	-0.034
H2O	5.551e+001	9.998e-001	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-133.521	-133.520	0.001
C(4)	9.112e-007				
HCO3-	6.030e-007	5.533e-007	-6.220	-6.257	-0.037
CO3-2	2.648e-007	1.877e-007	-6.577	-6.727	-0.150
NaCO3-	3.908e-008	3.576e-008	-7.408	-7.447	-0.039
NaHCO3	4.108e-009	4.115e-009	-8.386	-8.386	0.001
CO2	1.653e-010	1.656e-010	-9.782	-9.781	0.001
CaCO3	1.455e-013	1.457e-013	-12.837	-12.836	0.001
CaHCO3+	3.578e-015	3.283e-015	-14.446	-14.484	-0.037
MgCO3	9.522e-019	9.538e-019	-18.021	-18.021	0.001
MgHCO3+	3.990e-020	3.651e-020	-19.399	-19.438	-0.039
Ca	7.157e-010				
Ca+2	7.148e-010	5.063e-010	-9.146	-9.296	-0.150
CaOH+	7.393e-013	6.765e-013	-12.131	-12.170	-0.039
CaCO3	1.455e-013	1.457e-013	-12.837	-12.836	0.001
CaHCO3+	3.578e-015	3.283e-015	-14.446	-14.484	-0.037
CaSO4	4.459e-021	4.467e-021	-20.351	-20.350	0.001
CaHSO4+	3.346e-030	3.062e-030	-29.475	-29.514	-0.039
Cl	2.016e-014				
Cl-	2.016e-014	1.843e-014	-13.696	-13.735	-0.039
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.333	-40.332	0.001
K	6.444e-015				
K+	6.444e-015	5.889e-015	-14.191	-14.230	-0.039
KOH	1.641e-019	1.644e-019	-18.785	-18.784	0.001
KSO4-	1.919e-027	1.756e-027	-26.717	-26.756	-0.039
Mg	8.198e-015				
Mg+2	8.081e-015	5.751e-015	-14.093	-14.240	-0.148
MgOH+	1.161e-016	1.062e-016	-15.935	-15.974	-0.039
MgCO3	9.522e-019	9.538e-019	-18.021	-18.021	0.001
MgHCO3+	3.990e-020	3.651e-020	-19.399	-19.438	-0.039
MgSO4	5.475e-026	5.484e-026	-25.262	-25.261	0.001
N(5)	3.296e-013				
NO3-	3.296e-013	3.008e-013	-12.482	-12.522	-0.040
Na	1.444e-002				
Na+	1.444e-002	1.323e-002	-1.840	-1.879	-0.038
NaOH	7.024e-007	7.035e-007	-6.153	-6.153	0.001
NaCO3-	3.908e-008	3.576e-008	-7.408	-7.447	-0.039
NaHCO3	4.108e-009	4.115e-009	-8.386	-8.386	0.001
NaSO4-	3.252e-015	2.976e-015	-14.488	-14.526	-0.039
O(0)	8.769e-014				
O2	4.385e-014	4.392e-014	-13.358	-13.357	0.001
S(6)	6.894e-014				
SO4-2	6.569e-014	4.637e-014	-13.183	-13.334	-0.151
NaSO4-	3.252e-015	2.976e-015	-14.488	-14.526	-0.039
CaSO4	4.459e-021	4.467e-021	-20.351	-20.350	0.001
HSO4-	5.497e-022	5.030e-022	-21.260	-21.298	-0.039

MgSO4	5.475e-026	5.484e-026	-25.262	-25.261	0.001
KSO4-	1.919e-027	1.756e-027	-26.717	-26.756	-0.039
CaHSO4+	3.346e-030	3.062e-030	-29.475	-29.514	-0.039

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

Phase	SI	log IAP	log KT	
Anhydrite	-18.29	-22.63	-4.34	CaSO4
Aragonite	-7.72	-16.02	-8.31	CaCO3
Calcite	-7.57	-16.02	-8.45	CaCO3
CH4(g)	-130.70	-133.52	-2.82	CH4
CO2(g)	-8.37	-9.78	-1.41	CO2
Dolomite	-20.02	-36.99	-16.97	CaMg(CO3)2
Gypsum	-18.05	-22.63	-4.58	CaSO4:2H2O
H2(g)	-37.20	-40.33	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
Halite	-17.18	-15.61	1.57	NaCl
O2(g)	-10.50	-13.36	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Calcite	0.00	-8.45	-8.45	1.000e+001	9.998e+000	-1.904e-003
CO2(g)	-2.00	-3.41	-1.41	1.000e+001	9.998e+000	-2.345e-003

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

Elements	Molality	Moles
C	4.251e-003	4.251e-003
Ca	1.904e-003	1.904e-003
Cl	2.016e-014	2.016e-014
K	6.444e-015	6.444e-015
Mg	8.198e-015	8.198e-015
N	3.296e-013	3.296e-013
Na	1.444e-002	1.444e-002
S	6.894e-014	6.894e-014

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

pH	=	7.318	Charge balance
pe	=	11.295	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	1.282e-002	
Mass of water (kg)	=	1.000e+000	
Total alkalinity (eq/kg)	=	3.871e-003	
Total CO2 (mol/kg)	=	4.251e-003	
Temperature (deg C)	=	20.000	
Electrical balance (eq)	=	1.438e-002	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	65.53	
Iterations	=	9	
Total H	=	1.110125e+002	
Total O	=	5.551668e+001	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.585e-007	1.411e-007	-6.800	-6.850	-0.051
H+	5.309e-008	4.810e-008	-7.275	-7.318	-0.043
H2O	5.551e+001	9.997e-001	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-127.234	-127.233	0.001
C(4)	4.251e-003				
HCO3-	3.772e-003	3.380e-003	-2.423	-2.471	-0.048
CO2	3.907e-004	3.919e-004	-3.408	-3.407	0.001
CaHCO3+	5.260e-005	4.713e-005	-4.279	-4.327	-0.048
NaHCO3	2.442e-005	2.449e-005	-4.612	-4.611	0.001
CaCO3	5.385e-006	5.401e-006	-5.269	-5.268	0.001
CO3-2	4.590e-006	2.960e-006	-5.338	-5.529	-0.191
NaCO3-	6.156e-007	5.493e-007	-6.211	-6.260	-0.049
MgHCO3+	2.247e-016	2.005e-016	-15.648	-15.698	-0.049
MgCO3	1.348e-017	1.352e-017	-16.870	-16.869	0.001
Ca	1.904e-003				
Ca+2	1.846e-003	1.190e-003	-2.734	-2.925	-0.191
CaHCO3+	5.260e-005	4.713e-005	-4.279	-4.327	-0.048
CaCO3	5.385e-006	5.401e-006	-5.269	-5.268	0.001
CaOH+	4.598e-009	4.104e-009	-8.337	-8.387	-0.049
CaSO4	8.379e-015	8.404e-015	-14.077	-14.076	0.001
CaHSO4+	2.501e-021	2.232e-021	-20.602	-20.651	-0.049
Cl	2.016e-014				
Cl-	2.016e-014	1.795e-014	-13.695	-13.746	-0.050
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.355	-40.354	0.001
K	6.444e-015				
K+	6.444e-015	5.738e-015	-14.191	-14.241	-0.050
KOH	4.122e-022	4.135e-022	-21.385	-21.384	0.001
KSO4-	1.535e-027	1.370e-027	-26.814	-26.863	-0.049
Mg	8.198e-015				
Mg+2	7.960e-015	5.169e-015	-14.099	-14.287	-0.187
MgHCO3+	2.247e-016	2.005e-016	-15.648	-15.698	-0.049
MgCO3	1.348e-017	1.352e-017	-16.870	-16.869	0.001
MgOH+	2.762e-019	2.464e-019	-18.559	-18.608	-0.049
MgSO4	3.935e-026	3.946e-026	-25.405	-25.404	0.001
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-54.607	-54.660	-0.052
NH3	0.000e+000	0.000e+000	-56.743	-56.742	0.001
NH4SO4-	0.000e+000	0.000e+000	-66.931	-66.980	-0.049
N(0)	2.782e-015				
N2	1.391e-015	1.395e-015	-14.857	-14.855	0.001
N(3)	2.546e-021				
NO2-	2.546e-021	2.261e-021	-20.594	-20.646	-0.051
N(5)	3.268e-013				
NO3-	3.268e-013	2.903e-013	-12.486	-12.537	-0.051
Na	1.444e-002				
Na+	1.442e-002	1.288e-002	-1.841	-1.890	-0.049
NaHCO3	2.442e-005	2.449e-005	-4.612	-4.611	0.001
NaCO3-	6.156e-007	5.493e-007	-6.211	-6.260	-0.049
NaOH	1.764e-009	1.769e-009	-8.754	-8.752	0.001
NaSO4-	2.600e-015	2.321e-015	-14.585	-14.634	-0.049
O(0)	9.677e-014				
O2	4.838e-014	4.853e-014	-13.315	-13.314	0.001
S(-2)	0.000e+000				
HS-	0.000e+000	0.000e+000	-135.198	-135.249	-0.051
H2S	0.000e+000	0.000e+000	-135.558	-135.556	0.001
S-2	0.000e+000	0.000e+000	-140.807	-141.000	-0.193
S(6)	6.894e-014				
SO4-2	5.796e-014	3.712e-014	-13.237	-13.430	-0.194
CaSO4	8.379e-015	8.404e-015	-14.077	-14.076	0.001
NaSO4-	2.600e-015	2.321e-015	-14.585	-14.634	-0.049
HSO4-	1.748e-019	1.560e-019	-18.757	-18.807	-0.049

CaHSO4+	2.501e-021	2.232e-021	-20.602	-20.651	-0.049
MgSO4	3.935e-026	3.946e-026	-25.405	-25.404	0.001
KSO4-	1.535e-027	1.370e-027	-26.814	-26.863	-0.049
NH4SO4-	0.000e+000	0.000e+000	-66.931	-66.980	-0.049

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

Phase	SI	log IAP	log KT	
Anhydrite	-12.01	-16.35	-4.34	CaSO4
Aragonite	-0.15	-8.45	-8.31	CaCO3
Calcite	0.00	-8.45	-8.45	CaCO3
CH4(g)	-124.41	-127.23	-2.82	CH4
CO2(g)	-2.00	-3.41	-1.41	CO2
Dolomite	-11.30	-28.27	-16.97	CaMg(CO3)2
Gypsum	-11.77	-16.36	-4.58	CaSO4:2H2O
H2(g)	-37.23	-40.35	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
H2S(g)	-134.62	-135.56	-0.94	H2S
Halite	-17.21	-15.64	1.57	NaCl
N2(g)	-11.61	-14.86	-3.24	N2
NH3(g)	-58.61	-56.74	1.87	NH3
O2(g)	-10.46	-13.31	-2.85	O2
Sulfur	-103.33	-98.33	5.00	S

End of simulation.

Reading input data for simulation 2.

End of run.

Run 2 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\eqb mix 2 withmontmorillonite.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\eqb mix 2 withmontmorillonite.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          Ca-Montmorillonite 0 10
      SOLUTION 1
          temp      20
          pH        7.313
          pe        11.534
          redox     pe
          units     mmol/kgw
          density   1
          C         0.004154
          Ca        0.001866
          Cl        8.124e-013
          K         2.601e-013
          Mg        3.308e-013
          N(5)      1.329e-011
          Na        0.008832
          S(6)      2.785e-012
          water    1 # kg
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.

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

      Elements           Molality       Moles

      C                4.154e-006  4.154e-006
      Ca               1.866e-006  1.866e-006
      Cl               8.124e-016  8.124e-016
      K                2.601e-016  2.601e-016
      Mg               3.308e-016  3.308e-016
      N(5)             1.329e-014  1.329e-014
      Na               8.832e-006  8.832e-006
      S(6)             2.785e-015  2.785e-015

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

                                       pH  =   7.313
                                       pe  =  11.534
                         Activity of water  =   1.000
                            Ionic strength  =  1.011e-005
```

```
                    Mass of water (kg)  =  1.000e+000
              Total alkalinity (eq/kg)  =  3.815e-006
                    Total CO2 (mol/kg)  =  4.154e-006
                  Temperature (deg C)   =  20.000
             Electrical balance (eq)    =  8.749e-006
Percent error, 100*(Cat-|An|)/(Cat+|An|) =  53.10
                             Iterations =   3
                                Total H = 1.110124e+002
                                Total O = 5.550623e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.401e-007	1.396e-007	-6.854	-6.855	-0.002
H+	4.882e-008	4.864e-008	-7.311	-7.313	-0.002
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-132.062	-132.062	0.000
C(4)	4.154e-006				
HCO3-	3.717e-006	3.703e-006	-5.430	-5.431	-0.002
CO2	4.339e-007	4.339e-007	-6.363	-6.363	0.000
CO3-2	3.254e-009	3.206e-009	-8.488	-8.494	-0.006
CaHCO3+	8.009e-011	7.980e-011	-10.096	-10.098	-0.002
NaHCO3	1.832e-011	1.832e-011	-10.737	-10.737	0.000
CaCO3	9.042e-012	9.042e-012	-11.044	-11.044	0.000
NaCO3-	4.080e-013	4.065e-013	-12.389	-12.391	-0.002
MgHCO3+	1.390e-020	1.385e-020	-19.857	-19.859	-0.002
MgCO3	9.235e-022	9.235e-022	-21.035	-21.035	0.000
Ca	1.866e-006				
Ca+2	1.866e-006	1.839e-006	-5.729	-5.735	-0.006
CaHCO3+	8.009e-011	7.980e-011	-10.096	-10.098	-0.002
CaCO3	9.042e-012	9.042e-012	-11.044	-11.044	0.000
CaOH+	6.297e-012	6.273e-012	-11.201	-11.202	-0.002
CaSO4	9.597e-019	9.597e-019	-18.018	-18.018	0.000
CaHSO4+	2.587e-025	2.577e-025	-24.587	-24.589	-0.002
Cl	8.124e-016				
Cl-	8.124e-016	8.094e-016	-15.090	-15.092	-0.002
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.822	-40.822	0.000
K	2.601e-016				
K+	2.601e-016	2.591e-016	-15.585	-15.586	-0.002
KOH	1.847e-023	1.847e-023	-22.733	-22.733	0.000
KSO4-	4.588e-030	4.571e-030	-29.338	-29.340	-0.002
Mg	3.308e-016				
Mg+2	3.308e-016	3.259e-016	-15.480	-15.487	-0.006
MgOH+	1.543e-020	1.537e-020	-19.812	-19.813	-0.002
MgHCO3+	1.390e-020	1.385e-020	-19.857	-19.859	-0.002
MgCO3	9.235e-022	9.235e-022	-21.035	-21.035	0.000
MgSO4	1.839e-028	1.839e-028	-27.735	-27.735	0.000
N(5)	1.329e-014				
NO3-	1.329e-014	1.324e-014	-13.876	-13.878	-0.002
Na	8.832e-006				
Na+	8.832e-006	8.800e-006	-5.054	-5.056	-0.002
NaHCO3	1.832e-011	1.832e-011	-10.737	-10.737	0.000
NaOH	1.195e-012	1.195e-012	-11.923	-11.923	0.000
NaCO3-	4.080e-013	4.065e-013	-12.389	-12.391	-0.002
NaSO4-	1.176e-019	1.171e-019	-18.930	-18.931	-0.002
O(0)	8.393e-013				
O2	4.196e-013	4.196e-013	-12.377	-12.377	0.000
S(6)	2.785e-015				
SO4-2	2.784e-015	2.743e-015	-14.555	-14.562	-0.006
CaSO4	9.597e-019	9.597e-019	-18.018	-18.018	0.000
NaSO4-	1.176e-019	1.171e-019	-18.930	-18.931	-0.002
HSO4-	1.170e-020	1.166e-020	-19.932	-19.933	-0.002
CaHSO4+	2.587e-025	2.577e-025	-24.587	-24.589	-0.002

MgSO4	1.839e-028	1.839e-028	-27.735	-27.735	0.000
KSO4-	4.588e-030	4.571e-030	-29.338	-29.340	-0.002

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

Phase	SI	log IAP	log KT	
Anhydrite	-15.95	-20.30	-4.34	CaSO4
Aragonite	-5.92	-14.23	-8.31	CaCO3
Calcite	-5.78	-14.23	-8.45	CaCO3
CH4(g)	-129.24	-132.06	-2.82	CH4
CO2(g)	-4.96	-6.36	-1.41	CO2
Dolomite	-21.24	-38.21	-16.97	CaMg(CO3)2
Gypsum	-15.72	-20.30	-4.58	CaSO4:2H2O
H2(g)	-37.69	-40.82	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
Halite	-21.72	-20.15	1.57	NaCl
O2(g)	-9.52	-12.38	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca-Montmorillonite	0.00	-45.76	-45.76	1.000e+001	1.000e+001	-2.061e-006

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

Elements	Molality	Moles
Al	4.802e-006	4.802e-006
C	4.154e-006	4.154e-006
Ca	2.206e-006	2.206e-006
Cl	8.124e-016	8.124e-016
K	2.601e-016	2.601e-016
Mg	3.308e-016	3.308e-016
N	1.329e-014	1.329e-014
Na	8.832e-006	8.832e-006
S	2.785e-015	2.785e-015
Si	7.563e-006	7.563e-006

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

```
                                    pH  =   6.617      Charge balance
                                    pe  =  12.232      Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  1.255e-005
                   Mass of water (kg)   =  1.000e+000
            Total alkalinity (eq/kg)    =  1.890e-005
                   Total CO2 (mol/kg)   =  4.154e-006
                  Temperature (deg C)   =  20.000
             Electrical balance (eq)    =  8.749e-006
Percent error, 100*(Cat-|An|)/(Cat+|An|) =  42.54
                             Iterations =   9
                                Total H = 1.110124e+002
                                Total O = 5.550625e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.427e-007	2.417e-007	-6.615	-6.617	-0.002
OH-	2.821e-008	2.809e-008	-7.550	-7.551	-0.002
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Al	4.802e-006				
Al(OH)4-	3.246e-006	3.233e-006	-5.489	-5.490	-0.002
Al(OH)2+	1.061e-006	1.057e-006	-5.974	-5.976	-0.002
Al(OH)3	4.405e-007	4.405e-007	-6.356	-6.356	0.000
AlOH+2	5.195e-008	5.110e-008	-7.284	-7.292	-0.007
Al+3	1.792e-009	1.727e-009	-8.747	-8.763	-0.016
AlSO4+	1.406e-020	1.400e-020	-19.852	-19.854	-0.002
AlHSO4+2	2.928e-028	2.880e-028	-27.533	-27.541	-0.007
Al(SO4)2-	1.189e-033	1.184e-033	-32.925	-32.927	-0.002
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-131.527	-131.527	0.000
C(4)	4.154e-006				
HCO3-	2.629e-006	2.618e-006	-5.580	-5.582	-0.002
CO2	1.524e-006	1.524e-006	-5.817	-5.817	0.000
CO3-2	4.638e-010	4.563e-010	-9.334	-9.341	-0.007
CaHCO3+	6.687e-011	6.659e-011	-10.175	-10.177	-0.002
NaHCO3	1.295e-011	1.295e-011	-10.888	-10.888	0.000
CaCO3	1.519e-012	1.519e-012	-11.819	-11.819	0.000
NaCO3-	5.806e-014	5.782e-014	-13.236	-13.238	-0.002
MgHCO3+	9.816e-021	9.776e-021	-20.008	-20.010	-0.002
MgCO3	1.312e-022	1.312e-022	-21.882	-21.882	0.000
Ca	2.206e-006				
Ca+2	2.206e-006	2.170e-006	-5.656	-5.664	-0.007
CaHCO3+	6.687e-011	6.659e-011	-10.175	-10.177	-0.002
CaCO3	1.519e-012	1.519e-012	-11.819	-11.819	0.000
CaOH+	1.496e-012	1.490e-012	-11.825	-11.827	-0.002
CaSO4	1.131e-018	1.131e-018	-17.947	-17.947	0.000
CaHSO4+	1.515e-024	1.509e-024	-23.820	-23.821	-0.002
Cl	8.124e-016				
Cl-	8.124e-016	8.091e-016	-15.090	-15.092	-0.002
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.825	-40.825	0.000
K	2.601e-016				
K+	2.601e-016	2.590e-016	-15.585	-15.587	-0.002
KOH	3.717e-024	3.717e-024	-23.430	-23.430	0.000
KSO4-	4.580e-030	4.561e-030	-29.339	-29.341	-0.002
Mg	3.308e-016				
Mg+2	3.308e-016	3.254e-016	-15.480	-15.488	-0.007
MgHCO3+	9.816e-021	9.776e-021	-20.008	-20.010	-0.002
MgOH+	3.101e-021	3.089e-021	-20.508	-20.510	-0.002
MgCO3	1.312e-022	1.312e-022	-21.882	-21.882	0.000
MgSO4	1.833e-028	1.833e-028	-27.737	-27.737	0.000
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-56.482	-56.483	-0.002
NH3	0.000e+000	0.000e+000	-59.267	-59.267	0.000
NH4SO4-	0.000e+000	0.000e+000	-69.934	-69.936	-0.002
N(0)	6.446e-019				
N2	3.223e-019	3.223e-019	-18.492	-18.492	0.000
N(3)	3.498e-023				
NO2-	3.498e-023	3.484e-023	-22.456	-22.458	-0.002
N(5)	1.329e-014				
NO3-	1.329e-014	1.323e-014	-13.876	-13.878	-0.002
Na	8.832e-006				
Na+	8.832e-006	8.796e-006	-5.054	-5.056	-0.002
NaHCO3	1.295e-011	1.295e-011	-10.888	-10.888	0.000
NaOH	2.405e-013	2.405e-013	-12.619	-12.619	0.000
NaCO3-	5.806e-014	5.782e-014	-13.236	-13.238	-0.002
NaSO4-	1.174e-019	1.169e-019	-18.930	-18.932	-0.002
O(0)	8.500e-013				
O2	4.250e-013	4.250e-013	-12.372	-12.372	0.000

S(-2)	0.000e+000					
H2S		0.000e+000	0.000e+000	-137.171	-137.171	0.000
HS-		0.000e+000	0.000e+000	-137.563	-137.564	-0.002
S-2		0.000e+000	0.000e+000	-144.010	-144.017	-0.007
S(6)	2.785e-015					
SO4-2		2.784e-015	2.738e-015	-14.555	-14.562	-0.007
CaSO4		1.131e-018	1.131e-018	-17.947	-17.947	0.000
NaSO4-		1.174e-019	1.169e-019	-18.930	-18.932	-0.002
HSO4-		5.806e-020	5.782e-020	-19.236	-19.238	-0.002
AlSO4+		1.406e-020	1.400e-020	-19.852	-19.854	-0.002
CaHSO4+		1.515e-024	1.509e-024	-23.820	-23.821	-0.002
AlHSO4+2		2.928e-028	2.880e-028	-27.533	-27.541	-0.007
MgSO4		1.833e-028	1.833e-028	-27.737	-27.737	0.000
KSO4-		4.580e-030	4.561e-030	-29.339	-29.341	-0.002
Al(SO4)2-		1.189e-033	1.184e-033	-32.925	-32.927	-0.002
NH4SO4-		0.000e+000	0.000e+000	-69.934	-69.936	-0.002
Si	7.563e-006					
H4SiO4		7.559e-006	7.559e-006	-5.122	-5.122	0.000
H3SiO4-		3.869e-009	3.854e-009	-8.412	-8.414	-0.002
H2SiO4-2		7.884e-016	7.756e-016	-15.103	-15.110	-0.007

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

Phase	SI	log IAP	log KT	
Al(OH)3(a)	-0.04	11.09	11.13	Al(OH)3
Albite	-7.58	-25.91	-18.33	NaAlSi3O8
Alunite	-30.53	-31.30	-0.77	KAl3(SO4)2(OH)6
Anhydrite	-15.88	-20.23	-4.34	CaSO4
Anorthite	-7.03	-26.89	-19.86	CaAl2Si2O8
Aragonite	-6.70	-15.00	-8.31	CaCO3
Ca-Montmorillonite	0.00	-45.76	-45.76	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-6.55	-15.00	-8.45	CaCO3
CH4(g)	-128.71	-131.53	-2.82	CH4
Chalcedony	-1.51	-5.12	-3.61	SiO2
Chlorite(14A)	-74.73	-4.46	70.27	Mg5Al2Si3O10(OH)8
Chrysotile	-49.84	-17.01	32.83	Mg3Si2O5(OH)4
CO2(g)	-4.41	-5.82	-1.41	CO2
Dolomite	-22.86	-39.83	-16.97	CaMg(CO3)2
Gibbsite	2.69	11.09	8.40	Al(OH)3
Gypsum	-15.64	-20.23	-4.58	CaSO4:2H2O
H2(g)	-37.70	-40.82	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
H2S(g)	-136.23	-137.17	-0.94	H2S
Halite	-21.72	-20.15	1.57	NaCl
Illite	-10.77	-51.72	-40.95	K0.6Mg0.25Al2.3Si3.5O10(OH)2
K-feldspar	-15.48	-36.44	-20.96	KAlSi3O8
K-mica	-4.52	8.93	13.45	KAl3Si3O10(OH)2
Kaolinite	4.06	11.93	7.88	Al2Si2O5(OH)4
N2(g)	-15.25	-18.49	-3.24	N2
NH3(g)	-61.14	-59.27	1.87	NH3
O2(g)	-9.52	-12.37	-2.85	O2
Quartz	-1.07	-5.12	-4.06	SiO2
Sepiolite	-35.77	-19.87	15.89	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-38.53	-19.87	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-2.37	-5.12	-2.75	SiO2
Sulfur	-104.48	-99.47	5.00	S
Talc	-49.23	-27.25	21.98	Mg3Si4O10(OH)2

End of simulation.

Reading input data for simulation 2.

```
-----------
End of run.
-----------
```

Run 3

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\10%rainwater+90%NaOH.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\10%rainwater+90%NaOH.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          CO2(g)    -3.5 10
      SOLUTION 1 rainwater
          temp      25
          pH        5.24
          pe        4
          redox     pe
          units     mg/l
          density   1
          Ca        0.458
          Mg        0.034
          Na        0.082
          K         0.043
          Cl        0.122
          S(6)      1.131
          N(5)      1.004
          N(-3)     0.36
          water    1 # kg
      SOLUTION 2 NaOH
          temp      20
          pH        14
          pe        4
          redox     pe
          units     mmol/kgw
          density   1
          Na        24.9 mol/kgw
          water    1 # kg
      MIX 1
          1    0.1
          2    0.9
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.     rainwater

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

      Elements           Molality       Moles

      Ca                1.143e-005  1.143e-005
      Cl                3.441e-006  3.441e-006
      K                 1.100e-006  1.100e-006
```

Mg	1.398e-006	1.398e-006
N(-3)	2.570e-005	2.570e-005
N(5)	7.168e-005	7.168e-005
Na	3.567e-006	3.567e-006
S(6)	1.177e-005	1.177e-005

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

```
                                    pH  =   5.240
                                    pe  =   4.000
                     Activity of water  =   1.000
                        Ionic strength  =  1.047e-004
                   Mass of water (kg)   =  1.000e+000
            Total alkalinity (eq/kg)    = -5.824e-006
               Total carbon (mol/kg)    =  0.000e+000
                  Total CO2 (mol/kg)    =  0.000e+000
                 Temperature (deg C)    =  25.000
             Electrical balance (eq)    = -3.682e-005
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -22.96
                            Iterations  =   3
                               Total H  = 1.110125e+002
                               Total O  = 5.550648e+001
```

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

Redox couple	pe	Eh (volts)
N(-3)/N(5)	8.3903	0.4963

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	5.822e-006	5.754e-006	-5.235	-5.240	-0.005
OH-	1.760e-009	1.740e-009	-8.754	-8.760	-0.005
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Ca	1.143e-005				
Ca+2	1.140e-005	1.088e-005	-4.943	-4.963	-0.020
CaSO4	2.429e-008	2.429e-008	-7.614	-7.614	0.000
CaHSO4+	8.288e-013	8.190e-013	-12.082	-12.087	-0.005
CaOH+	3.174e-013	3.137e-013	-12.498	-12.503	-0.005
Cl	3.441e-006				
Cl-	3.441e-006	3.401e-006	-5.463	-5.468	-0.005
H(0)	4.688e-022				
H2	2.344e-022	2.344e-022	-21.630	-21.630	0.000
K	1.100e-006				
K+	1.100e-006	1.087e-006	-5.959	-5.964	-0.005
KSO4-	8.649e-011	8.547e-011	-10.063	-10.068	-0.005
KOH	6.547e-016	6.548e-016	-15.184	-15.184	0.000
Mg	1.398e-006				
Mg+2	1.395e-006	1.331e-006	-5.855	-5.876	-0.020
MgSO4	3.492e-009	3.492e-009	-8.457	-8.457	0.000
MgOH+	8.497e-013	8.397e-013	-12.071	-12.076	-0.005
N(-3)	2.570e-005				
NH4+	2.570e-005	2.539e-005	-4.590	-4.595	-0.005
NH4SO4-	3.705e-009	3.662e-009	-8.431	-8.436	-0.005
NH3	2.515e-009	2.515e-009	-8.600	-8.600	0.000
N(5)	7.168e-005				
NO3-	7.168e-005	7.083e-005	-4.145	-4.150	-0.005
Na	3.567e-006				
Na+	3.567e-006	3.525e-006	-5.448	-5.453	-0.005
NaSO4-	2.001e-010	1.977e-010	-9.699	-9.704	-0.005
NaOH	4.047e-015	4.047e-015	-14.393	-14.393	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-49.120	-49.120	0.000
S(6)	1.177e-005				

SO4-2	1.174e-005	1.119e-005	-4.931	-4.951	-0.021
CaSO4	2.429e-008	2.429e-008	-7.614	-7.614	0.000
HSO4-	6.337e-009	6.263e-009	-8.198	-8.203	-0.005
NH4SO4-	3.705e-009	3.662e-009	-8.431	-8.436	-0.005
MgSO4	3.492e-009	3.492e-009	-8.457	-8.457	0.000
NaSO4-	2.001e-010	1.977e-010	-9.699	-9.704	-0.005
KSO4-	8.649e-011	8.547e-011	-10.063	-10.068	-0.005
CaHSO4+	8.288e-013	8.190e-013	-12.082	-12.087	-0.005

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

Phase	SI	log IAP	log KT	
Anhydrite	-5.55	-9.91	-4.36	CaSO4
Gypsum	-5.33	-9.91	-4.58	CaSO4:2H2O
H2(g)	-18.48	-21.63	-3.15	H2
H2O(g)	-1.51	-0.00	1.51	H2O
Halite	-12.50	-10.92	1.58	NaCl
NH3(g)	-10.37	-8.60	1.77	NH3
O2(g)	-46.23	-49.12	-2.89	O2

Initial solution 2. NaOH

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

Elements	Molality	Moles
Na	2.490e+001	2.490e+001

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

pH	=	14.000
pe	=	4.000
Activity of water	=	0.562
Ionic strength	=	1.184e+001
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	2.931e+000
Total carbon (mol/kg)	=	0.000e+000
Total CO2 (mol/kg)	=	0.000e+000
Temperature (deg C)	=	20.000
Electrical balance (eq)	=	2.197e+001
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	92.76
Iterations	=	6
Total H	=	1.139431e+002
Total O	=	5.843693e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	8.574e-001	3.816e-001	-0.067	-0.418	-0.352
H+	1.432e-014	1.000e-014	-13.844	-14.000	-0.156
H2O	5.551e+001	5.621e-001	1.744	-0.250	0.000
H(0)	0.000e+000				
H2	0.000e+000	7.447e-040	-40.312	-39.128	1.184
Na	2.490e+001				
Na+	2.283e+001	8.532e+001	1.358	1.931	0.573
NaOH	2.073e+000	3.169e+001	0.317	1.501	1.184
O(0)	7.102e-018				
O2	3.551e-018	5.427e-017	-17.450	-16.265	1.184

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

Phase	SI	log IAP	log KT	
H2(g)	-36.00	-39.13	-3.13	H2

```
      H2O(g)            -1.89   -0.25    1.64  H2O
      O2(g)            -13.41  -16.27   -2.85  O2

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

 Reaction step 1.

 Using mix 1.
 Using pure phase assemblage 1.

 Mixture 1.

       1.000e-001 Solution 1  rainwater
       9.000e-001 Solution 2  NaOH

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

                                                        Moles in assemblage
 Phase                  SI log IAP  log KT      Initial       Final       Delta

 CO2(g)              -3.50   -4.91   -1.41   1.000e+001  8.588e+000 -1.412e+000

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

      Elements           Molality       Moles

      C                1.382e+000  1.412e+000
      Ca               1.118e-006  1.143e-006
      Cl               3.367e-007  3.441e-007
      K                1.076e-007  1.100e-007
      Mg               1.368e-007  1.398e-007
      N                9.528e-006  9.738e-006
      Na               2.193e+001  2.241e+001
      S                1.152e-006  1.177e-006

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

                                      pH  =  10.088      Charge balance
                                      pe  =   8.402      Adjusted to redox equilibrium
                         Activity of water  =   0.623
                            Ionic strength  =  1.133e+001
                       Mass of water (kg)   =  1.022e+000
                 Total alkalinity (eq/kg)   =  2.581e+000
                       Total CO2 (mol/kg)   =  1.382e+000
                     Temperature (deg C)    =  20.500
                  Electrical balance (eq)   =  1.977e+001
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   =  86.89
                                Iterations  =  24
                                   Total H  = 1.136501e+002
                                   Total O  = 6.096855e+001

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

                                                   Log        Log         Log
   Species                Molality    Activity  Molality  Activity     Gamma

   OH-                  1.206e-004  5.383e-005    -3.919    -4.269    -0.350
   H+                   1.170e-010  8.174e-011    -9.932   -10.088    -0.156
   H2O                  5.551e+001  6.228e-001     1.744    -0.206     0.000
C(-4)           0.000e+000
   CH4                  0.000e+000  0.000e+000  -128.547  -127.415     1.133
C(4)            1.382e+000
   NaCO3-               1.005e+000  2.139e+001     0.002     1.330     1.328
   CO3-2                1.931e-001  2.028e-002    -0.714    -1.693    -0.979
   NaHCO3               1.150e-001  1.561e+000    -0.939     0.193     1.133
```

HCO3-	6.837e-002	3.892e-002	-1.165	-1.410	-0.245
CO2	9.000e-007	1.221e-005	-6.046	-4.913	1.133
CaCO3	7.902e-007	1.072e-005	-6.102	-4.970	1.133
CaHCO3+	2.765e-007	1.574e-007	-6.558	-6.803	-0.245
MgCO3	1.298e-007	1.762e-006	-6.887	-5.754	1.133
MgHCO3+	2.051e-009	4.363e-008	-8.688	-7.360	1.328
Ca	1.118e-006				
CaCO3	7.902e-007	1.072e-005	-6.102	-4.970	1.133
CaHCO3+	2.765e-007	1.574e-007	-6.558	-6.803	-0.245
Ca+2	5.129e-008	3.419e-007	-7.290	-6.466	0.824
CaOH+	2.032e-011	4.323e-010	-10.692	-9.364	1.328
CaSO4	1.161e-013	1.576e-012	-12.935	-11.803	1.133
CaHSO4+	3.360e-023	7.150e-022	-22.474	-21.146	1.328
Cl	3.367e-007				
Cl-	3.367e-007	2.223e-007	-6.473	-6.653	-0.180
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-41.243	-40.110	1.133
K	1.076e-007				
K+	1.076e-007	7.105e-008	-6.968	-7.148	-0.180
KOH	1.383e-013	1.877e-012	-12.859	-11.727	1.133
KSO4-	5.222e-016	1.111e-014	-15.282	-13.954	1.328
Mg	1.368e-007				
MgCO3	1.298e-007	1.762e-006	-6.887	-5.754	1.133
Mg+2	4.868e-009	9.754e-008	-8.313	-7.011	1.302
MgHCO3+	2.051e-009	4.363e-008	-8.688	-7.360	1.328
MgOH+	8.395e-011	1.786e-009	-10.076	-8.748	1.328
MgSO4	3.610e-014	4.899e-013	-13.442	-12.310	1.133
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-51.502	-51.954	-0.453
NH3	0.000e+000	0.000e+000	-52.384	-51.251	1.133
NH4SO4-	0.000e+000	0.000e+000	-59.790	-58.462	1.328
N(0)	4.024e-006				
N2	2.012e-006	2.730e-005	-5.696	-4.564	1.133
N(3)	1.066e-013				
NO2-	1.066e-013	4.295e-014	-12.972	-13.367	-0.395
N(5)	5.504e-006				
NO3-	5.504e-006	2.217e-006	-5.259	-5.654	-0.395
Na	2.193e+001				
Na+	2.081e+001	7.131e+001	1.318	1.853	0.535
NaCO3-	1.005e+000	2.139e+001	0.002	1.330	1.328
NaHCO3	1.150e-001	1.561e+000	-0.939	0.193	1.133
NaOH	2.646e-004	3.590e-003	-3.577	-2.445	1.133
NaSO4-	3.933e-007	8.369e-006	-6.405	-5.077	1.328
O(0)	1.328e-015				
O2	6.639e-016	9.010e-015	-15.178	-14.045	1.133
S(-2)	0.000e+000				
HS-	0.000e+000	0.000e+000	-130.127	-130.477	-0.350
S-2	0.000e+000	0.000e+000	-132.399	-133.444	-1.045
H2S	0.000e+000	0.000e+000	-134.695	-133.562	1.133
S(6)	1.152e-006				
SO4-2	7.586e-007	2.410e-008	-6.120	-7.618	-1.498
NaSO4-	3.933e-007	8.369e-006	-6.405	-5.077	1.328
CaSO4	1.161e-013	1.576e-012	-12.935	-11.803	1.133
MgSO4	3.610e-014	4.899e-013	-13.442	-12.310	1.133
KSO4-	5.222e-016	1.111e-014	-15.282	-13.954	1.328
HSO4-	8.176e-018	1.739e-016	-17.087	-15.760	1.328
CaHSO4+	3.360e-023	7.150e-022	-22.474	-21.146	1.328
NH4SO4-	0.000e+000	0.000e+000	-59.790	-58.462	1.328

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

Phase	SI	log IAP	log KT	
Anhydrite	-9.74	-14.08	-4.35	CaSO4
Aragonite	0.15	-8.16	-8.31	CaCO3
Calcite	0.30	-8.16	-8.46	CaCO3
CH4(g)	-124.59	-127.41	-2.82	CH4

```
CO2(g)            -3.50   -4.91   -1.41  CO2
Dolomite           0.12  -16.86  -16.98  CaMg(CO3)2
Gypsum            -9.91  -14.50   -4.58  CaSO4:2H2O
H2(g)            -36.98  -40.11   -3.13  H2
H2O(g)            -1.83   -0.21    1.63  H2O
H2S(g)          -132.62 -133.56   -0.95  H2S
Halite            -6.37   -4.80    1.57  NaCl
N2(g)             -1.32   -4.56   -3.24  N2
NH3(g)           -53.11  -51.25    1.86  NH3
O2(g)            -11.19  -14.05   -2.86  O2
Sulfur          -101.57  -96.58    4.99  S

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 2.
------------------------------------

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End of run.
-----------
```

Run 3 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\mix 10-90rain NaOH + calcite GW.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\mix 10-90rain NaOH + calcite GW.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-------------------------------------
Reading input data for simulation 1.
-------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      MIX 1
          1    0.1
          2    0.9
      SOLUTION 1
          temp      25
          pH        10.088
          pe        8.273
          redox     pe
          units     mmol/kgw
          density   1
          C         1.516
          Ca        1.116e-007
          Cl        3.36e-008
          K         1.074e-008
          Mg        1.365e-008
          N(5)      5.493e-007
          Na        24.07
          S(6)      1.149e-007
          water    1 # kg
      SOLUTION 2
          temp      20
          pH        7.301
          pe        -1.841
          redox     pe
          units     mmol/kgw
          density   1
          C         0.003961
          Ca        0.001789
          water    1 # kg
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

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

      Elements           Molality       Moles

      C                 1.516e-003  1.516e-003
      Ca                1.116e-010  1.116e-010
      Cl                3.360e-011  3.360e-011
      K                 1.074e-011  1.074e-011
```

Mg	1.365e-011	1.365e-011
N(5)	5.493e-010	5.493e-010
Na	2.407e-002	2.407e-002
S(6)	1.149e-010	1.149e-010

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

pH	=	10.088
pe	=	8.273
Activity of water	=	1.000
Ionic strength	=	1.367e-002
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	2.423e-003
Total CO2 (mol/kg)	=	1.516e-003
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	2.165e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	82.83
Iterations	=	5
Total H	=	1.110133e+002
Total O	=	5.551090e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.383e-004	1.225e-004	-3.859	-3.912	-0.052
H+	9.042e-011	8.166e-011	-10.044	-10.088	-0.044
H2O	5.551e+001	9.996e-001	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-129.414	-129.413	0.001
C(4)	1.516e-003				
HCO3-	7.407e-004	6.612e-004	-3.130	-3.180	-0.049
CO3-2	5.981e-004	3.797e-004	-3.223	-3.421	-0.197
NaCO3-	1.692e-004	1.504e-004	-3.772	-3.823	-0.051
NaHCO3	7.882e-006	7.907e-006	-5.103	-5.102	0.001
CO2	1.211e-007	1.215e-007	-6.917	-6.916	0.001
CaCO3	3.192e-011	3.202e-011	-10.496	-10.495	0.001
MgCO3	2.487e-012	2.495e-012	-11.604	-11.603	0.001
CaHCO3+	4.743e-013	4.234e-013	-12.324	-12.373	-0.049
MgHCO3+	5.993e-014	5.326e-014	-13.222	-13.274	-0.051
Ca	1.116e-010				
Ca+2	7.910e-011	5.019e-011	-10.102	-10.299	-0.198
CaCO3	3.192e-011	3.202e-011	-10.496	-10.495	0.001
CaHCO3+	4.743e-013	4.234e-013	-12.324	-12.373	-0.049
CaOH+	1.147e-013	1.020e-013	-12.940	-12.992	-0.051
CaSO4	6.723e-019	6.744e-019	-18.172	-18.171	0.001
CaHSO4+	3.630e-028	3.226e-028	-27.440	-27.491	-0.051
Cl	3.360e-011				
Cl-	3.360e-011	2.979e-011	-10.474	-10.526	-0.052
H(0)	2.677e-040				
H2	1.339e-040	1.343e-040	-39.873	-39.872	0.001
K	1.074e-011				
K+	1.074e-011	9.522e-012	-10.969	-11.021	-0.052
KOH	4.029e-016	4.041e-016	-15.395	-15.393	0.001
KSO4-	5.070e-021	4.506e-021	-20.295	-20.346	-0.051
Mg	1.365e-011				
Mg+2	1.076e-011	6.884e-012	-10.968	-11.162	-0.194
MgCO3	2.487e-012	2.495e-012	-11.604	-11.603	0.001
MgOH+	3.443e-013	3.060e-013	-12.463	-12.514	-0.051
MgHCO3+	5.993e-014	5.326e-014	-13.222	-13.274	-0.051
MgSO4	1.083e-019	1.087e-019	-18.965	-18.964	0.001
N(5)	5.493e-010				
NO3-	5.493e-010	4.858e-010	-9.260	-9.314	-0.053
Na	2.407e-002				
Na+	2.389e-002	2.126e-002	-1.622	-1.672	-0.051
NaCO3-	1.692e-004	1.504e-004	-3.772	-3.823	-0.051

```
   NaHCO3                 7.882e-006  7.907e-006    -5.103    -5.102     0.001
   NaOH                   1.714e-006  1.720e-006    -5.766    -5.765     0.001
   NaSO4-                 8.076e-012  7.177e-012   -11.093   -11.144    -0.051
O(0)             4.606e-013
   O2                     2.303e-013  2.310e-013   -12.638   -12.636     0.001
S(6)             1.149e-010
   SO4-2                  1.068e-010  6.735e-011    -9.971   -10.172    -0.200
   NaSO4-                 8.076e-012  7.177e-012   -11.093   -11.144    -0.051
   CaSO4                  6.723e-019  6.744e-019   -18.172   -18.171     0.001
   HSO4-                  6.016e-019  5.347e-019   -18.221   -18.272    -0.051
   MgSO4                  1.083e-019  1.087e-019   -18.965   -18.964     0.001
   KSO4-                  5.070e-021  4.506e-021   -20.295   -20.346    -0.051
   CaHSO4+                3.630e-028  3.226e-028   -27.440   -27.491    -0.051

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

      Phase               SI log IAP  log KT

      Anhydrite       -16.11  -20.47   -4.36  CaSO4
      Aragonite        -5.38  -13.72   -8.34  CaCO3
      Calcite          -5.24  -13.72   -8.48  CaCO3
      CH4(g)        -126.55 -129.41   -2.86  CH4
      CO2(g)           -5.45   -6.92   -1.47  CO2
      Dolomite        -11.21  -28.30  -17.09  CaMg(CO3)2
      Gypsum          -15.89  -20.47   -4.58  CaSO4:2H2O
      H2(g)           -36.72  -39.87   -3.15  H2
      H2O(g)           -1.51   -0.00    1.51  H2O
      Halite          -13.78  -12.20    1.58  NaCl
      O2(g)            -9.74  -12.64   -2.89  O2

Initial solution 2.

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

      Elements           Molality       Moles

      C                3.961e-006  3.961e-006
      Ca               1.789e-006  1.789e-006

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

                                       pH  =   7.301
                                       pe  =  -1.841
                         Activity of water  =   1.000
                            Ionic strength  =  5.444e-006
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  3.626e-006
                       Total CO2 (mol/kg)   =  3.961e-006
                      Temperature (deg C)   =  20.000
                  Electrical balance (eq)   = -4.751e-008
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   =  -0.65
                                Iterations  =   3
                                   Total H  = 1.110124e+002
                                   Total O  = 5.550623e+001

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

                                                  Log       Log        Log
   Species                 Molality    Activity  Molality  Activity   Gamma

   OH-                   1.361e-007  1.358e-007    -6.866    -6.867    -0.001
   H+                    5.014e-008  5.000e-008    -7.300    -7.301    -0.001
   H2O                   5.551e+001  1.000e+000     1.744    -0.000     0.000
C(-4)            1.058e-025
   CH4                   1.058e-025  1.058e-025   -24.975   -24.975     0.000
C(4)             3.961e-006
   HCO3-                 3.533e-006  3.524e-006    -5.452    -5.453    -0.001
```

```
    CO2                     4.245e-007  4.245e-007    -6.372    -6.372     0.000
    CO3-2                   3.000e-009  2.968e-009    -8.523    -8.528    -0.005
    CaHCO3+                 7.328e-011  7.309e-011   -10.135   -10.136    -0.001
    CaCO3                   8.056e-012  8.056e-012   -11.094   -11.094     0.000
 Ca                 1.789e-006
    Ca+2                    1.789e-006  1.770e-006    -5.747    -5.752    -0.005
    CaHCO3+                 7.328e-011  7.309e-011   -10.135   -10.136    -0.001
    CaCO3                   8.056e-012  8.056e-012   -11.094   -11.094     0.000
    CaOH+                   5.889e-012  5.873e-012   -11.230   -11.231    -0.001
 H(0)               1.791e-014
    H2                      8.953e-015  8.953e-015   -14.048   -14.048     0.000
 O(0)               0.000e+000
    O2                      0.000e+000  0.000e+000   -65.925   -65.925     0.000

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

      Phase               SI log IAP  log KT

      Aragonite        -5.97  -14.28   -8.31  CaCO3
      Calcite          -5.83  -14.28   -8.45  CaCO3
      CH4(g)          -22.16  -24.98   -2.82  CH4
      CO2(g)           -4.97   -6.37   -1.41  CO2
      H2(g)           -10.92  -14.05   -3.13  H2
      H2O(g)           -1.64   -0.00    1.64  H2O
      O2(g)           -63.07  -65.93   -2.85  O2

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

 Reaction step 1.

 Using mix 1.

 Mixture 1.

       1.000e-001 Solution 1
       9.000e-001 Solution 2

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

      Elements           Molality       Moles

      C                1.552e-004  1.552e-004
      Ca               1.610e-006  1.610e-006
      Cl               3.360e-012  3.360e-012
      K                1.074e-012  1.074e-012
      Mg               1.365e-012  1.365e-012
      N                5.493e-011  5.493e-011
      Na               2.407e-003  2.407e-003
      S                1.149e-011  1.149e-011

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

                                      pH  =   9.839      Charge balance
                                      pe  =   8.649      Adjusted to redox equilibrium
                         Activity of water  =   1.000
                            Ionic strength  =  1.366e-003
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  2.456e-004
                       Total CO2 (mol/kg)   =  1.552e-004
                     Temperature (deg C)    =  20.500
                  Electrical balance (eq)   =  2.165e-003
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   =  81.60
                                Iterations  =  20
                                   Total H  = 1.110125e+002
                                   Total O  = 5.550670e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	5.081e-005	4.875e-005	-4.294	-4.312	-0.018
H+	1.506e-010	1.449e-010	-9.822	-9.839	-0.017
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-130.308	-130.308	0.000
C(4)	1.552e-004				
HCO3-	1.154e-004	1.109e-004	-3.938	-3.955	-0.018
CO3-2	3.831e-005	3.260e-005	-4.417	-4.487	-0.070
NaCO3-	1.160e-006	1.113e-006	-5.936	-5.953	-0.018
NaHCO3	1.439e-007	1.440e-007	-6.842	-6.842	0.000
CaCO3	6.604e-008	6.606e-008	-7.180	-7.180	0.000
CO2	3.840e-008	3.841e-008	-7.416	-7.416	0.000
CaHCO3+	1.790e-009	1.719e-009	-8.747	-8.765	-0.018
MgCO3	3.241e-014	3.242e-014	-13.489	-13.489	0.000
MgHCO3+	1.483e-015	1.423e-015	-14.829	-14.847	-0.018
Ca	1.610e-006				
Ca+2	1.541e-006	1.311e-006	-5.812	-5.883	-0.070
CaCO3	6.604e-008	6.606e-008	-7.180	-7.180	0.000
CaHCO3+	1.790e-009	1.719e-009	-8.747	-8.765	-0.018
CaOH+	1.564e-009	1.501e-009	-8.806	-8.824	-0.018
CaSO4	2.422e-015	2.423e-015	-14.616	-14.616	0.000
CaHSO4+	2.031e-024	1.949e-024	-23.692	-23.710	-0.018
Cl	3.360e-012				
Cl-	3.360e-012	3.224e-012	-11.474	-11.492	-0.018
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.105	-40.105	0.000
K	1.074e-012				
K+	1.074e-012	1.031e-012	-11.969	-11.987	-0.018
KOH	2.465e-017	2.466e-017	-16.608	-16.608	0.000
KSO4-	6.736e-023	6.465e-023	-22.172	-22.189	-0.018
Mg	1.365e-012				
Mg+2	1.312e-012	1.117e-012	-11.882	-11.952	-0.070
MgCO3	3.241e-014	3.242e-014	-13.489	-13.489	0.000
MgOH+	1.930e-014	1.853e-014	-13.714	-13.732	-0.018
MgHCO3+	1.483e-015	1.423e-015	-14.829	-14.847	-0.018
MgSO4	2.250e-021	2.251e-021	-20.648	-20.648	0.000
N(-3)	0.000e+000				
NH3	0.000e+000	0.000e+000	-56.223	-56.223	0.000
NH4+	0.000e+000	0.000e+000	-56.660	-56.678	-0.018
NH4SO4-	0.000e+000	0.000e+000	-66.565	-66.582	-0.018
N(0)	5.995e-015				
N2	2.998e-015	2.999e-015	-14.523	-14.523	0.000
N(3)	6.704e-019				
NO2-	6.704e-019	6.432e-019	-18.174	-18.192	-0.018
N(5)	5.492e-011				
NO3-	5.492e-011	5.269e-011	-10.260	-10.278	-0.018
Na	2.407e-003				
Na+	2.406e-003	2.309e-003	-2.619	-2.636	-0.018
NaCO3-	1.160e-006	1.113e-006	-5.936	-5.953	-0.018
NaHCO3	1.439e-007	1.440e-007	-6.842	-6.842	0.000
NaOH	1.053e-007	1.053e-007	-6.978	-6.978	0.000
NaSO4-	1.133e-013	1.087e-013	-12.946	-12.964	-0.018
O(0)	4.537e-014				
O2	2.268e-014	2.269e-014	-13.644	-13.644	0.000
S(-2)	0.000e+000				
HS-	0.000e+000	0.000e+000	-134.410	-134.428	-0.018
H2S	0.000e+000	0.000e+000	-137.264	-137.264	0.000
S-2	0.000e+000	0.000e+000	-137.572	-137.643	-0.070
S(6)	1.149e-011				
SO4-2	1.137e-011	9.669e-012	-10.944	-11.015	-0.071
NaSO4-	1.133e-013	1.087e-013	-12.946	-12.964	-0.018

CaSO4	2.422e-015	2.423e-015	-14.616	-14.616	0.000
HSO4-	1.289e-019	1.237e-019	-18.890	-18.908	-0.018
MgSO4	2.250e-021	2.251e-021	-20.648	-20.648	0.000
KSO4-	6.736e-023	6.465e-023	-22.172	-22.189	-0.018
CaHSO4+	2.031e-024	1.949e-024	-23.692	-23.710	-0.018
NH4SO4-	0.000e+000	0.000e+000	-66.565	-66.582	-0.018

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

Phase	SI	log IAP	log KT	
Anhydrite	-12.55	-16.90	-4.35	CaSO4
Aragonite	-2.06	-10.37	-8.31	CaCO3
Calcite	-1.91	-10.37	-8.46	CaCO3
CH4(g)	-127.49	-130.31	-2.82	CH4
CO2(g)	-6.00	-7.42	-1.41	CO2
Dolomite	-9.82	-26.81	-16.98	CaMg(CO3)2
Gypsum	-12.32	-16.90	-4.58	CaSO4:2H2O
H2(g)	-36.97	-40.11	-3.13	H2
H2O(g)	-1.63	-0.00	1.63	H2O
H2S(g)	-136.32	-137.26	-0.95	H2S
Halite	-15.70	-14.13	1.57	NaCl
N2(g)	-11.28	-14.52	-3.24	N2
NH3(g)	-58.09	-56.22	1.86	NH3
O2(g)	-10.79	-13.64	-2.86	O2
Sulfur	-105.28	-100.29	4.99	S

End of simulation.

Reading input data for simulation 2.

End of run.

Run 3 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\10-90\eqb mix 1 with calcite and co2.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\10-90\eqb mix 1 with calcite and co2.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          CO2(g)    -2 10
          Calcite   0 10
      SOLUTION 1
          temp      20
          pH        9.839
          pe        8.649
          redox     pe
          units     mmol/kgw
          density   1
          C         0.0001552
          Ca        1.61e-006
          Cl        3.36e-012
          K         1.074e-012
          Mg        1.365e-012
          N(5)      5.492e-011
          Na        0.002407
          S(6)      1.149e-011
          water    1 # kg
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

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

      Elements           Molality       Moles

      C                1.552e-007  1.552e-007
      Ca               1.610e-009  1.610e-009
      Cl               3.360e-015  3.360e-015
      K                1.074e-015  1.074e-015
      Mg               1.365e-015  1.365e-015
      N(5)             5.492e-014  5.492e-014
      Na               2.407e-006  2.407e-006
      S(6)             1.149e-014  1.149e-014

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

                                     pH  =   9.839
                                     pe  =   8.649
                        Activity of water  =   1.000
```

```
                    Ionic strength  =  2.490e-005
                Mass of water (kg)  =  1.000e+000
           Total alkalinity (eq/kg) =  4.732e-005
                 Total CO2 (mol/kg) =  1.552e-007
               Temperature (deg C)  =  20.000
            Electrical balance (eq) = -4.491e-005
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -90.31
                         Iterations =   3
                            Total H = 1.110125e+002
                            Total O = 5.550626e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	4.713e-005	4.686e-005	-4.327	-4.329	-0.003
H+	1.457e-010	1.449e-010	-9.837	-9.839	-0.002
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-133.209	-133.209	0.000
C(4)	1.552e-007				
HCO3-	1.197e-007	1.191e-007	-6.922	-6.924	-0.002
CO3-2	3.541e-008	3.461e-008	-7.451	-7.461	-0.010
CO2	4.155e-011	4.155e-011	-10.381	-10.381	0.000
NaCO3-	1.200e-012	1.193e-012	-11.921	-11.923	-0.003
NaHCO3	1.602e-013	1.602e-013	-12.795	-12.795	0.000
CaCO3	8.342e-014	8.342e-014	-13.079	-13.079	0.000
CaHCO3+	2.205e-015	2.193e-015	-14.657	-14.659	-0.002
MgCO3	4.017e-020	4.017e-020	-19.396	-19.396	0.000
MgHCO3+	1.805e-021	1.794e-021	-20.744	-20.746	-0.003
Ca	1.610e-009				
Ca+2	1.608e-009	1.572e-009	-8.794	-8.804	-0.010
CaOH+	1.811e-012	1.800e-012	-11.742	-11.745	-0.003
CaCO3	8.342e-014	8.342e-014	-13.079	-13.079	0.000
CaHCO3+	2.205e-015	2.193e-015	-14.657	-14.659	-0.002
CaSO4	3.357e-021	3.357e-021	-20.474	-20.474	0.000
CaHSO4+	2.701e-030	2.685e-030	-29.568	-29.571	-0.003
Cl	3.360e-015				
Cl-	3.360e-015	3.341e-015	-14.474	-14.476	-0.003
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.104	-40.104	0.000
K	1.074e-015				
K+	1.074e-015	1.068e-015	-14.969	-14.972	-0.003
KOH	2.556e-020	2.556e-020	-19.593	-19.593	0.000
KSO4-	7.754e-029	7.709e-029	-28.110	-28.113	-0.003
Mg	1.365e-015				
Mg+2	1.344e-015	1.313e-015	-14.872	-14.882	-0.010
MgOH+	2.092e-017	2.080e-017	-16.680	-16.682	-0.003
MgCO3	4.017e-020	4.017e-020	-19.396	-19.396	0.000
MgHCO3+	1.805e-021	1.794e-021	-20.744	-20.746	-0.003
MgSO4	3.033e-027	3.033e-027	-26.518	-26.518	0.000
N(5)	5.492e-014				
NO3-	5.492e-014	5.460e-014	-13.260	-13.263	-0.003
Na	2.407e-006				
Na+	2.407e-006	2.393e-006	-5.619	-5.621	-0.003
NaOH	1.091e-010	1.091e-010	-9.962	-9.962	0.000
NaCO3-	1.200e-012	1.193e-012	-11.921	-11.923	-0.003
NaHCO3	1.602e-013	1.602e-013	-12.795	-12.795	0.000
NaSO4-	1.312e-019	1.304e-019	-18.882	-18.885	-0.003
O(0)	3.075e-014				
O2	1.538e-014	1.538e-014	-13.813	-13.813	0.000
S(6)	1.149e-014				
SO4-2	1.149e-014	1.123e-014	-13.940	-13.950	-0.010
NaSO4-	1.312e-019	1.304e-019	-18.882	-18.885	-0.003
CaSO4	3.357e-021	3.357e-021	-20.474	-20.474	0.000
HSO4-	1.430e-022	1.421e-022	-21.845	-21.847	-0.003

```
    MgSO4                  3.033e-027  3.033e-027   -26.518   -26.518     0.000
    KSO4-                  7.754e-029  7.709e-029   -28.110   -28.113    -0.003
    CaHSO4+                2.701e-030  2.685e-030   -29.568   -29.571    -0.003

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

      Phase               SI log IAP  log KT

      Anhydrite       -18.41  -22.75   -4.34  CaSO4
      Aragonite        -7.96  -16.26   -8.31  CaCO3
      Calcite          -7.81  -16.26   -8.45  CaCO3
      CH4(g)        -130.39 -133.21   -2.82  CH4
      CO2(g)           -8.97  -10.38   -1.41  CO2
      Dolomite        -21.63  -38.61  -16.97  CaMg(CO3)2
      Gypsum          -18.17  -22.75   -4.58  CaSO4:2H2O
      H2(g)           -36.98  -40.10   -3.13  H2
      H2O(g)           -1.64   -0.00    1.64  H2O
      Halite          -21.67  -20.10    1.57  NaCl
      O2(g)           -10.96  -13.81   -2.85  O2

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

Reaction step 1.

Using solution 1.
Using pure phase assemblage 1.

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

                                                      Moles in assemblage
Phase                  SI log IAP  log KT      Initial       Final       Delta

Calcite              0.00   -8.45   -8.45   1.000e+001  9.998e+000 -1.773e-003
CO2(g)              -2.00   -3.41   -1.41   1.000e+001  9.998e+000 -2.202e-003

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

      Elements           Molality       Moles

      C                 3.976e-003  3.975e-003
      Ca                1.773e-003  1.773e-003
      Cl                3.360e-015  3.360e-015
      K                 1.074e-015  1.074e-015
      Mg                1.365e-015  1.365e-015
      N                 5.492e-014  5.492e-014
      Na                2.407e-006  2.407e-006
      S                 1.149e-014  1.149e-014

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

                                       pH  =   7.303      Charge balance
                                       pe  =  11.197      Adjusted to redox equilibrium
                         Activity of water  =   1.000
                            Ionic strength  =  5.226e-003
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  3.593e-003
                       Total CO2 (mol/kg)   =  3.976e-003
                     Temperature (deg C)    =  20.000
                  Electrical balance (eq)   = -4.491e-005
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   =  -0.64
                                Iterations  =  11
                                   Total H  = 1.110125e+002
                                   Total O  = 5.551599e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.475e-007	1.365e-007	-6.831	-6.865	-0.034
H+	5.331e-008	4.974e-008	-7.273	-7.303	-0.030
H2O	5.551e+001	9.999e-001	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-126.333	-126.332	0.001
C(4)	3.976e-003				
HCO3-	3.522e-003	3.269e-003	-2.453	-2.486	-0.032
CO2	3.914e-004	3.919e-004	-3.407	-3.407	0.001
CaHCO3+	5.252e-005	4.875e-005	-4.280	-4.312	-0.032
CaCO3	5.394e-006	5.401e-006	-5.268	-5.268	0.001
CO3-2	3.730e-006	2.768e-006	-5.428	-5.558	-0.130
NaHCO3	4.090e-009	4.095e-009	-8.388	-8.388	0.001
NaCO3-	9.589e-011	8.882e-011	-10.018	-10.051	-0.033
MgHCO3+	3.988e-017	3.694e-017	-16.399	-16.433	-0.033
MgCO3	2.406e-018	2.408e-018	-17.619	-17.618	0.001
Ca	1.773e-003				
Ca+2	1.715e-003	1.272e-003	-2.766	-2.895	-0.130
CaHCO3+	5.252e-005	4.875e-005	-4.280	-4.312	-0.032
CaCO3	5.394e-006	5.401e-006	-5.268	-5.268	0.001
CaOH+	4.582e-009	4.244e-009	-8.339	-8.372	-0.033
CaSO4	1.744e-015	1.746e-015	-14.759	-14.758	0.001
CaHSO4+	5.176e-022	4.794e-022	-21.286	-21.319	-0.033
Cl	3.360e-015				
Cl-	3.360e-015	3.110e-015	-14.474	-14.507	-0.034
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.129	-40.129	0.001
K	1.074e-015				
K+	1.074e-015	9.940e-016	-14.969	-15.003	-0.034
KOH	6.919e-023	6.928e-023	-22.160	-22.159	0.001
KSO4-	4.976e-029	4.609e-029	-28.303	-28.336	-0.033
Mg	1.365e-015				
Mg+2	1.323e-015	9.846e-016	-14.879	-15.007	-0.128
MgHCO3+	3.988e-017	3.694e-017	-16.399	-16.433	-0.033
MgCO3	2.406e-018	2.408e-018	-17.619	-17.618	0.001
MgOH+	4.901e-020	4.540e-020	-19.310	-19.343	-0.033
MgSO4	1.459e-027	1.460e-027	-26.836	-26.836	0.001
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-54.462	-54.497	-0.034
NH3	0.000e+000	0.000e+000	-56.594	-56.594	0.001
NH4SO4-	0.000e+000	0.000e+000	-67.496	-67.529	-0.033
N(0)	1.165e-015				
N2	5.823e-016	5.830e-016	-15.235	-15.234	0.001
N(3)	7.030e-022				
NO2-	7.030e-022	6.499e-022	-21.153	-21.187	-0.034
N(5)	5.376e-014				
NO3-	5.376e-014	4.970e-014	-13.270	-13.304	-0.034
Na	2.407e-006				
Na+	2.403e-006	2.227e-006	-5.619	-5.652	-0.033
NaHCO3	4.090e-009	4.095e-009	-8.388	-8.388	0.001
NaCO3-	9.589e-011	8.882e-011	-10.018	-10.051	-0.033
NaOH	2.954e-013	2.958e-013	-12.530	-12.529	0.001
NaSO4-	8.415e-020	7.795e-020	-19.075	-19.108	-0.033
O(0)	3.439e-014				
O2	1.720e-014	1.722e-014	-13.765	-13.764	0.001
S(-2)	0.000e+000				
HS-	0.000e+000	0.000e+000	-135.012	-135.046	-0.034
H2S	0.000e+000	0.000e+000	-135.339	-135.339	0.001
S-2	0.000e+000	0.000e+000	-140.681	-140.812	-0.131
S(6)	1.149e-014				
SO4-2	9.747e-015	7.212e-015	-14.011	-14.142	-0.131
CaSO4	1.744e-015	1.746e-015	-14.759	-14.758	0.001
NaSO4-	8.415e-020	7.795e-020	-19.075	-19.108	-0.033
HSO4-	3.384e-020	3.135e-020	-19.471	-19.504	-0.033

CaHSO4+	5.176e-022	4.794e-022	-21.286	-21.319	-0.033
MgSO4	1.459e-027	1.460e-027	-26.836	-26.836	0.001
KSO4-	4.976e-029	4.609e-029	-28.303	-28.336	-0.033
NH4SO4-	0.000e+000	0.000e+000	-67.496	-67.529	-0.033

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

Phase	SI	log IAP	log KT	
Anhydrite	-12.69	-17.04	-4.34	CaSO4
Aragonite	-0.15	-8.45	-8.31	CaCO3
Calcite	0.00	-8.45	-8.45	CaCO3
CH4(g)	-123.51	-126.33	-2.82	CH4
CO2(g)	-2.00	-3.41	-1.41	CO2
Dolomite	-12.05	-29.02	-16.97	CaMg(CO3)2
Gypsum	-12.46	-17.04	-4.58	CaSO4:2H2O
H2(g)	-37.00	-40.13	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
H2S(g)	-134.40	-135.34	-0.94	H2S
Halite	-21.73	-20.16	1.57	NaCl
N2(g)	-11.99	-15.23	-3.24	N2
NH3(g)	-58.47	-56.59	1.87	NH3
O2(g)	-10.91	-13.76	-2.85	O2
Sulfur	-103.34	-98.34	5.00	S

End of simulation.

Reading input data for simulation 2.

End of run.

Run 3 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\eqb mix 2 10-90withmontmorillonite.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\eqb mix 2 10-90withmontmorillonite.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          Ca-Montmorillonite 0 10
      SOLUTION 1
          temp      20
          pH        7.313
          pe        11.534
          redox     pe
          units     mmol/kgw
          density   1
          C         0.004154
          Ca        0.001866
          Cl        8.124e-013
          K         2.601e-013
          Mg        3.308e-013
          N(5)      1.329e-011
          Na        0.008832
          S(6)      2.785e-012
          water    1 # kg
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

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

      Elements           Molality       Moles

      C                4.154e-006  4.154e-006
      Ca               1.866e-006  1.866e-006
      Cl               8.124e-016  8.124e-016
      K                2.601e-016  2.601e-016
      Mg               3.308e-016  3.308e-016
      N(5)             1.329e-014  1.329e-014
      Na               8.832e-006  8.832e-006
      S(6)             2.785e-015  2.785e-015

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

                                     pH  =   7.313
                                     pe  =  11.534
                        Activity of water  =   1.000
                           Ionic strength  =  1.011e-005
```

```
                    Mass of water (kg)  =  1.000e+000
              Total alkalinity (eq/kg)  =  3.815e-006
                    Total CO2 (mol/kg)  =  4.154e-006
                  Temperature (deg C)   =  20.000
             Electrical balance (eq)    =  8.749e-006
Percent error, 100*(Cat-|An|)/(Cat+|An|) =  53.10
                             Iterations =   3
                                Total H = 1.110124e+002
                                Total O = 5.550623e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.401e-007	1.396e-007	-6.854	-6.855	-0.002
H+	4.882e-008	4.864e-008	-7.311	-7.313	-0.002
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-132.062	-132.062	0.000
C(4)	4.154e-006				
HCO3-	3.717e-006	3.703e-006	-5.430	-5.431	-0.002
CO2	4.339e-007	4.339e-007	-6.363	-6.363	0.000
CO3-2	3.254e-009	3.206e-009	-8.488	-8.494	-0.006
CaHCO3+	8.009e-011	7.980e-011	-10.096	-10.098	-0.002
NaHCO3	1.832e-011	1.832e-011	-10.737	-10.737	0.000
CaCO3	9.042e-012	9.042e-012	-11.044	-11.044	0.000
NaCO3-	4.080e-013	4.065e-013	-12.389	-12.391	-0.002
MgHCO3+	1.390e-020	1.385e-020	-19.857	-19.859	-0.002
MgCO3	9.235e-022	9.235e-022	-21.035	-21.035	0.000
Ca	1.866e-006				
Ca+2	1.866e-006	1.839e-006	-5.729	-5.735	-0.006
CaHCO3+	8.009e-011	7.980e-011	-10.096	-10.098	-0.002
CaCO3	9.042e-012	9.042e-012	-11.044	-11.044	0.000
CaOH+	6.297e-012	6.273e-012	-11.201	-11.202	-0.002
CaSO4	9.597e-019	9.597e-019	-18.018	-18.018	0.000
CaHSO4+	2.587e-025	2.577e-025	-24.587	-24.589	-0.002
Cl	8.124e-016				
Cl-	8.124e-016	8.094e-016	-15.090	-15.092	-0.002
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.822	-40.822	0.000
K	2.601e-016				
K+	2.601e-016	2.591e-016	-15.585	-15.586	-0.002
KOH	1.847e-023	1.847e-023	-22.733	-22.733	0.000
KSO4-	4.588e-030	4.571e-030	-29.338	-29.340	-0.002
Mg	3.308e-016				
Mg+2	3.308e-016	3.259e-016	-15.480	-15.487	-0.006
MgOH+	1.543e-020	1.537e-020	-19.812	-19.813	-0.002
MgHCO3+	1.390e-020	1.385e-020	-19.857	-19.859	-0.002
MgCO3	9.235e-022	9.235e-022	-21.035	-21.035	0.000
MgSO4	1.839e-028	1.839e-028	-27.735	-27.735	0.000
N(5)	1.329e-014				
NO3-	1.329e-014	1.324e-014	-13.876	-13.878	-0.002
Na	8.832e-006				
Na+	8.832e-006	8.800e-006	-5.054	-5.056	-0.002
NaHCO3	1.832e-011	1.832e-011	-10.737	-10.737	0.000
NaOH	1.195e-012	1.195e-012	-11.923	-11.923	0.000
NaCO3-	4.080e-013	4.065e-013	-12.389	-12.391	-0.002
NaSO4-	1.176e-019	1.171e-019	-18.930	-18.931	-0.002
O(0)	8.393e-013				
O2	4.196e-013	4.196e-013	-12.377	-12.377	0.000
S(6)	2.785e-015				
SO4-2	2.784e-015	2.743e-015	-14.555	-14.562	-0.006
CaSO4	9.597e-019	9.597e-019	-18.018	-18.018	0.000
NaSO4-	1.176e-019	1.171e-019	-18.930	-18.931	-0.002
HSO4-	1.170e-020	1.166e-020	-19.932	-19.933	-0.002
CaHSO4+	2.587e-025	2.577e-025	-24.587	-24.589	-0.002

MgSO4	1.839e-028	1.839e-028	-27.735	-27.735	0.000
KSO4-	4.588e-030	4.571e-030	-29.338	-29.340	-0.002

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

Phase	SI	log IAP	log KT	
Anhydrite	-15.95	-20.30	-4.34	CaSO4
Aragonite	-5.92	-14.23	-8.31	CaCO3
Calcite	-5.78	-14.23	-8.45	CaCO3
CH4(g)	-129.24	-132.06	-2.82	CH4
CO2(g)	-4.96	-6.36	-1.41	CO2
Dolomite	-21.24	-38.21	-16.97	CaMg(CO3)2
Gypsum	-15.72	-20.30	-4.58	CaSO4:2H2O
H2(g)	-37.69	-40.82	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
Halite	-21.72	-20.15	1.57	NaCl
O2(g)	-9.52	-12.38	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca-Montmorillonite	0.00	-45.76	-45.76	1.000e+001	1.000e+001	-2.061e-006

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

Elements	Molality	Moles
Al	4.802e-006	4.802e-006
C	4.154e-006	4.154e-006
Ca	2.206e-006	2.206e-006
Cl	8.124e-016	8.124e-016
K	2.601e-016	2.601e-016
Mg	3.308e-016	3.308e-016
N	1.329e-014	1.329e-014
Na	8.832e-006	8.832e-006
S	2.785e-015	2.785e-015
Si	7.563e-006	7.563e-006

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

pH	=	6.617	Charge balance
pe	=	12.232	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	1.255e-005	
Mass of water (kg)	=	1.000e+000	
Total alkalinity (eq/kg)	=	1.890e-005	
Total CO2 (mol/kg)	=	4.154e-006	
Temperature (deg C)	=	20.000	
Electrical balance (eq)	=	8.749e-006	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	42.54	
Iterations	=	9	
Total H	=	1.110124e+002	
Total O	=	5.550625e+001	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.427e-007	2.417e-007	-6.615	-6.617	-0.002
OH-	2.821e-008	2.809e-008	-7.550	-7.551	-0.002
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Al	4.802e-006				
Al(OH)4-	3.246e-006	3.233e-006	-5.489	-5.490	-0.002
Al(OH)2+	1.061e-006	1.057e-006	-5.974	-5.976	-0.002
Al(OH)3	4.405e-007	4.405e-007	-6.356	-6.356	0.000
AlOH+2	5.195e-008	5.110e-008	-7.284	-7.292	-0.007
Al+3	1.792e-009	1.727e-009	-8.747	-8.763	-0.016
AlSO4+	1.406e-020	1.400e-020	-19.852	-19.854	-0.002
AlHSO4+2	2.928e-028	2.880e-028	-27.533	-27.541	-0.007
Al(SO4)2-	1.189e-033	1.184e-033	-32.925	-32.927	-0.002
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-131.527	-131.527	0.000
C(4)	4.154e-006				
HCO3-	2.629e-006	2.618e-006	-5.580	-5.582	-0.002
CO2	1.524e-006	1.524e-006	-5.817	-5.817	0.000
CO3-2	4.638e-010	4.563e-010	-9.334	-9.341	-0.007
CaHCO3+	6.687e-011	6.659e-011	-10.175	-10.177	-0.002
NaHCO3	1.295e-011	1.295e-011	-10.888	-10.888	0.000
CaCO3	1.519e-012	1.519e-012	-11.819	-11.819	0.000
NaCO3-	5.806e-014	5.782e-014	-13.236	-13.238	-0.002
MgHCO3+	9.816e-021	9.776e-021	-20.008	-20.010	-0.002
MgCO3	1.312e-022	1.312e-022	-21.882	-21.882	0.000
Ca	2.206e-006				
Ca+2	2.206e-006	2.170e-006	-5.656	-5.664	-0.007
CaHCO3+	6.687e-011	6.659e-011	-10.175	-10.177	-0.002
CaCO3	1.519e-012	1.519e-012	-11.819	-11.819	0.000
CaOH+	1.496e-012	1.490e-012	-11.825	-11.827	-0.002
CaSO4	1.131e-018	1.131e-018	-17.947	-17.947	0.000
CaHSO4+	1.515e-024	1.509e-024	-23.820	-23.821	-0.002
Cl	8.124e-016				
Cl-	8.124e-016	8.091e-016	-15.090	-15.092	-0.002
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.825	-40.825	0.000
K	2.601e-016				
K+	2.601e-016	2.590e-016	-15.585	-15.587	-0.002
KOH	3.717e-024	3.717e-024	-23.430	-23.430	0.000
KSO4-	4.580e-030	4.561e-030	-29.339	-29.341	-0.002
Mg	3.308e-016				
Mg+2	3.308e-016	3.254e-016	-15.480	-15.488	-0.007
MgHCO3+	9.816e-021	9.776e-021	-20.008	-20.010	-0.002
MgOH+	3.101e-021	3.089e-021	-20.508	-20.510	-0.002
MgCO3	1.312e-022	1.312e-022	-21.882	-21.882	0.000
MgSO4	1.833e-028	1.833e-028	-27.737	-27.737	0.000
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-56.482	-56.483	-0.002
NH3	0.000e+000	0.000e+000	-59.267	-59.267	0.000
NH4SO4-	0.000e+000	0.000e+000	-69.934	-69.936	-0.002
N(0)	6.446e-019				
N2	3.223e-019	3.223e-019	-18.492	-18.492	0.000
N(3)	3.498e-023				
NO2-	3.498e-023	3.484e-023	-22.456	-22.458	-0.002
N(5)	1.329e-014				
NO3-	1.329e-014	1.323e-014	-13.876	-13.878	-0.002
Na	8.832e-006				
Na+	8.832e-006	8.796e-006	-5.054	-5.056	-0.002
NaHCO3	1.295e-011	1.295e-011	-10.888	-10.888	0.000
NaOH	2.405e-013	2.405e-013	-12.619	-12.619	0.000
NaCO3-	5.806e-014	5.782e-014	-13.236	-13.238	-0.002
NaSO4-	1.174e-019	1.169e-019	-18.930	-18.932	-0.002
O(0)	8.500e-013				
O2	4.250e-013	4.250e-013	-12.372	-12.372	0.000

S(-2)	0.000e+000					
H2S		0.000e+000	0.000e+000	-137.171	-137.171	0.000
HS-		0.000e+000	0.000e+000	-137.563	-137.564	-0.002
S-2		0.000e+000	0.000e+000	-144.010	-144.017	-0.007
S(6)	2.785e-015					
SO4-2		2.784e-015	2.738e-015	-14.555	-14.562	-0.007
CaSO4		1.131e-018	1.131e-018	-17.947	-17.947	0.000
NaSO4-		1.174e-019	1.169e-019	-18.930	-18.932	-0.002
HSO4-		5.806e-020	5.782e-020	-19.236	-19.238	-0.002
AlSO4+		1.406e-020	1.400e-020	-19.852	-19.854	-0.002
CaHSO4+		1.515e-024	1.509e-024	-23.820	-23.821	-0.002
AlHSO4+2		2.928e-028	2.880e-028	-27.533	-27.541	-0.007
MgSO4		1.833e-028	1.833e-028	-27.737	-27.737	0.000
KSO4-		4.580e-030	4.561e-030	-29.339	-29.341	-0.002
Al(SO4)2-		1.189e-033	1.184e-033	-32.925	-32.927	-0.002
NH4SO4-		0.000e+000	0.000e+000	-69.934	-69.936	-0.002
Si	7.563e-006					
H4SiO4		7.559e-006	7.559e-006	-5.122	-5.122	0.000
H3SiO4-		3.869e-009	3.854e-009	-8.412	-8.414	-0.002
H2SiO4-2		7.884e-016	7.756e-016	-15.103	-15.110	-0.007

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

Phase	SI	log IAP	log KT	
Al(OH)3(a)	-0.04	11.09	11.13	Al(OH)3
Albite	-7.58	-25.91	-18.33	NaAlSi3O8
Alunite	-30.53	-31.30	-0.77	KAl3(SO4)2(OH)6
Anhydrite	-15.88	-20.23	-4.34	CaSO4
Anorthite	-7.03	-26.89	-19.86	CaAl2Si2O8
Aragonite	-6.70	-15.00	-8.31	CaCO3
Ca-Montmorillonite	0.00	-45.76	-45.76	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-6.55	-15.00	-8.45	CaCO3
CH4(g)	-128.71	-131.53	-2.82	CH4
Chalcedony	-1.51	-5.12	-3.61	SiO2
Chlorite(14A)	-74.73	-4.46	70.27	Mg5Al2Si3O10(OH)8
Chrysotile	-49.84	-17.01	32.83	Mg3Si2O5(OH)4
CO2(g)	-4.41	-5.82	-1.41	CO2
Dolomite	-22.86	-39.83	-16.97	CaMg(CO3)2
Gibbsite	2.69	11.09	8.40	Al(OH)3
Gypsum	-15.64	-20.23	-4.58	CaSO4:2H2O
H2(g)	-37.70	-40.82	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
H2S(g)	-136.23	-137.17	-0.94	H2S
Halite	-21.72	-20.15	1.57	NaCl
Illite	-10.77	-51.72	-40.95	K0.6Mg0.25Al2.3Si3.5O10(OH)2
K-feldspar	-15.48	-36.44	-20.96	KAlSi3O8
K-mica	-4.52	8.93	13.45	KAl3Si3O10(OH)2
Kaolinite	4.06	11.93	7.88	Al2Si2O5(OH)4
N2(g)	-15.25	-18.49	-3.24	N2
NH3(g)	-61.14	-59.27	1.87	NH3
O2(g)	-9.52	-12.37	-2.85	O2
Quartz	-1.07	-5.12	-4.06	SiO2
Sepiolite	-35.77	-19.87	15.89	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-38.53	-19.87	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-2.37	-5.12	-2.75	SiO2
Sulfur	-104.48	-99.47	5.00	S
Talc	-49.23	-27.25	21.98	Mg3Si4O10(OH)2

End of simulation.

Reading input data for simulation 2.

```
-----------
End of run.
-----------
```

Run 4

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\25-75\25%rainwater+75%NaOH.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\25-75\25%rainwater+75%NaOH.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          CO2(g)     -3.5 10
      SOLUTION 1 rainwater
          temp       25
          pH         5.24
          pe         4
          redox      pe
          units      mg/l
          density    1
          Ca         0.458
          Mg         0.034
          Na         0.082
          K          0.043
          Cl         0.122
          S(6)       1.131
          N(5)       1.004
          N(-3)      0.36
          water     1 # kg
     SOLUTION 2 NaOH
          temp       20
          pH         14
          pe         4
          redox      pe
          units      mmol/kgw
          density    1
          Na         24.9 mol/kgw
          water     1 # kg
     MIX 1
          1    0.25
          2    0.75
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     rainwater

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

      Elements           Molality       Moles

      Ca                1.143e-005  1.143e-005
      Cl                3.441e-006  3.441e-006
      K                 1.100e-006  1.100e-006
```

Mg	1.398e-006	1.398e-006
N(-3)	2.570e-005	2.570e-005
N(5)	7.168e-005	7.168e-005
Na	3.567e-006	3.567e-006
S(6)	1.177e-005	1.177e-005

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

pH	=	5.240
pe	=	4.000
Activity of water	=	1.000
Ionic strength	=	1.047e-004
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	-5.824e-006
Total carbon (mol/kg)	=	0.000e+000
Total CO2 (mol/kg)	=	0.000e+000
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	-3.682e-005
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-22.96
Iterations	=	3
Total H	=	1.110125e+002
Total O	=	5.550648e+001

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

Redox couple	pe	Eh (volts)
N(-3)/N(5)	8.3903	0.4963

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	5.822e-006	5.754e-006	-5.235	-5.240	-0.005
OH-	1.760e-009	1.740e-009	-8.754	-8.760	-0.005
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Ca	1.143e-005				
Ca+2	1.140e-005	1.088e-005	-4.943	-4.963	-0.020
CaSO4	2.429e-008	2.429e-008	-7.614	-7.614	0.000
CaHSO4+	8.288e-013	8.190e-013	-12.082	-12.087	-0.005
CaOH+	3.174e-013	3.137e-013	-12.498	-12.503	-0.005
Cl	3.441e-006				
Cl-	3.441e-006	3.401e-006	-5.463	-5.468	-0.005
H(0)	4.688e-022				
H2	2.344e-022	2.344e-022	-21.630	-21.630	0.000
K	1.100e-006				
K+	1.100e-006	1.087e-006	-5.959	-5.964	-0.005
KSO4-	8.649e-011	8.547e-011	-10.063	-10.068	-0.005
KOH	6.547e-016	6.548e-016	-15.184	-15.184	0.000
Mg	1.398e-006				
Mg+2	1.395e-006	1.331e-006	-5.855	-5.876	-0.020
MgSO4	3.492e-009	3.492e-009	-8.457	-8.457	0.000
MgOH+	8.497e-013	8.397e-013	-12.071	-12.076	-0.005
N(-3)	2.570e-005				
NH4+	2.570e-005	2.539e-005	-4.590	-4.595	-0.005
NH4SO4-	3.705e-009	3.662e-009	-8.431	-8.436	-0.005
NH3	2.515e-009	2.515e-009	-8.600	-8.600	0.000
N(5)	7.168e-005				
NO3-	7.168e-005	7.083e-005	-4.145	-4.150	-0.005
Na	3.567e-006				
Na+	3.567e-006	3.525e-006	-5.448	-5.453	-0.005
NaSO4-	2.001e-010	1.977e-010	-9.699	-9.704	-0.005
NaOH	4.047e-015	4.047e-015	-14.393	-14.393	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-49.120	-49.120	0.000
S(6)	1.177e-005				

SO4-2	1.174e-005	1.119e-005	-4.931	-4.951	-0.021
CaSO4	2.429e-008	2.429e-008	-7.614	-7.614	0.000
HSO4-	6.337e-009	6.263e-009	-8.198	-8.203	-0.005
NH4SO4-	3.705e-009	3.662e-009	-8.431	-8.436	-0.005
MgSO4	3.492e-009	3.492e-009	-8.457	-8.457	0.000
NaSO4-	2.001e-010	1.977e-010	-9.699	-9.704	-0.005
KSO4-	8.649e-011	8.547e-011	-10.063	-10.068	-0.005
CaHSO4+	8.288e-013	8.190e-013	-12.082	-12.087	-0.005

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

Phase	SI	log IAP	log KT	
Anhydrite	-5.55	-9.91	-4.36	CaSO4
Gypsum	-5.33	-9.91	-4.58	CaSO4:2H2O
H2(g)	-18.48	-21.63	-3.15	H2
H2O(g)	-1.51	-0.00	1.51	H2O
Halite	-12.50	-10.92	1.58	NaCl
NH3(g)	-10.37	-8.60	1.77	NH3
O2(g)	-46.23	-49.12	-2.89	O2

Initial solution 2. NaOH

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

Elements	Molality	Moles
Na	2.490e+001	2.490e+001

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

pH	=	14.000
pe	=	4.000
Activity of water	=	0.562
Ionic strength	=	1.184e+001
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	2.931e+000
Total carbon (mol/kg)	=	0.000e+000
Total CO2 (mol/kg)	=	0.000e+000
Temperature (deg C)	=	20.000
Electrical balance (eq)	=	2.197e+001
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	92.76
Iterations	=	6
Total H	=	1.139431e+002
Total O	=	5.843693e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	8.574e-001	3.816e-001	-0.067	-0.418	-0.352
H+	1.432e-014	1.000e-014	-13.844	-14.000	-0.156
H2O	5.551e+001	5.621e-001	1.744	-0.250	0.000
H(0)	0.000e+000				
H2	0.000e+000	7.447e-040	-40.312	-39.128	1.184
Na	2.490e+001				
Na+	2.283e+001	8.532e+001	1.358	1.931	0.573
NaOH	2.073e+000	3.169e+001	0.317	1.501	1.184
O(0)	7.102e-018				
O2	3.551e-018	5.427e-017	-17.450	-16.265	1.184

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

Phase	SI	log IAP	log KT	
H2(g)	-36.00	-39.13	-3.13	H2

```
      H2O(g)            -1.89   -0.25    1.64  H2O
      O2(g)            -13.41  -16.27   -2.85  O2

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

 Reaction step 1.

 Using mix 1.
 Using pure phase assemblage 1.

 Mixture 1.

       2.500e-001 Solution 1  rainwater
       7.500e-001 Solution 2  NaOH

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

                                                        Moles in assemblage
 Phase                   SI log IAP  log KT      Initial       Final       Delta

 CO2(g)               -3.50   -4.92   -1.42   1.000e+001  8.822e+000 -1.178e+000

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

      Elements           Molality       Moles

      C                1.156e+000  1.178e+000
      Ca               2.805e-006  2.857e-006
      Cl               8.448e-007  8.603e-007
      K                2.700e-007  2.749e-007
      Mg               3.433e-007  3.496e-007
      N                2.391e-005  2.435e-005
      Na               1.834e+001  1.868e+001
      S                2.890e-006  2.943e-006

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

                                      pH  =   9.993      Charge balance
                                      pe  =   8.492      Adjusted to redox equilibrium
                         Activity of water  =   0.685
                            Ionic strength  =  9.420e+000
                       Mass of water (kg)   =  1.018e+000
                 Total alkalinity (eq/kg)   =  2.158e+000
                       Total CO2 (mol/kg)   =  1.156e+000
                     Temperature (deg C)    =  21.250
                  Electrical balance (eq)   =  1.648e+001
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   =  87.12
                              Iterations    =  19
                                 Total H    = 1.132105e+002
                                 Total O    = 6.005934e+001

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

                                                      Log       Log        Log
   Species                 Molality    Activity  Molality  Activity     Gamma

   OH-                   1.116e-004  5.056e-005    -3.953    -4.296    -0.344
   H+                    1.449e-010  1.015e-010    -9.839    -9.993    -0.155
   H2O                   5.551e+001  6.850e-001     1.744    -0.164     0.000
C(-4)            0.000e+000
   CH4                   0.000e+000  0.000e+000  -128.517  -127.575     0.942
C(4)             1.156e+000
   NaCO3-                8.672e-001  9.699e+000    -0.062     0.987     1.049
   CO3-2                 1.345e-001  1.454e-002    -0.871    -1.837    -0.966
   NaHCO3                9.503e-002  8.316e-001    -1.022    -0.080     0.942
```

	HCO3-	5.946e-002	3.409e-002	-1.226	-1.467	-0.242
	CaCO3	2.020e-006	1.767e-005	-5.695	-4.753	0.942
	CO2	1.366e-006	1.195e-005	-5.865	-4.923	0.942
	CaHCO3+	5.532e-007	3.172e-007	-6.257	-6.499	-0.242
	MgCO3	3.114e-007	2.725e-006	-6.507	-5.565	0.942
	MgHCO3+	7.306e-009	8.171e-008	-8.136	-7.088	1.049
Ca	2.805e-006					
	CaCO3	2.020e-006	1.767e-005	-5.695	-4.753	0.942
	CaHCO3+	5.532e-007	3.172e-007	-6.257	-6.499	-0.242
	Ca+2	2.323e-007	7.758e-007	-6.634	-6.110	0.524
	CaOH+	7.766e-011	8.685e-010	-10.110	-9.061	1.049
	CaSO4	1.108e-012	9.698e-012	-11.955	-11.013	0.942
	CaHSO4+	4.931e-022	5.515e-021	-21.307	-20.258	1.049
Cl	8.448e-007					
	Cl-	8.448e-007	5.301e-007	-6.073	-6.276	-0.202
H(0)	0.000e+000					
	H2	0.000e+000	0.000e+000	-41.047	-40.105	0.942
K	2.700e-007					
	K+	2.700e-007	1.694e-007	-6.569	-6.771	-0.202
	KOH	4.529e-013	3.963e-012	-12.344	-11.402	0.942
	KSO4-	6.466e-015	7.232e-014	-14.189	-13.141	1.049
Mg	3.433e-007					
	MgCO3	3.114e-007	2.725e-006	-6.507	-5.565	0.942
	Mg+2	2.428e-008	2.080e-007	-7.615	-6.682	0.933
	MgHCO3+	7.306e-009	8.171e-008	-8.136	-7.088	1.049
	MgOH+	3.232e-010	3.615e-009	-9.491	-8.442	1.049
	MgSO4	3.280e-013	2.870e-012	-12.484	-11.542	0.942
N(-3)	0.000e+000					
	NH4+	0.000e+000	0.000e+000	-51.359	-51.801	-0.442
	NH3	0.000e+000	0.000e+000	-52.111	-51.169	0.942
	NH4SO4-	0.000e+000	0.000e+000	-58.927	-57.879	1.049
N(0)	1.010e-005					
	N2	5.048e-006	4.417e-005	-5.297	-4.355	0.942
N(3)	2.051e-013					
	NO2-	2.051e-013	8.421e-014	-12.688	-13.075	-0.387
N(5)	1.381e-005					
	NO3-	1.381e-005	5.670e-006	-4.860	-5.246	-0.387
Na	1.834e+001					
	Na+	1.738e+001	4.337e+001	1.240	1.637	0.397
	NaCO3-	8.672e-001	9.699e+000	-0.062	0.987	1.049
	NaHCO3	9.503e-002	8.316e-001	-1.022	-0.080	0.942
	NaOH	2.209e-004	1.933e-003	-3.656	-2.714	0.942
	NaSO4-	1.232e-006	1.377e-005	-5.910	-4.861	1.049
O(0)	4.306e-015					
	O2	2.153e-015	1.884e-014	-14.667	-13.725	0.942
S(-2)	0.000e+000					
	HS-	0.000e+000	0.000e+000	-129.853	-130.197	-0.344
	S-2	0.000e+000	0.000e+000	-132.204	-133.234	-1.031
	H2S	0.000e+000	0.000e+000	-134.140	-133.198	0.942
S(6)	2.890e-006					
	SO4-2	1.659e-006	6.491e-008	-5.780	-7.188	-1.407
	NaSO4-	1.232e-006	1.377e-005	-5.910	-4.861	1.049
	CaSO4	1.108e-012	9.698e-012	-11.955	-11.013	0.942
	MgSO4	3.280e-013	2.870e-012	-12.484	-11.542	0.942
	KSO4-	6.466e-015	7.232e-014	-14.189	-13.141	1.049
	HSO4-	5.286e-017	5.912e-016	-16.277	-15.228	1.049
	CaHSO4+	4.931e-022	5.515e-021	-21.307	-20.258	1.049
	NH4SO4-	0.000e+000	0.000e+000	-58.927	-57.879	1.049

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

Phase	SI	log IAP	log KT	
Anhydrite	-8.95	-13.30	-4.35	CaSO4
Aragonite	0.37	-7.95	-8.31	CaCO3
Calcite	0.51	-7.95	-8.46	CaCO3
CH4(g)	-124.75	-127.57	-2.83	CH4

```
      CO2(g)            -3.50   -4.92   -1.42  CO2
      Dolomite           0.54  -16.47  -17.00  CaMg(CO3)2
      Gypsum            -9.05  -13.63   -4.58  CaSO4:2H2O
      H2(g)            -36.97  -40.10   -3.13  H2
      H2O(g)            -1.77   -0.16    1.61  H2O
      H2S(g)          -132.24 -133.20   -0.95  H2S
      Halite            -6.21   -4.64    1.57  NaCl
      N2(g)             -1.11   -4.35   -3.25  N2
      NH3(g)           -53.01  -51.17    1.85  NH3
      O2(g)            -10.86  -13.72   -2.86  O2
      Sulfur          -101.20  -96.23    4.97  S

------------------
End of simulation.
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-----------------------------------
Reading input data for simulation 2.
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-----------
End of run.
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```

Run 4 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\25-75\mix rain NaOH and calcite GW.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\25-75\mix rain NaOH and calcite GW.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 2 NaOH
          temp      20
          pH        9.993
          pe        8.492
          redox     pe
          units     mmol/kgw
          density   1
          Na        18.34 Mol/kgw
          C         1.156
          Ca        2.805e-006
          Cl        8.448e-007
          K         2.7e-007
          Mg        3.433e-007
          N(5)      1.381e-005
          S(6)      2.89e-006
          water    1 # kg
     SOLUTION 1 GW @ eqb w/ Calcite
          temp      20
          pH        7.301
          pe        -1.841
          redox     pe
          units     mmol/kgw
          density   1
          Ca        0.001789
          C         0.003961
          water    1 # kg
     SAVE solution 1-2
     MIX 1 Mix NaOH and GW @ equ w/ calcite
          1    0.4
          2    0.6
------------------------------------------
Beginning of initial solution calculations.
------------------------------------------

Initial solution 1.     GW @ eqb w/ Calcite

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

     Elements           Molality       Moles

     C                 3.961e-006  3.961e-006
     Ca                1.789e-006  1.789e-006
```

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

pH	=	7.301
pe	=	-1.841
Activity of water	=	1.000
Ionic strength	=	5.444e-006
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	3.626e-006
Total CO2 (mol/kg)	=	3.961e-006
Temperature (deg C)	=	20.000
Electrical balance (eq)	=	-4.751e-008
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-0.65
Iterations	=	3
Total H	=	1.110124e+002
Total O	=	5.550623e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.361e-007	1.358e-007	-6.866	-6.867	-0.001
H+	5.014e-008	5.000e-008	-7.300	-7.301	-0.001
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	1.058e-025				
CH4	1.058e-025	1.058e-025	-24.975	-24.975	0.000
C(4)	3.961e-006				
HCO3-	3.533e-006	3.524e-006	-5.452	-5.453	-0.001
CO2	4.245e-007	4.245e-007	-6.372	-6.372	0.000
CO3-2	3.000e-009	2.968e-009	-8.523	-8.528	-0.005
CaHCO3+	7.328e-011	7.309e-011	-10.135	-10.136	-0.001
CaCO3	8.056e-012	8.056e-012	-11.094	-11.094	0.000
Ca	1.789e-006				
Ca+2	1.789e-006	1.770e-006	-5.747	-5.752	-0.005
CaHCO3+	7.328e-011	7.309e-011	-10.135	-10.136	-0.001
CaCO3	8.056e-012	8.056e-012	-11.094	-11.094	0.000
CaOH+	5.889e-012	5.873e-012	-11.230	-11.231	-0.001
H(0)	1.791e-014				
H2	8.953e-015	8.953e-015	-14.048	-14.048	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-65.925	-65.925	0.000

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

Phase	SI	log IAP	log KT	
Aragonite	-5.97	-14.28	-8.31	CaCO3
Calcite	-5.83	-14.28	-8.45	CaCO3
CH4(g)	-22.16	-24.98	-2.82	CH4
CO2(g)	-4.97	-6.37	-1.41	CO2
H2(g)	-10.92	-14.05	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.07	-65.93	-2.85	O2

Initial solution 2. NaOH

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

Elements	Molality	Moles
C	1.156e-003	1.156e-003
Ca	2.805e-009	2.805e-009
Cl	8.448e-010	8.448e-010
K	2.700e-010	2.700e-010
Mg	3.433e-010	3.433e-010
N(5)	1.381e-008	1.381e-008
Na	1.834e+001	1.834e+001

S(6) 2.890e-009 2.890e-009

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

pH	=	9.993
pe	=	8.492
Activity of water	=	0.688
Ionic strength	=	9.170e+000
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	2.491e-003
Total CO2 (mol/kg)	=	1.156e-003
Temperature (deg C)	=	20.000
Electrical balance (eq)	=	1.834e+001
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	99.99
Iterations	=	8
Total H	=	1.110129e+002
Total O	=	5.551002e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.011e-004	4.598e-005	-3.995	-4.337	-0.342
H+	1.449e-010	1.016e-010	-9.839	-9.993	-0.154
H2O	5.551e+001	6.882e-001	1.744	-0.162	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-131.316	-130.399	0.917
C(4)	1.156e-003				
NaCO3-	8.675e-004	8.874e-003	-3.062	-2.052	1.010
CO3-2	1.285e-004	1.401e-005	-3.891	-4.854	-0.963
NaHCO3	1.012e-004	8.358e-004	-3.995	-3.078	0.917
HCO3-	5.882e-005	3.380e-005	-4.230	-4.471	-0.241
CO2	1.455e-009	1.202e-008	-8.837	-7.920	0.917
CaCO3	2.212e-011	1.827e-010	-10.655	-9.738	0.917
CaHCO3+	5.865e-012	3.370e-012	-11.232	-11.472	-0.241
MgCO3	3.867e-012	3.194e-011	-11.413	-10.496	0.917
MgHCO3+	9.784e-014	1.001e-012	-13.009	-12.000	1.010
Ca	2.805e-009				
Ca+2	2.776e-009	8.507e-009	-8.557	-8.070	0.486
CaCO3	2.212e-011	1.827e-010	-10.655	-9.738	0.917
CaHCO3+	5.865e-012	3.370e-012	-11.232	-11.472	-0.241
CaOH+	9.347e-013	9.561e-012	-12.029	-11.019	1.010
CaSO4	1.242e-017	1.026e-016	-16.906	-15.989	0.917
CaHSO4+	5.626e-027	5.755e-026	-26.250	-25.240	1.010
Cl	8.448e-010				
Cl-	8.448e-010	5.275e-010	-9.073	-9.278	-0.205
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-41.015	-40.098	0.917
K	2.700e-010				
K+	2.700e-010	1.686e-010	-9.569	-9.773	-0.205
KOH	4.792e-016	3.959e-015	-15.319	-14.402	0.917
KSO4-	6.715e-021	6.869e-020	-20.173	-19.163	1.010
Mg	3.433e-010				
Mg+2	3.354e-010	2.581e-009	-9.474	-8.588	0.886
MgOH+	3.919e-012	4.009e-011	-11.407	-10.397	1.010
MgCO3	3.867e-012	3.194e-011	-11.413	-10.496	0.917
MgHCO3+	9.784e-014	1.001e-012	-13.009	-12.000	1.010
MgSO4	4.071e-018	3.363e-017	-17.390	-16.473	0.917
N(5)	1.381e-008				
NO3-	1.381e-008	5.694e-009	-7.860	-8.245	-0.385
Na	1.834e+001				
Na+	1.834e+001	4.397e+001	1.263	1.643	0.380
NaCO3-	8.675e-004	8.874e-003	-3.062	-2.052	1.010
NaOH	2.382e-004	1.968e-003	-3.623	-2.706	0.917
NaHCO3	1.012e-004	8.358e-004	-3.995	-3.078	0.917
NaSO4-	1.322e-009	1.352e-008	-8.879	-7.869	1.010

```
O(0)            1.715e-015
   O2                   8.576e-016  7.085e-015   -15.067   -14.150     0.917
S(6)            2.890e-009
   SO4-2                1.568e-009  6.337e-011    -8.805   -10.198    -1.394
   NaSO4-               1.322e-009  1.352e-008    -8.879    -7.869     1.010
   CaSO4                1.242e-017  1.026e-016   -16.906   -15.989     0.917
   MgSO4                4.071e-018  3.363e-017   -17.390   -16.473     0.917
   HSO4-                5.500e-020  5.626e-019   -19.260   -18.250     1.010
   KSO4-                6.715e-021  6.869e-020   -20.173   -19.163     1.010
   CaHSO4+              5.626e-027  5.755e-026   -26.250   -25.240     1.010

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

      Phase               SI log IAP  log KT

      Anhydrite       -13.92  -18.27   -4.34  CaSO4
      Aragonite        -4.62  -12.92   -8.31  CaCO3
      Calcite          -4.47  -12.92   -8.45  CaCO3
      CH4(g)        -127.58 -130.40   -2.82  CH4
      CO2(g)           -6.51   -7.92   -1.41  CO2
      Dolomite         -9.39  -26.37  -16.97  CaMg(CO3)2
      Gypsum          -14.01  -18.59   -4.58  CaSO4:2H2O
      H2(g)           -36.97  -40.10   -3.13  H2
      H2O(g)           -1.80   -0.16    1.64  H2O
      Halite           -9.21   -7.63    1.57  NaCl
      O2(g)           -11.30  -14.15   -2.85  O2

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

Reaction step 1.

Using mix 1.      Mix NaOH and GW @ equ w/ calcite

Mixture 1.  Mix NaOH and GW @ equ w/ calcite

       4.000e-001 Solution 1  GW @ eqb w/ Calcite
       6.000e-001 Solution 2  NaOH

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

      Elements           Molality       Moles

      C                6.952e-004  6.952e-004
      Ca               7.173e-007  7.173e-007
      Cl               5.069e-010  5.069e-010
      K                1.620e-010  1.620e-010
      Mg               2.060e-010  2.060e-010
      N                8.286e-009  8.286e-009
      Na               1.100e+001  1.100e+001
      S                1.734e-009  1.734e-009

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

                                     pH  =   9.809      Charge balance
                                     pe  =   9.884      Adjusted to redox equilibrium
                       Activity of water  =   0.813
                          Ionic strength  =  5.502e+000
                     Mass of water (kg)   =  1.000e+000
                Total alkalinity (eq/kg)  =  1.496e-003
                      Total CO2 (mol/kg)  =  6.952e-004
                     Temperature (deg C)  =  20.000
                  Electrical balance (eq) =  1.100e+001
 Percent error, 100*(Cat-|An|)/(Cat+|An|) =  99.99
                              Iterations  =  12
                                 Total H  = 1.110127e+002
```

Total O = 5.550851e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	7.453e-005	3.558e-005	-4.128	-4.449	-0.321
H+	2.190e-010	1.551e-010	-9.660	-9.809	-0.150
H2O	5.551e+001	8.129e-001	1.744	-0.090	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-140.739	-140.189	0.550
C(4)	6.952e-004				
NaCO3-	5.219e-004	1.575e-003	-3.282	-2.803	0.480
NaHCO3	6.378e-005	2.264e-004	-4.195	-3.645	0.550
CO3-2	6.249e-005	7.505e-006	-4.204	-5.125	-0.920
HCO3-	4.696e-005	2.764e-005	-4.328	-4.558	-0.230
CO2	3.580e-009	1.271e-008	-8.446	-7.896	0.550
CaCO3	1.968e-009	6.986e-009	-8.706	-8.156	0.550
CaHCO3+	3.340e-010	1.966e-010	-9.476	-9.706	-0.230
MgCO3	5.953e-013	2.113e-012	-12.225	-11.675	0.550
MgHCO3+	3.349e-014	1.011e-013	-13.475	-12.995	0.480
Ca	7.173e-007				
Ca+2	7.148e-007	6.069e-007	-6.146	-6.217	-0.071
CaCO3	1.968e-009	6.986e-009	-8.706	-8.156	0.550
CaHCO3+	3.340e-010	1.966e-010	-9.476	-9.706	-0.230
CaOH+	1.749e-010	5.278e-010	-9.757	-9.278	0.480
CaSO4	1.438e-015	5.103e-015	-14.842	-14.292	0.550
CaHSO4+	1.449e-024	4.371e-024	-23.839	-23.359	0.480
Cl	5.069e-010				
Cl-	5.069e-010	2.926e-010	-9.295	-9.534	-0.239
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-43.066	-42.515	0.550
K	1.620e-010				
K+	1.620e-010	9.351e-011	-9.790	-10.029	-0.239
KOH	4.786e-016	1.699e-015	-15.320	-14.770	0.550
KSO4-	8.807e-021	2.657e-020	-20.055	-19.576	0.480
Mg	2.060e-010				
Mg+2	2.041e-010	3.186e-010	-9.690	-9.497	0.193
MgOH+	1.269e-012	3.830e-012	-11.896	-11.417	0.480
MgCO3	5.953e-013	2.113e-012	-12.225	-11.675	0.550
MgHCO3+	3.349e-014	1.011e-013	-13.475	-12.995	0.480
MgSO4	8.157e-019	2.896e-018	-18.088	-17.538	0.550
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-63.517	-63.923	-0.406
NH3	0.000e+000	0.000e+000	-64.064	-63.514	0.550
NH4SO4-	0.000e+000	0.000e+000	-73.647	-73.167	0.480
N(0)	6.875e-023				
N2	3.437e-023	1.220e-022	-22.464	-21.914	0.550
N(3)	5.471e-019				
NO2-	5.471e-019	2.396e-019	-18.262	-18.620	-0.359
N(5)	8.286e-009				
NO3-	8.286e-009	3.629e-009	-8.082	-8.440	-0.359
Na	1.100e+001				
Na+	1.100e+001	1.456e+001	1.042	1.163	0.122
NaCO3-	5.219e-004	1.575e-003	-3.282	-2.803	0.480
NaOH	1.420e-004	5.042e-004	-3.848	-3.297	0.550
NaHCO3	6.378e-005	2.264e-004	-4.195	-3.645	0.550
NaSO4-	1.035e-009	3.123e-009	-8.985	-8.505	0.480
O(0)	3.805e-010				
O2	1.903e-010	6.754e-010	-9.721	-9.170	0.550
S(-2)	0.000e+000				
HS-	0.000e+000	0.000e+000	-142.630	-142.952	-0.321
S-2	0.000e+000	0.000e+000	-145.233	-146.211	-0.979
H2S	0.000e+000	0.000e+000	-146.301	-145.751	0.550
S(6)	1.734e-009				
NaSO4-	1.035e-009	3.123e-009	-8.985	-8.505	0.480

SO4-2	6.988e-010	4.419e-011	-9.156	-10.355	-1.199
CaSO4	1.438e-015	5.103e-015	-14.842	-14.292	0.550
MgSO4	8.157e-019	2.896e-018	-18.088	-17.538	0.550
HSO4-	1.985e-019	5.990e-019	-18.702	-18.223	0.480
KSO4-	8.807e-021	2.657e-020	-20.055	-19.576	0.480
CaHSO4+	1.449e-024	4.371e-024	-23.839	-23.359	0.480
NH4SO4-	0.000e+000	0.000e+000	-73.647	-73.167	0.480

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

Phase	SI	log IAP	log KT	
Anhydrite	-12.23	-16.57	-4.34	CaSO4
Aragonite	-3.04	-11.34	-8.31	CaCO3
Calcite	-2.89	-11.34	-8.45	CaCO3
CH4(g)	-137.37	-140.19	-2.82	CH4
CO2(g)	-6.49	-7.90	-1.41	CO2
Dolomite	-8.99	-25.96	-16.97	CaMg(CO3)2
Gypsum	-12.17	-16.75	-4.58	CaSO4:2H2O
H2(g)	-39.39	-42.52	-3.13	H2
H2O(g)	-1.73	-0.09	1.64	H2O
H2S(g)	-144.81	-145.75	-0.94	H2S
Halite	-9.94	-8.37	1.57	NaCl
N2(g)	-18.67	-21.91	-3.24	N2
NH3(g)	-65.39	-63.51	1.87	NH3
O2(g)	-6.32	-9.17	-2.85	O2
Sulfur	-111.36	-106.36	5.00	S

End of simulation.

Reading input data for simulation 2.

End of run.

Run 4 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\eqb mix 2 withmontmorillonite.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\eqb mix 2 withmontmorillonite.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          Ca-Montmorillonite 0 10
      SOLUTION 1
          temp      20
          pH        7.313
          pe        11.534
          redox     pe
          units     mmol/kgw
          density   1
          C         0.004154
          Ca        0.001866
          Cl        8.124e-013
          K         2.601e-013
          Mg        3.308e-013
          N(5)      1.329e-011
          Na        0.008832
          S(6)      2.785e-012
          water    1 # kg
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.

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

      Elements           Molality       Moles

      C                4.154e-006  4.154e-006
      Ca               1.866e-006  1.866e-006
      Cl               8.124e-016  8.124e-016
      K                2.601e-016  2.601e-016
      Mg               3.308e-016  3.308e-016
      N(5)             1.329e-014  1.329e-014
      Na               8.832e-006  8.832e-006
      S(6)             2.785e-015  2.785e-015

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

                                       pH  =   7.313
                                       pe  =  11.534
                          Activity of water  =   1.000
                             Ionic strength  =  1.011e-005
```

```
                    Mass of water (kg)  =  1.000e+000
              Total alkalinity (eq/kg)  =  3.815e-006
                    Total CO2 (mol/kg)  =  4.154e-006
                  Temperature (deg C)   =  20.000
               Electrical balance (eq)  =  8.749e-006
Percent error, 100*(Cat-|An|)/(Cat+|An|) =  53.10
                            Iterations  =   3
                               Total H  = 1.110124e+002
                               Total O  = 5.550623e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.401e-007	1.396e-007	-6.854	-6.855	-0.002
H+	4.882e-008	4.864e-008	-7.311	-7.313	-0.002
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-132.062	-132.062	0.000
C(4)	4.154e-006				
HCO3-	3.717e-006	3.703e-006	-5.430	-5.431	-0.002
CO2	4.339e-007	4.339e-007	-6.363	-6.363	0.000
CO3-2	3.254e-009	3.206e-009	-8.488	-8.494	-0.006
CaHCO3+	8.009e-011	7.980e-011	-10.096	-10.098	-0.002
NaHCO3	1.832e-011	1.832e-011	-10.737	-10.737	0.000
CaCO3	9.042e-012	9.042e-012	-11.044	-11.044	0.000
NaCO3-	4.080e-013	4.065e-013	-12.389	-12.391	-0.002
MgHCO3+	1.390e-020	1.385e-020	-19.857	-19.859	-0.002
MgCO3	9.235e-022	9.235e-022	-21.035	-21.035	0.000
Ca	1.866e-006				
Ca+2	1.866e-006	1.839e-006	-5.729	-5.735	-0.006
CaHCO3+	8.009e-011	7.980e-011	-10.096	-10.098	-0.002
CaCO3	9.042e-012	9.042e-012	-11.044	-11.044	0.000
CaOH+	6.297e-012	6.273e-012	-11.201	-11.202	-0.002
CaSO4	9.597e-019	9.597e-019	-18.018	-18.018	0.000
CaHSO4+	2.587e-025	2.577e-025	-24.587	-24.589	-0.002
Cl	8.124e-016				
Cl-	8.124e-016	8.094e-016	-15.090	-15.092	-0.002
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.822	-40.822	0.000
K	2.601e-016				
K+	2.601e-016	2.591e-016	-15.585	-15.586	-0.002
KOH	1.847e-023	1.847e-023	-22.733	-22.733	0.000
KSO4-	4.588e-030	4.571e-030	-29.338	-29.340	-0.002
Mg	3.308e-016				
Mg+2	3.308e-016	3.259e-016	-15.480	-15.487	-0.006
MgOH+	1.543e-020	1.537e-020	-19.812	-19.813	-0.002
MgHCO3+	1.390e-020	1.385e-020	-19.857	-19.859	-0.002
MgCO3	9.235e-022	9.235e-022	-21.035	-21.035	0.000
MgSO4	1.839e-028	1.839e-028	-27.735	-27.735	0.000
N(5)	1.329e-014				
NO3-	1.329e-014	1.324e-014	-13.876	-13.878	-0.002
Na	8.832e-006				
Na+	8.832e-006	8.800e-006	-5.054	-5.056	-0.002
NaHCO3	1.832e-011	1.832e-011	-10.737	-10.737	0.000
NaOH	1.195e-012	1.195e-012	-11.923	-11.923	0.000
NaCO3-	4.080e-013	4.065e-013	-12.389	-12.391	-0.002
NaSO4-	1.176e-019	1.171e-019	-18.930	-18.931	-0.002
O(0)	8.393e-013				
O2	4.196e-013	4.196e-013	-12.377	-12.377	0.000
S(6)	2.785e-015				
SO4-2	2.784e-015	2.743e-015	-14.555	-14.562	-0.006
CaSO4	9.597e-019	9.597e-019	-18.018	-18.018	0.000
NaSO4-	1.176e-019	1.171e-019	-18.930	-18.931	-0.002
HSO4-	1.170e-020	1.166e-020	-19.932	-19.933	-0.002
CaHSO4+	2.587e-025	2.577e-025	-24.587	-24.589	-0.002

MgSO4	1.839e-028	1.839e-028	-27.735	-27.735	0.000
KSO4-	4.588e-030	4.571e-030	-29.338	-29.340	-0.002

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

Phase	SI	log IAP	log KT	
Anhydrite	-15.95	-20.30	-4.34	CaSO4
Aragonite	-5.92	-14.23	-8.31	CaCO3
Calcite	-5.78	-14.23	-8.45	CaCO3
CH4(g)	-129.24	-132.06	-2.82	CH4
CO2(g)	-4.96	-6.36	-1.41	CO2
Dolomite	-21.24	-38.21	-16.97	CaMg(CO3)2
Gypsum	-15.72	-20.30	-4.58	CaSO4:2H2O
H2(g)	-37.69	-40.82	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
Halite	-21.72	-20.15	1.57	NaCl
O2(g)	-9.52	-12.38	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca-Montmorillonite	0.00	-45.76	-45.76	1.000e+001	1.000e+001	-2.061e-006

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

Elements	Molality	Moles
Al	4.802e-006	4.802e-006
C	4.154e-006	4.154e-006
Ca	2.206e-006	2.206e-006
Cl	8.124e-016	8.124e-016
K	2.601e-016	2.601e-016
Mg	3.308e-016	3.308e-016
N	1.329e-014	1.329e-014
Na	8.832e-006	8.832e-006
S	2.785e-015	2.785e-015
Si	7.563e-006	7.563e-006

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

```
                                    pH  =   6.617      Charge balance
                                    pe  =  12.232      Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  1.255e-005
                    Mass of water (kg)  =  1.000e+000
            Total alkalinity (eq/kg)    =  1.890e-005
                   Total CO2 (mol/kg)   =  4.154e-006
                  Temperature (deg C)   =  20.000
             Electrical balance (eq)    =  8.749e-006
Percent error, 100*(Cat-|An|)/(Cat+|An|) =  42.54
                             Iterations =   9
                                Total H = 1.110124e+002
                                Total O = 5.550625e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.427e-007	2.417e-007	-6.615	-6.617	-0.002
OH-	2.821e-008	2.809e-008	-7.550	-7.551	-0.002
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Al	4.802e-006				
Al(OH)4-	3.246e-006	3.233e-006	-5.489	-5.490	-0.002
Al(OH)2+	1.061e-006	1.057e-006	-5.974	-5.976	-0.002
Al(OH)3	4.405e-007	4.405e-007	-6.356	-6.356	0.000
AlOH+2	5.195e-008	5.110e-008	-7.284	-7.292	-0.007
Al+3	1.792e-009	1.727e-009	-8.747	-8.763	-0.016
AlSO4+	1.406e-020	1.400e-020	-19.852	-19.854	-0.002
AlHSO4+2	2.928e-028	2.880e-028	-27.533	-27.541	-0.007
Al(SO4)2-	1.189e-033	1.184e-033	-32.925	-32.927	-0.002
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-131.527	-131.527	0.000
C(4)	4.154e-006				
HCO3-	2.629e-006	2.618e-006	-5.580	-5.582	-0.002
CO2	1.524e-006	1.524e-006	-5.817	-5.817	0.000
CO3-2	4.638e-010	4.563e-010	-9.334	-9.341	-0.007
CaHCO3+	6.687e-011	6.659e-011	-10.175	-10.177	-0.002
NaHCO3	1.295e-011	1.295e-011	-10.888	-10.888	0.000
CaCO3	1.519e-012	1.519e-012	-11.819	-11.819	0.000
NaCO3-	5.806e-014	5.782e-014	-13.236	-13.238	-0.002
MgHCO3+	9.816e-021	9.776e-021	-20.008	-20.010	-0.002
MgCO3	1.312e-022	1.312e-022	-21.882	-21.882	0.000
Ca	2.206e-006				
Ca+2	2.206e-006	2.170e-006	-5.656	-5.664	-0.007
CaHCO3+	6.687e-011	6.659e-011	-10.175	-10.177	-0.002
CaCO3	1.519e-012	1.519e-012	-11.819	-11.819	0.000
CaOH+	1.496e-012	1.490e-012	-11.825	-11.827	-0.002
CaSO4	1.131e-018	1.131e-018	-17.947	-17.947	0.000
CaHSO4+	1.515e-024	1.509e-024	-23.820	-23.821	-0.002
Cl	8.124e-016				
Cl-	8.124e-016	8.091e-016	-15.090	-15.092	-0.002
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.825	-40.825	0.000
K	2.601e-016				
K+	2.601e-016	2.590e-016	-15.585	-15.587	-0.002
KOH	3.717e-024	3.717e-024	-23.430	-23.430	0.000
KSO4-	4.580e-030	4.561e-030	-29.339	-29.341	-0.002
Mg	3.308e-016				
Mg+2	3.308e-016	3.254e-016	-15.480	-15.488	-0.007
MgHCO3+	9.816e-021	9.776e-021	-20.008	-20.010	-0.002
MgOH+	3.101e-021	3.089e-021	-20.508	-20.510	-0.002
MgCO3	1.312e-022	1.312e-022	-21.882	-21.882	0.000
MgSO4	1.833e-028	1.833e-028	-27.737	-27.737	0.000
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-56.482	-56.483	-0.002
NH3	0.000e+000	0.000e+000	-59.267	-59.267	0.000
NH4SO4-	0.000e+000	0.000e+000	-69.934	-69.936	-0.002
N(0)	6.446e-019				
N2	3.223e-019	3.223e-019	-18.492	-18.492	0.000
N(3)	3.498e-023				
NO2-	3.498e-023	3.484e-023	-22.456	-22.458	-0.002
N(5)	1.329e-014				
NO3-	1.329e-014	1.323e-014	-13.876	-13.878	-0.002
Na	8.832e-006				
Na+	8.832e-006	8.796e-006	-5.054	-5.056	-0.002
NaHCO3	1.295e-011	1.295e-011	-10.888	-10.888	0.000
NaOH	2.405e-013	2.405e-013	-12.619	-12.619	0.000
NaCO3-	5.806e-014	5.782e-014	-13.236	-13.238	-0.002
NaSO4-	1.174e-019	1.169e-019	-18.930	-18.932	-0.002
O(0)	8.500e-013				
O2	4.250e-013	4.250e-013	-12.372	-12.372	0.000

S(-2)	0.000e+000					
H2S		0.000e+000	0.000e+000	-137.171	-137.171	0.000
HS-		0.000e+000	0.000e+000	-137.563	-137.564	-0.002
S-2		0.000e+000	0.000e+000	-144.010	-144.017	-0.007
S(6)	2.785e-015					
SO4-2		2.784e-015	2.738e-015	-14.555	-14.562	-0.007
CaSO4		1.131e-018	1.131e-018	-17.947	-17.947	0.000
NaSO4-		1.174e-019	1.169e-019	-18.930	-18.932	-0.002
HSO4-		5.806e-020	5.782e-020	-19.236	-19.238	-0.002
AlSO4+		1.406e-020	1.400e-020	-19.852	-19.854	-0.002
CaHSO4+		1.515e-024	1.509e-024	-23.820	-23.821	-0.002
AlHSO4+2		2.928e-028	2.880e-028	-27.533	-27.541	-0.007
MgSO4		1.833e-028	1.833e-028	-27.737	-27.737	0.000
KSO4-		4.580e-030	4.561e-030	-29.339	-29.341	-0.002
Al(SO4)2-		1.189e-033	1.184e-033	-32.925	-32.927	-0.002
NH4SO4-		0.000e+000	0.000e+000	-69.934	-69.936	-0.002
Si	7.563e-006					
H4SiO4		7.559e-006	7.559e-006	-5.122	-5.122	0.000
H3SiO4-		3.869e-009	3.854e-009	-8.412	-8.414	-0.002
H2SiO4-2		7.884e-016	7.756e-016	-15.103	-15.110	-0.007

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

Phase	SI	log IAP	log KT	
Al(OH)3(a)	-0.04	11.09	11.13	Al(OH)3
Albite	-7.58	-25.91	-18.33	NaAlSi3O8
Alunite	-30.53	-31.30	-0.77	KAl3(SO4)2(OH)6
Anhydrite	-15.88	-20.23	-4.34	CaSO4
Anorthite	-7.03	-26.89	-19.86	CaAl2Si2O8
Aragonite	-6.70	-15.00	-8.31	CaCO3
Ca-Montmorillonite	0.00	-45.76	-45.76	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-6.55	-15.00	-8.45	CaCO3
CH4(g)	-128.71	-131.53	-2.82	CH4
Chalcedony	-1.51	-5.12	-3.61	SiO2
Chlorite(14A)	-74.73	-4.46	70.27	Mg5Al2Si3O10(OH)8
Chrysotile	-49.84	-17.01	32.83	Mg3Si2O5(OH)4
CO2(g)	-4.41	-5.82	-1.41	CO2
Dolomite	-22.86	-39.83	-16.97	CaMg(CO3)2
Gibbsite	2.69	11.09	8.40	Al(OH)3
Gypsum	-15.64	-20.23	-4.58	CaSO4:2H2O
H2(g)	-37.70	-40.82	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
H2S(g)	-136.23	-137.17	-0.94	H2S
Halite	-21.72	-20.15	1.57	NaCl
Illite	-10.77	-51.72	-40.95	K0.6Mg0.25Al2.3Si3.5O10(OH)2
K-feldspar	-15.48	-36.44	-20.96	KAlSi3O8
K-mica	-4.52	8.93	13.45	KAl3Si3O10(OH)2
Kaolinite	4.06	11.93	7.88	Al2Si2O5(OH)4
N2(g)	-15.25	-18.49	-3.24	N2
NH3(g)	-61.14	-59.27	1.87	NH3
O2(g)	-9.52	-12.37	-2.85	O2
Quartz	-1.07	-5.12	-4.06	SiO2
Sepiolite	-35.77	-19.87	15.89	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-38.53	-19.87	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-2.37	-5.12	-2.75	SiO2
Sulfur	-104.48	-99.47	5.00	S
Talc	-49.23	-27.25	21.98	Mg3Si4O10(OH)2

End of simulation.

Reading input data for simulation 2.

```
-----------
End of run.
-----------
```

Run 5

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\40%rainwater+60%NaOH.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\40%rainwater+60%NaOH.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          CO2(g)    -3.5 10
      SOLUTION 1 rainwater
          temp      25
          pH        5.24
          pe        4
          redox     pe
          units     mg/l
          density   1
          Ca        0.458
          Mg        0.034
          Na        0.082
          K         0.043
          Cl        0.122
          S(6)      1.131
          N(5)      1.004
          N(-3)     0.36
          water    1 # kg
      SOLUTION 2 NaOH
          temp      20
          pH        14
          pe        4
          redox     pe
          units     mmol/kgw
          density   1
          Na        24.9 mol/kgw
          water    1 # kg
      MIX 1
          1    0.4
          2    0.6
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     rainwater

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

      Elements           Molality       Moles

      Ca               1.143e-005  1.143e-005
      Cl               3.441e-006  3.441e-006
      K                1.100e-006  1.100e-006
```

Mg	1.398e-006	1.398e-006
N(-3)	2.570e-005	2.570e-005
N(5)	7.168e-005	7.168e-005
Na	3.567e-006	3.567e-006
S(6)	1.177e-005	1.177e-005

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

pH	=	5.240
pe	=	4.000
Activity of water	=	1.000
Ionic strength	=	1.047e-004
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	-5.824e-006
Total carbon (mol/kg)	=	0.000e+000
Total CO2 (mol/kg)	=	0.000e+000
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	-3.682e-005
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-22.96
Iterations	=	3
Total H	=	1.110125e+002
Total O	=	5.550648e+001

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

Redox couple	pe	Eh (volts)
N(-3)/N(5)	8.3903	0.4963

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	5.822e-006	5.754e-006	-5.235	-5.240	-0.005
OH-	1.760e-009	1.740e-009	-8.754	-8.760	-0.005
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Ca	1.143e-005				
Ca+2	1.140e-005	1.088e-005	-4.943	-4.963	-0.020
CaSO4	2.429e-008	2.429e-008	-7.614	-7.614	0.000
CaHSO4+	8.288e-013	8.190e-013	-12.082	-12.087	-0.005
CaOH+	3.174e-013	3.137e-013	-12.498	-12.503	-0.005
Cl	3.441e-006				
Cl-	3.441e-006	3.401e-006	-5.463	-5.468	-0.005
H(0)	4.688e-022				
H2	2.344e-022	2.344e-022	-21.630	-21.630	0.000
K	1.100e-006				
K+	1.100e-006	1.087e-006	-5.959	-5.964	-0.005
KSO4-	8.649e-011	8.547e-011	-10.063	-10.068	-0.005
KOH	6.547e-016	6.548e-016	-15.184	-15.184	0.000
Mg	1.398e-006				
Mg+2	1.395e-006	1.331e-006	-5.855	-5.876	-0.020
MgSO4	3.492e-009	3.492e-009	-8.457	-8.457	0.000
MgOH+	8.497e-013	8.397e-013	-12.071	-12.076	-0.005
N(-3)	2.570e-005				
NH4+	2.570e-005	2.539e-005	-4.590	-4.595	-0.005
NH4SO4-	3.705e-009	3.662e-009	-8.431	-8.436	-0.005
NH3	2.515e-009	2.515e-009	-8.600	-8.600	0.000
N(5)	7.168e-005				
NO3-	7.168e-005	7.083e-005	-4.145	-4.150	-0.005
Na	3.567e-006				
Na+	3.567e-006	3.525e-006	-5.448	-5.453	-0.005
NaSO4-	2.001e-010	1.977e-010	-9.699	-9.704	-0.005
NaOH	4.047e-015	4.047e-015	-14.393	-14.393	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-49.120	-49.120	0.000
S(6)	1.177e-005				

SO4-2	1.174e-005	1.119e-005	-4.931	-4.951	-0.021
CaSO4	2.429e-008	2.429e-008	-7.614	-7.614	0.000
HSO4-	6.337e-009	6.263e-009	-8.198	-8.203	-0.005
NH4SO4-	3.705e-009	3.662e-009	-8.431	-8.436	-0.005
MgSO4	3.492e-009	3.492e-009	-8.457	-8.457	0.000
NaSO4-	2.001e-010	1.977e-010	-9.699	-9.704	-0.005
KSO4-	8.649e-011	8.547e-011	-10.063	-10.068	-0.005
CaHSO4+	8.288e-013	8.190e-013	-12.082	-12.087	-0.005

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

Phase	SI	log IAP	log KT	
Anhydrite	-5.55	-9.91	-4.36	CaSO4
Gypsum	-5.33	-9.91	-4.58	CaSO4:2H2O
H2(g)	-18.48	-21.63	-3.15	H2
H2O(g)	-1.51	-0.00	1.51	H2O
Halite	-12.50	-10.92	1.58	NaCl
NH3(g)	-10.37	-8.60	1.77	NH3
O2(g)	-46.23	-49.12	-2.89	O2

Initial solution 2. NaOH

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

Elements	Molality	Moles
Na	2.490e+001	2.490e+001

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

pH	=	14.000
pe	=	4.000
Activity of water	=	0.562
Ionic strength	=	1.184e+001
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	2.931e+000
Total carbon (mol/kg)	=	0.000e+000
Total CO2 (mol/kg)	=	0.000e+000
Temperature (deg C)	=	20.000
Electrical balance (eq)	=	2.197e+001
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	92.76
Iterations	=	6
Total H	=	1.139431e+002
Total O	=	5.843693e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	8.574e-001	3.816e-001	-0.067	-0.418	-0.352
H+	1.432e-014	1.000e-014	-13.844	-14.000	-0.156
H2O	5.551e+001	5.621e-001	1.744	-0.250	0.000
H(0)	0.000e+000				
H2	0.000e+000	7.447e-040	-40.312	-39.128	1.184
Na	2.490e+001				
Na+	2.283e+001	8.532e+001	1.358	1.931	0.573
NaOH	2.073e+000	3.169e+001	0.317	1.501	1.184
O(0)	7.102e-018				
O2	3.551e-018	5.427e-017	-17.450	-16.265	1.184

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

Phase	SI	log IAP	log KT	
H2(g)	-36.00	-39.13	-3.13	H2

```
      H2O(g)            -1.89   -0.25    1.64  H2O
      O2(g)            -13.41  -16.27   -2.85  O2

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

 Reaction step 1.

 Using mix 1.
 Using pure phase assemblage 1.

 Mixture 1.

       4.000e-001 Solution 1  rainwater
       6.000e-001 Solution 2  NaOH

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

                                                        Moles in assemblage
 Phase                    SI log IAP  log KT      Initial       Final       Delta

 CO2(g)               -3.50   -4.93   -1.43   1.000e+001  9.057e+000 -9.431e-001

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

      Elements           Molality       Moles

      C                9.295e-001  9.431e-001
      Ca               4.505e-006  4.571e-006
      Cl               1.357e-006  1.376e-006
      K                4.335e-007  4.399e-007
      Mg               5.513e-007  5.594e-007
      N                3.839e-005  3.895e-005
      Na               1.472e+001  1.494e+001
      S                4.641e-006  4.709e-006

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

                                       pH  =   9.900      Charge balance
                                       pe  =   8.565      Adjusted to redox equilibrium
                          Activity of water  =   0.747
                             Ionic strength  =  7.534e+000
                        Mass of water (kg)   =  1.015e+000
                  Total alkalinity (eq/kg)   =  1.733e+000
                        Total CO2 (mol/kg)   =  9.295e-001
                      Temperature (deg C)    =  22.000
                   Electrical balance (eq)   =  1.318e+001
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   =  87.28
                                Iterations   =  22
                                   Total H   = 1.127709e+002
                                   Total O   = 5.915103e+001

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

                                                   Log       Log        Log
   Species                 Molality    Activity  Molality  Activity    Gamma

   OH-                   1.020e-004  4.713e-005    -3.991    -4.327    -0.335
   H+                    1.792e-010  1.260e-010    -9.747    -9.900    -0.153
   H2O                   5.551e+001  7.473e-001     1.744    -0.127     0.000
C(-4)            0.000e+000
   CH4                   0.000e+000  0.000e+000  -128.346  -127.593     0.753
C(4)             9.295e-001
   NaCO3-                7.110e-001  4.225e+000    -0.148     0.626     0.774
   CO3-2                 9.225e-002  1.036e-002    -1.035    -1.985    -0.950
   NaHCO3                7.506e-002  4.255e-001    -1.125    -0.371     0.753
```

HCO3-	5.122e-002	2.965e-002	-1.291	-1.528	-0.237
CaCO3	3.179e-006	1.802e-005	-5.498	-4.744	0.753
CO2	2.064e-006	1.170e-005	-5.685	-4.932	0.753
CaHCO3+	6.821e-007	3.949e-007	-6.166	-6.404	-0.237
MgCO3	4.605e-007	2.610e-006	-6.337	-5.583	0.753
MgHCO3+	1.594e-008	9.473e-008	-7.798	-7.024	0.774
Ca	4.505e-006				
CaCO3	3.179e-006	1.802e-005	-5.498	-4.744	0.753
CaHCO3+	6.821e-007	3.949e-007	-6.166	-6.404	-0.237
Ca+2	6.433e-007	1.096e-006	-6.192	-5.960	0.231
CaOH+	1.815e-010	1.078e-009	-9.741	-8.967	0.774
CaSO4	4.177e-012	2.368e-011	-11.379	-10.626	0.753
CaHSO4+	2.836e-021	1.686e-020	-20.547	-19.773	0.774
Cl	1.357e-006				
Cl-	1.357e-006	8.133e-007	-5.868	-6.090	-0.222
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.819	-40.066	0.753
K	4.335e-007				
K+	4.335e-007	2.599e-007	-6.363	-6.585	-0.222
KOH	9.426e-013	5.343e-012	-12.026	-11.272	0.753
KSO4-	3.246e-014	1.929e-013	-13.489	-12.715	0.774
Mg	5.513e-007				
MgCO3	4.605e-007	2.610e-006	-6.337	-5.583	0.753
Mg+2	7.413e-008	2.765e-007	-7.130	-6.558	0.572
MgHCO3+	1.594e-008	9.473e-008	-7.798	-7.024	0.774
MgOH+	7.617e-010	4.526e-009	-9.118	-8.344	0.774
MgSO4	1.178e-012	6.675e-012	-11.929	-11.176	0.753
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-51.265	-51.693	-0.428
NH3	0.000e+000	0.000e+000	-51.885	-51.131	0.753
NH4SO4-	0.000e+000	0.000e+000	-58.311	-57.537	0.774
N(0)	1.621e-005				
N2	8.106e-006	4.594e-005	-5.091	-4.338	0.753
N(3)	2.753e-013				
NO2-	2.753e-013	1.158e-013	-12.560	-12.936	-0.376
N(5)	2.218e-005				
NO3-	2.218e-005	9.331e-006	-4.654	-5.030	-0.376
Na	1.472e+001				
Na+	1.394e+001	2.552e+001	1.144	1.407	0.263
NaCO3-	7.110e-001	4.225e+000	-0.148	0.626	0.774
NaHCO3	7.506e-002	4.255e-001	-1.125	-0.371	0.753
NaOH	1.764e-004	9.996e-004	-3.754	-3.000	0.753
NaSO4-	2.351e-006	1.397e-005	-5.629	-4.855	0.774
O(0)	1.168e-014				
O2	5.842e-015	3.312e-014	-14.233	-13.480	0.753
S(-2)	0.000e+000				
HS-	0.000e+000	0.000e+000	-129.628	-129.963	-0.335
S-2	0.000e+000	0.000e+000	-132.060	-133.072	-1.012
H2S	0.000e+000	0.000e+000	-133.634	-132.881	0.753
S(6)	4.641e-006				
NaSO4-	2.351e-006	1.397e-005	-5.629	-4.855	0.774
SO4-2	2.290e-006	1.114e-007	-5.640	-6.953	-1.313
CaSO4	4.177e-012	2.368e-011	-11.379	-10.626	0.753
MgSO4	1.178e-012	6.675e-012	-11.929	-11.176	0.753
KSO4-	3.246e-014	1.929e-013	-13.489	-12.715	0.774
HSO4-	2.153e-016	1.279e-015	-15.667	-14.893	0.774
CaHSO4+	2.836e-021	1.686e-020	-20.547	-19.773	0.774
NH4SO4-	0.000e+000	0.000e+000	-58.311	-57.537	0.774

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

Phase	SI	log IAP	log KT	
Anhydrite	-8.56	-12.91	-4.35	CaSO4
Aragonite	0.37	-7.94	-8.32	CaCO3
Calcite	0.52	-7.94	-8.46	CaCO3
CH4(g)	-124.76	-127.59	-2.83	CH4

CO2(g)	-3.50	-4.93	-1.43	CO2
Dolomite	0.53	-16.49	-17.02	CaMg(CO3)2
Gypsum	-8.59	-13.17	-4.58	CaSO4:2H2O
H2(g)	-36.93	-40.07	-3.14	H2
H2O(g)	-1.71	-0.13	1.59	H2O
H2S(g)	-131.92	-132.88	-0.96	H2S
Halite	-6.26	-4.68	1.58	NaCl
N2(g)	-1.09	-4.34	-3.25	N2
NH3(g)	-52.96	-51.13	1.83	NH3
O2(g)	-10.61	-13.48	-2.87	O2
Sulfur	-100.90	-95.95	4.95	S

```
------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 2.
------------------------------------

-----------
End of run.
-----------
```

```
    Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\mix rain NaOH and calcite GW.pqi
   Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\mix rain NaOH and calcite GW.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 2 NaOH
          temp      20
          pH        9.9
          pe        8.565
          redox     pe
          units     mmol/kgw
          density   1
          Na        14.72 Mol/kgw
          C         0.9295
          Ca        4.505e-006
          Cl        1.354e-006
          K         4.335e-007
          Mg        5.513e-007
          N(5)      2.218e-005
          S(6)      4.641e-006
          water    1 # kg
      SOLUTION 1 GW @ eqb w/ Calcite
          temp      20
          pH        7.301
          pe        -1.841
          redox     pe
          units     mmol/kgw
          density   1
          Ca        0.001789
          C         0.003961
          water    1 # kg
      SAVE solution 1-2
      MIX 1 Mix NaOH and GW @ equ w/ calcite
          1    0.4
          2    0.6
------------------------------------------
Beginning of initial solution calculations.
------------------------------------------

Initial solution 1.     GW @ eqb w/ Calcite

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

      Elements           Molality       Moles

      C                 3.961e-006  3.961e-006
      Ca                1.789e-006  1.789e-006
```

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

pH	=	7.301
pe	=	-1.841
Activity of water	=	1.000
Ionic strength	=	5.444e-006
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	3.626e-006
Total CO2 (mol/kg)	=	3.961e-006
Temperature (deg C)	=	20.000
Electrical balance (eq)	=	-4.751e-008
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-0.65
Iterations	=	3
Total H	=	1.110124e+002
Total O	=	5.550623e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.361e-007	1.358e-007	-6.866	-6.867	-0.001
H+	5.014e-008	5.000e-008	-7.300	-7.301	-0.001
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	1.058e-025				
CH4	1.058e-025	1.058e-025	-24.975	-24.975	0.000
C(4)	3.961e-006				
HCO3-	3.533e-006	3.524e-006	-5.452	-5.453	-0.001
CO2	4.245e-007	4.245e-007	-6.372	-6.372	0.000
CO3-2	3.000e-009	2.968e-009	-8.523	-8.528	-0.005
CaHCO3+	7.328e-011	7.309e-011	-10.135	-10.136	-0.001
CaCO3	8.056e-012	8.056e-012	-11.094	-11.094	0.000
Ca	1.789e-006				
Ca+2	1.789e-006	1.770e-006	-5.747	-5.752	-0.005
CaHCO3+	7.328e-011	7.309e-011	-10.135	-10.136	-0.001
CaCO3	8.056e-012	8.056e-012	-11.094	-11.094	0.000
CaOH+	5.889e-012	5.873e-012	-11.230	-11.231	-0.001
H(0)	1.791e-014				
H2	8.953e-015	8.953e-015	-14.048	-14.048	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-65.925	-65.925	0.000

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

Phase	SI	log IAP	log KT	
Aragonite	-5.97	-14.28	-8.31	CaCO3
Calcite	-5.83	-14.28	-8.45	CaCO3
CH4(g)	-22.16	-24.98	-2.82	CH4
CO2(g)	-4.97	-6.37	-1.41	CO2
H2(g)	-10.92	-14.05	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.07	-65.93	-2.85	O2

Initial solution 2. NaOH

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

Elements	Molality	Moles
C	9.295e-004	9.295e-004
Ca	4.505e-009	4.505e-009
Cl	1.354e-009	1.354e-009
K	4.335e-010	4.335e-010
Mg	5.513e-010	5.513e-010
N(5)	2.218e-008	2.218e-008
Na	1.472e+001	1.472e+001

S(6) 4.641e-009 4.641e-009

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

pH	=	9.900
pe	=	8.565
Activity of water	=	0.750
Ionic strength	=	7.360e+000
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	1.999e-003
Total CO2 (mol/kg)	=	9.295e-004
Temperature (deg C)	=	20.000
Electrical balance (eq)	=	1.472e+001
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	99.99
Iterations	=	8
Total H	=	1.110128e+002
Total O	=	5.550928e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	8.713e-005	4.043e-005	-4.060	-4.393	-0.333
H+	1.788e-010	1.259e-010	-9.748	-9.900	-0.152
H2O	5.551e+001	7.498e-001	1.744	-0.125	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-131.032	-130.296	0.736
C(4)	9.295e-004				
NaCO3-	7.013e-004	3.910e-003	-3.154	-2.408	0.746
CO3-2	9.117e-005	1.034e-005	-4.040	-4.985	-0.945
NaHCO3	8.377e-005	4.561e-004	-4.077	-3.341	0.736
HCO3-	5.326e-005	3.091e-005	-4.274	-4.510	-0.236
CO2	2.296e-009	1.250e-008	-8.639	-7.903	0.736
CaCO3	2.102e-011	1.145e-010	-10.677	-9.941	0.736
CaHCO3+	4.506e-012	2.615e-012	-11.346	-11.583	-0.236
MgCO3	3.169e-012	1.725e-011	-11.499	-10.763	0.736
MgHCO3+	1.201e-013	6.696e-013	-12.920	-12.174	0.746
Ca	4.505e-009				
Ca+2	4.478e-009	7.219e-009	-8.349	-8.142	0.207
CaCO3	2.102e-011	1.145e-010	-10.677	-9.941	0.736
CaHCO3+	4.506e-012	2.615e-012	-11.346	-11.583	-0.236
CaOH+	1.280e-012	7.135e-012	-11.893	-11.147	0.746
CaSO4	2.731e-017	1.487e-016	-16.564	-15.828	0.736
CaHSO4+	1.854e-026	1.034e-025	-25.732	-24.986	0.746
Cl	1.354e-009				
Cl-	1.354e-009	8.102e-010	-8.868	-9.091	-0.223
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.794	-40.058	0.736
K	4.335e-010				
K+	4.335e-010	2.594e-010	-9.363	-9.586	-0.223
KOH	9.837e-016	5.357e-015	-15.007	-14.271	0.736
KSO4-	3.239e-020	1.806e-019	-19.490	-18.743	0.746
Mg	5.513e-010				
Mg+2	5.434e-010	1.888e-009	-9.265	-8.724	0.541
MgOH+	4.627e-012	2.580e-011	-11.335	-10.588	0.746
MgCO3	3.169e-012	1.725e-011	-11.499	-10.763	0.736
MgHCO3+	1.201e-013	6.696e-013	-12.920	-12.174	0.746
MgSO4	7.721e-018	4.204e-017	-17.112	-16.376	0.736
N(5)	2.218e-008				
NO3-	2.218e-008	9.379e-009	-7.654	-8.028	-0.374
Na	1.472e+001				
Na+	1.472e+001	2.624e+001	1.168	1.419	0.251
NaCO3-	7.013e-004	3.910e-003	-3.154	-2.408	0.746
NaOH	1.896e-004	1.033e-003	-3.722	-2.986	0.736
NaHCO3	8.377e-005	4.561e-004	-4.077	-3.341	0.736
NaSO4-	2.473e-009	1.379e-008	-8.607	-7.860	0.746

```
O(0)            2.569e-015
   O2                   1.284e-015  6.994e-015   -14.891   -14.155     0.736
S(6)            4.641e-009
   NaSO4-               2.473e-009  1.379e-008    -8.607    -7.860     0.746
   SO4-2                2.168e-009  1.083e-010    -8.664    -9.965    -1.301
   CaSO4                2.731e-017  1.487e-016   -16.564   -15.828     0.736
   MgSO4                7.721e-018  4.204e-017   -17.112   -16.376     0.736
   HSO4-                2.136e-019  1.191e-018   -18.670   -17.924     0.746
   KSO4-                3.239e-020  1.806e-019   -19.490   -18.743     0.746
   CaHSO4+              1.854e-026  1.034e-025   -25.732   -24.986     0.746

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

      Phase               SI log IAP  log KT

      Anhydrite       -13.76  -18.11   -4.34  CaSO4
      Aragonite        -4.82  -13.13   -8.31  CaCO3
      Calcite          -4.67  -13.13   -8.45  CaCO3
      CH4(g)        -127.48 -130.30   -2.82  CH4
      CO2(g)           -6.50   -7.90   -1.41  CO2
      Dolomite         -9.86  -26.84  -16.97  CaMg(CO3)2
      Gypsum          -13.78  -18.36   -4.58  CaSO4:2H2O
      H2(g)           -36.93  -40.06   -3.13  H2
      H2O(g)           -1.77   -0.13    1.64  H2O
      Halite           -9.24   -7.67    1.57  NaCl
      O2(g)           -11.30  -14.16   -2.85  O2

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

Reaction step 1.

Using mix 1.      Mix NaOH and GW @ equ w/ calcite

Mixture 1.  Mix NaOH and GW @ equ w/ calcite

       4.000e-001 Solution 1  GW @ eqb w/ Calcite
       6.000e-001 Solution 2  NaOH

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

      Elements           Molality       Moles

      C                5.593e-004  5.593e-004
      Ca               7.183e-007  7.183e-007
      Cl               8.124e-010  8.124e-010
      K                2.601e-010  2.601e-010
      Mg               3.308e-010  3.308e-010
      N                1.331e-008  1.331e-008
      Na               8.832e+000  8.832e+000
      S                2.785e-009  2.785e-009

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

                                     pH  =   9.748      Charge balance
                                     pe  =   9.092      Adjusted to redox equilibrium
                       Activity of water  =   0.850
                          Ionic strength  =  4.416e+000
                     Mass of water (kg)   =  1.000e+000
                Total alkalinity (eq/kg)  =  1.201e-003
                      Total CO2 (mol/kg)  =  5.593e-004
                    Temperature (deg C)   =  20.000
                 Electrical balance (eq)  =  8.831e+000
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  99.99
                              Iterations  =  22
                                 Total H  = 1.110127e+002
```

Total O = 5.550806e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.623e-005	3.233e-005	-4.179	-4.490	-0.311
H+	2.506e-010	1.784e-010	-9.601	-9.748	-0.148
H2O	5.551e+001	8.499e-001	1.744	-0.071	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-133.826	-133.385	0.442
C(4)	5.593e-004				
NaCO3-	4.137e-004	8.783e-004	-3.383	-3.056	0.327
NaHCO3	5.254e-005	1.453e-004	-4.279	-3.838	0.442
CO3-2	4.907e-005	6.175e-006	-4.309	-5.209	-0.900
HCO3-	4.393e-005	2.616e-005	-4.357	-4.582	-0.225
CO2	4.788e-009	1.324e-008	-8.320	-7.878	0.442
CaCO3	1.454e-009	4.020e-009	-8.837	-8.396	0.442
CaHCO3+	2.186e-010	1.302e-010	-9.660	-9.885	-0.225
MgCO3	6.423e-013	1.776e-012	-12.192	-11.751	0.442
MgHCO3+	4.601e-014	9.768e-014	-13.337	-13.010	0.327
Ca	7.183e-007				
Ca+2	7.165e-007	4.245e-007	-6.145	-6.372	-0.227
CaCO3	1.454e-009	4.020e-009	-8.837	-8.396	0.442
CaHCO3+	2.186e-010	1.302e-010	-9.660	-9.885	-0.225
CaOH+	1.581e-010	3.355e-010	-9.801	-9.474	0.327
CaSO4	2.251e-015	6.224e-015	-14.648	-14.206	0.442
CaHSO4+	2.888e-024	6.131e-024	-23.539	-23.212	0.327
Cl	8.124e-010				
Cl-	8.124e-010	4.620e-010	-9.090	-9.335	-0.245
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-41.251	-40.809	0.442
K	2.601e-010				
K+	2.601e-010	1.479e-010	-9.585	-9.830	-0.245
KOH	8.836e-016	2.443e-015	-15.054	-14.612	0.442
KSO4-	3.452e-020	7.328e-020	-19.462	-19.135	0.327
Mg	3.308e-010				
Mg+2	3.284e-010	3.254e-010	-9.484	-9.488	-0.004
MgOH+	1.675e-012	3.555e-012	-11.776	-11.449	0.327
MgCO3	6.423e-013	1.776e-012	-12.192	-11.751	0.442
MgHCO3+	4.601e-014	9.768e-014	-13.337	-13.010	0.327
MgSO4	1.865e-018	5.156e-018	-17.729	-17.288	0.442
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-56.426	-56.816	-0.390
NH3	0.000e+000	0.000e+000	-56.909	-56.468	0.442
NH4SO4-	0.000e+000	0.000e+000	-66.146	-65.819	0.327
N(0)	8.293e-014				
N2	4.147e-014	1.146e-013	-13.382	-12.941	0.442
N(3)	4.273e-017				
NO2-	4.273e-017	1.925e-017	-16.369	-16.716	-0.346
N(5)	1.331e-008				
NO3-	1.331e-008	5.995e-009	-7.876	-8.222	-0.346
Na	8.832e+000				
Na+	8.831e+000	9.872e+000	0.946	0.994	0.048
NaCO3-	4.137e-004	8.783e-004	-3.383	-3.056	0.327
NaOH	1.124e-004	3.106e-004	-3.949	-3.508	0.442
NaHCO3	5.254e-005	1.453e-004	-4.279	-3.838	0.442
NaSO4-	1.739e-009	3.692e-009	-8.760	-8.433	0.327
O(0)	2.066e-013				
O2	1.033e-013	2.856e-013	-12.986	-12.544	0.442
S(-2)	0.000e+000				
HS-	0.000e+000	0.000e+000	-135.590	-135.902	-0.311
S-2	0.000e+000	0.000e+000	-138.266	-139.222	-0.956
H2S	0.000e+000	0.000e+000	-139.082	-138.640	0.442
S(6)	2.785e-009				
NaSO4-	1.739e-009	3.692e-009	-8.760	-8.433	0.327

SO4-2	1.046e-009	7.705e-011	-8.981	-10.113	-1.133
CaSO4	2.251e-015	6.224e-015	-14.648	-14.206	0.442
MgSO4	1.865e-018	5.156e-018	-17.729	-17.288	0.442
HSO4-	5.659e-019	1.201e-018	-18.247	-17.920	0.327
KSO4-	3.452e-020	7.328e-020	-19.462	-19.135	0.327
CaHSO4+	2.888e-024	6.131e-024	-23.539	-23.212	0.327
NH4SO4-	0.000e+000	0.000e+000	-66.146	-65.819	0.327

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

Phase	SI	log IAP	log KT	
Anhydrite	-12.14	-16.49	-4.34	CaSO4
Aragonite	-3.28	-11.58	-8.31	CaCO3
Calcite	-3.13	-11.58	-8.45	CaCO3
CH4(g)	-130.57	-133.38	-2.82	CH4
CO2(g)	-6.47	-7.88	-1.41	CO2
Dolomite	-9.31	-26.28	-16.97	CaMg(CO3)2
Gypsum	-12.05	-16.63	-4.58	CaSO4:2H2O
H2(g)	-37.68	-40.81	-3.13	H2
H2O(g)	-1.71	-0.07	1.64	H2O
H2S(g)	-137.70	-138.64	-0.94	H2S
Halite	-9.91	-8.34	1.57	NaCl
N2(g)	-9.70	-12.94	-3.24	N2
NH3(g)	-58.34	-56.47	1.87	NH3
O2(g)	-9.69	-12.54	-2.85	O2
Sulfur	-105.96	-100.96	5.00	S

End of simulation.

Reading input data for simulation 2.

End of run.

Run 5 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\eqb mix 1 with calcite and co2.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\eqb mix 1 with calcite and co2.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          CO2(g)     -2 10
          Calcite    0 10
      SOLUTION 1
          temp       20
          pH         9.748
          pe         9.092
          redox      pe
          units      mmol/kgw
          density    1
          C          0.0005593
          Ca         7.183e-007
          Cl         8.124e-010
          K          2.601e-010
          Mg         3.308e-010
          N(5)       1.331e-008
          Na         8.832
          S(6)       2.785e-009
          water     1 # kg
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.

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

      Elements           Molality       Moles

      C                 5.593e-007  5.593e-007
      Ca                7.183e-010  7.183e-010
      Cl                8.124e-013  8.124e-013
      K                 2.601e-013  2.601e-013
      Mg                3.308e-013  3.308e-013
      N(5)              1.331e-011  1.331e-011
      Na                8.832e-003  8.832e-003
      S(6)              2.785e-012  2.785e-012

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

                                     pH  =   9.748
                                     pe  =   9.092
                        Activity of water  =   1.000
```

```
                    Ionic strength  =  4.437e-003
                Mass of water (kg)  =  1.000e+000
          Total alkalinity (eq/kg)  =  4.183e-005
                Total CO2 (mol/kg)  =  5.593e-007
              Temperature (deg C)   =  20.000
           Electrical balance (eq)  =  8.790e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  99.06
                         Iterations  =   4
                            Total H  = 1.110125e+002
                            Total O  = 5.550626e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	4.083e-005	3.800e-005	-4.389	-4.420	-0.031
H+	1.906e-010	1.786e-010	-9.720	-9.748	-0.028
H2O	5.551e+001	9.998e-001	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-135.414	-135.413	0.000
C(4)	5.593e-007				
HCO3-	4.228e-007	3.945e-007	-6.374	-6.404	-0.030
CO3-2	1.227e-007	9.299e-008	-6.911	-7.032	-0.120
NaCO3-	1.184e-008	1.103e-008	-7.927	-7.958	-0.031
NaHCO3	1.824e-009	1.826e-009	-8.739	-8.739	0.000
CO2	1.696e-010	1.698e-010	-9.771	-9.770	0.000
CaCO3	7.746e-014	7.754e-014	-13.111	-13.110	0.000
CaHCO3+	2.694e-015	2.513e-015	-14.570	-14.600	-0.030
MgCO3	2.042e-017	2.044e-017	-16.690	-16.690	0.000
MgHCO3+	1.209e-018	1.126e-018	-17.918	-17.949	-0.031
Ca	7.183e-010				
Ca+2	7.177e-010	5.437e-010	-9.144	-9.265	-0.121
CaOH+	5.422e-013	5.050e-013	-12.266	-12.297	-0.031
CaCO3	7.746e-014	7.754e-014	-13.111	-13.110	0.000
CaHCO3+	2.694e-015	2.513e-015	-14.570	-14.600	-0.030
CaSO4	2.107e-019	2.109e-019	-18.676	-18.676	0.000
CaHSO4+	2.234e-028	2.080e-028	-27.651	-27.682	-0.031
Cl	8.124e-013				
Cl-	8.124e-013	7.561e-013	-12.090	-12.121	-0.031
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.808	-40.808	0.000
K	2.601e-013				
K+	2.601e-013	2.421e-013	-12.585	-12.616	-0.031
KOH	4.693e-018	4.698e-018	-17.329	-17.328	0.000
KSO4-	3.408e-024	3.174e-024	-23.468	-23.498	-0.031
Mg	3.308e-013				
Mg+2	3.273e-013	2.487e-013	-12.485	-12.604	-0.119
MgOH+	3.429e-015	3.193e-015	-14.465	-14.496	-0.031
MgCO3	2.042e-017	2.044e-017	-16.690	-16.690	0.000
MgHCO3+	1.209e-018	1.126e-018	-17.918	-17.949	-0.031
MgSO4	1.042e-022	1.043e-022	-21.982	-21.982	0.000
N(5)	1.331e-011				
NO3-	1.331e-011	1.238e-011	-10.876	-10.907	-0.032
Na	8.832e-003				
Na+	8.832e-003	8.231e-003	-2.054	-2.085	-0.031
NaOH	3.040e-007	3.043e-007	-6.517	-6.517	0.000
NaCO3-	1.184e-008	1.103e-008	-7.927	-7.958	-0.031
NaHCO3	1.824e-009	1.826e-009	-8.739	-8.739	0.000
NaSO4-	8.745e-014	8.145e-014	-13.058	-13.089	-0.031
O(0)	7.858e-013				
O2	3.929e-013	3.933e-013	-12.406	-12.405	0.000
S(6)	2.785e-012				
SO4-2	2.698e-012	2.039e-012	-11.569	-11.691	-0.122
NaSO4-	8.745e-014	8.145e-014	-13.058	-13.089	-0.031
CaSO4	2.107e-019	2.109e-019	-18.676	-18.676	0.000
HSO4-	3.417e-020	3.183e-020	-19.466	-19.497	-0.031

MgSO4	1.042e-022	1.043e-022	-21.982	-21.982	0.000
KSO4-	3.408e-024	3.174e-024	-23.468	-23.498	-0.031
CaHSO4+	2.234e-028	2.080e-028	-27.651	-27.682	-0.031

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

Phase	SI	log IAP	log KT	
Anhydrite	-16.61	-20.96	-4.34	CaSO4
Aragonite	-7.99	-16.30	-8.31	CaCO3
Calcite	-7.84	-16.30	-8.45	CaCO3
CH4(g)	-132.60	-135.41	-2.82	CH4
CO2(g)	-8.36	-9.77	-1.41	CO2
Dolomite	-18.96	-35.93	-16.97	CaMg(CO3)2
Gypsum	-16.37	-20.96	-4.58	CaSO4:2H2O
H2(g)	-37.68	-40.81	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
Halite	-15.78	-14.21	1.57	NaCl
O2(g)	-9.55	-12.41	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Calcite	0.00	-8.45	-8.45	1.000e+001	9.998e+000	-1.866e-003
CO2(g)	-2.00	-3.41	-1.41	1.000e+001	9.998e+000	-2.288e-003

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

Elements	Molality	Moles
C	4.154e-003	4.154e-003
Ca	1.866e-003	1.866e-003
Cl	8.124e-013	8.124e-013
K	2.601e-013	2.601e-013
Mg	3.308e-013	3.308e-013
N	1.331e-011	1.331e-011
Na	8.832e-003	8.832e-003
S	2.785e-012	2.785e-012

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

```
                                    pH  =   7.313      Charge balance
                                    pe  =  11.534      Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  9.902e-003
                    Mass of water (kg)  =  1.000e+000
            Total alkalinity (eq/kg)    =  3.773e-003
                  Total CO2 (mol/kg)    =  4.154e-003
                 Temperature (deg C)    =  20.000
             Electrical balance (eq)    =  8.790e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) =  54.33
                            Iterations  =   9
                               Total H  = 1.110125e+002
                               Total O  = 5.551643e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.547e-007	1.394e-007	-6.811	-6.856	-0.045
H+	5.324e-008	4.868e-008	-7.274	-7.313	-0.039
H2O	5.551e+001	9.997e-001	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-129.107	-129.106	0.001
C(4)	4.154e-003				
HCO3-	3.686e-003	3.340e-003	-2.433	-2.476	-0.043
CO2	3.910e-004	3.919e-004	-3.408	-3.407	0.001
CaHCO3+	5.264e-005	4.771e-005	-4.279	-4.321	-0.043
NaHCO3	1.494e-005	1.497e-005	-4.826	-4.825	0.001
CaCO3	5.388e-006	5.401e-006	-5.269	-5.268	0.001
CO3-2	4.283e-006	2.889e-006	-5.368	-5.539	-0.171
NaCO3-	3.675e-007	3.319e-007	-6.435	-6.479	-0.044
MgHCO3+	9.240e-015	8.346e-015	-14.034	-14.079	-0.044
MgCO3	5.548e-016	5.561e-016	-15.256	-15.255	0.001
Ca	1.866e-003				
Ca+2	1.808e-003	1.219e-003	-2.743	-2.914	-0.171
CaHCO3+	5.264e-005	4.771e-005	-4.279	-4.321	-0.043
CaCO3	5.388e-006	5.401e-006	-5.269	-5.268	0.001
CaOH+	4.598e-009	4.153e-009	-8.337	-8.382	-0.044
CaSO4	3.652e-013	3.660e-013	-12.438	-12.437	0.001
CaHSO4+	1.089e-019	9.837e-020	-18.963	-19.007	-0.044
Cl	8.124e-013				
Cl-	8.124e-013	7.325e-013	-12.090	-12.135	-0.045
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.823	-40.822	0.001
K	2.601e-013				
K+	2.601e-013	2.345e-013	-12.585	-12.630	-0.045
KOH	1.666e-020	1.670e-020	-19.778	-19.777	0.001
KSO4-	2.635e-024	2.380e-024	-23.579	-23.623	-0.044
Mg	3.308e-013				
Mg+2	3.210e-013	2.178e-013	-12.493	-12.662	-0.169
MgHCO3+	9.240e-015	8.346e-015	-14.034	-14.079	-0.044
MgCO3	5.548e-016	5.561e-016	-15.256	-15.255	0.001
MgOH+	1.136e-017	1.026e-017	-16.945	-16.989	-0.044
MgSO4	7.053e-023	7.069e-023	-22.152	-22.151	0.001
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-54.861	-54.908	-0.046
NH3	0.000e+000	0.000e+000	-56.996	-56.995	0.001
NH4SO4-	0.000e+000	0.000e+000	-65.555	-65.599	-0.044
N(0)	2.204e-014				
N2	1.102e-014	1.104e-014	-13.958	-13.957	0.001
N(3)	3.521e-020				
NO2-	3.521e-020	3.169e-020	-19.453	-19.499	-0.046
N(5)	1.329e-011				
NO3-	1.329e-011	1.196e-011	-10.877	-10.922	-0.046
Na	8.832e-003				
Na+	8.817e-003	7.973e-003	-2.055	-2.098	-0.044
NaHCO3	1.494e-005	1.497e-005	-4.826	-4.825	0.001
NaCO3-	3.675e-007	3.319e-007	-6.435	-6.479	-0.044
NaOH	1.079e-009	1.082e-009	-8.967	-8.966	0.001
NaSO4-	6.761e-014	6.107e-014	-13.170	-13.214	-0.044
O(0)	8.368e-013				
O2	4.184e-013	4.194e-013	-12.378	-12.377	0.001
S(-2)	0.000e+000				
HS-	0.000e+000	0.000e+000	-135.443	-135.488	-0.045
H2S	0.000e+000	0.000e+000	-135.792	-135.791	0.001
S-2	0.000e+000	0.000e+000	-141.072	-141.245	-0.173
S(6)	2.785e-012				
SO4-2	2.352e-012	1.578e-012	-11.629	-11.802	-0.173
CaSO4	3.652e-013	3.660e-013	-12.438	-12.437	0.001
NaSO4-	6.761e-014	6.107e-014	-13.170	-13.214	-0.044
HSO4-	7.434e-018	6.714e-018	-17.129	-17.173	-0.044

CaHSO4+	1.089e-019	9.837e-020	-18.963	-19.007	-0.044
MgSO4	7.053e-023	7.069e-023	-22.152	-22.151	0.001
KSO4-	2.635e-024	2.380e-024	-23.579	-23.623	-0.044
NH4SO4-	0.000e+000	0.000e+000	-65.555	-65.599	-0.044

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

Phase	SI	log IAP	log KT	
Anhydrite	-10.37	-14.72	-4.34	CaSO4
Aragonite	-0.15	-8.45	-8.31	CaCO3
Calcite	0.00	-8.45	-8.45	CaCO3
CH4(g)	-126.29	-129.11	-2.82	CH4
CO2(g)	-2.00	-3.41	-1.41	CO2
Dolomite	-9.68	-26.65	-16.97	CaMg(CO3)2
Gypsum	-10.13	-14.72	-4.58	CaSO4:2H2O
H2(g)	-37.69	-40.82	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
H2S(g)	-134.85	-135.79	-0.94	H2S
Halite	-15.80	-14.23	1.57	NaCl
N2(g)	-10.71	-13.96	-3.24	N2
NH3(g)	-58.87	-57.00	1.87	NH3
O2(g)	-9.52	-12.38	-2.85	O2
Sulfur	-103.10	-98.10	5.00	S

End of simulation.

Reading input data for simulation 2.

End of run.

Run 5 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\eqb mix 2 withmontmorillonite.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\rain\eqb mix 2 withmontmorillonite.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          Ca-Montmorillonite 0 10
      SOLUTION 1
          temp      20
          pH        7.313
          pe        11.534
          redox     pe
          units     mmol/kgw
          density   1
          C         0.004154
          Ca        0.001866
          Cl        8.124e-013
          K         2.601e-013
          Mg        3.308e-013
          N(5)      1.329e-011
          Na        0.008832
          S(6)      2.785e-012
          water    1 # kg
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

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

      Elements           Molality       Moles

      C                 4.154e-006  4.154e-006
      Ca                1.866e-006  1.866e-006
      Cl                8.124e-016  8.124e-016
      K                 2.601e-016  2.601e-016
      Mg                3.308e-016  3.308e-016
      N(5)              1.329e-014  1.329e-014
      Na                8.832e-006  8.832e-006
      S(6)              2.785e-015  2.785e-015

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

                                       pH  =   7.313
                                       pe  =  11.534
                          Activity of water  =   1.000
                             Ionic strength  =  1.011e-005
```

```
                    Mass of water (kg)  =  1.000e+000
              Total alkalinity (eq/kg)  =  3.815e-006
                    Total CO2 (mol/kg)  =  4.154e-006
                  Temperature (deg C)   =  20.000
             Electrical balance (eq)    =  8.749e-006
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  53.10
                            Iterations  =   3
                               Total H  = 1.110124e+002
                               Total O  = 5.550623e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.401e-007	1.396e-007	-6.854	-6.855	-0.002
H+	4.882e-008	4.864e-008	-7.311	-7.313	-0.002
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-132.062	-132.062	0.000
C(4)	4.154e-006				
HCO3-	3.717e-006	3.703e-006	-5.430	-5.431	-0.002
CO2	4.339e-007	4.339e-007	-6.363	-6.363	0.000
CO3-2	3.254e-009	3.206e-009	-8.488	-8.494	-0.006
CaHCO3+	8.009e-011	7.980e-011	-10.096	-10.098	-0.002
NaHCO3	1.832e-011	1.832e-011	-10.737	-10.737	0.000
CaCO3	9.042e-012	9.042e-012	-11.044	-11.044	0.000
NaCO3-	4.080e-013	4.065e-013	-12.389	-12.391	-0.002
MgHCO3+	1.390e-020	1.385e-020	-19.857	-19.859	-0.002
MgCO3	9.235e-022	9.235e-022	-21.035	-21.035	0.000
Ca	1.866e-006				
Ca+2	1.866e-006	1.839e-006	-5.729	-5.735	-0.006
CaHCO3+	8.009e-011	7.980e-011	-10.096	-10.098	-0.002
CaCO3	9.042e-012	9.042e-012	-11.044	-11.044	0.000
CaOH+	6.297e-012	6.273e-012	-11.201	-11.202	-0.002
CaSO4	9.597e-019	9.597e-019	-18.018	-18.018	0.000
CaHSO4+	2.587e-025	2.577e-025	-24.587	-24.589	-0.002
Cl	8.124e-016				
Cl-	8.124e-016	8.094e-016	-15.090	-15.092	-0.002
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.822	-40.822	0.000
K	2.601e-016				
K+	2.601e-016	2.591e-016	-15.585	-15.586	-0.002
KOH	1.847e-023	1.847e-023	-22.733	-22.733	0.000
KSO4-	4.588e-030	4.571e-030	-29.338	-29.340	-0.002
Mg	3.308e-016				
Mg+2	3.308e-016	3.259e-016	-15.480	-15.487	-0.006
MgOH+	1.543e-020	1.537e-020	-19.812	-19.813	-0.002
MgHCO3+	1.390e-020	1.385e-020	-19.857	-19.859	-0.002
MgCO3	9.235e-022	9.235e-022	-21.035	-21.035	0.000
MgSO4	1.839e-028	1.839e-028	-27.735	-27.735	0.000
N(5)	1.329e-014				
NO3-	1.329e-014	1.324e-014	-13.876	-13.878	-0.002
Na	8.832e-006				
Na+	8.832e-006	8.800e-006	-5.054	-5.056	-0.002
NaHCO3	1.832e-011	1.832e-011	-10.737	-10.737	0.000
NaOH	1.195e-012	1.195e-012	-11.923	-11.923	0.000
NaCO3-	4.080e-013	4.065e-013	-12.389	-12.391	-0.002
NaSO4-	1.176e-019	1.171e-019	-18.930	-18.931	-0.002
O(0)	8.393e-013				
O2	4.196e-013	4.196e-013	-12.377	-12.377	0.000
S(6)	2.785e-015				
SO4-2	2.784e-015	2.743e-015	-14.555	-14.562	-0.006
CaSO4	9.597e-019	9.597e-019	-18.018	-18.018	0.000
NaSO4-	1.176e-019	1.171e-019	-18.930	-18.931	-0.002
HSO4-	1.170e-020	1.166e-020	-19.932	-19.933	-0.002
CaHSO4+	2.587e-025	2.577e-025	-24.587	-24.589	-0.002

MgSO4	1.839e-028	1.839e-028	-27.735	-27.735	0.000
KSO4-	4.588e-030	4.571e-030	-29.338	-29.340	-0.002

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

Phase	SI	log IAP	log KT	
Anhydrite	-15.95	-20.30	-4.34	CaSO4
Aragonite	-5.92	-14.23	-8.31	CaCO3
Calcite	-5.78	-14.23	-8.45	CaCO3
CH4(g)	-129.24	-132.06	-2.82	CH4
CO2(g)	-4.96	-6.36	-1.41	CO2
Dolomite	-21.24	-38.21	-16.97	CaMg(CO3)2
Gypsum	-15.72	-20.30	-4.58	CaSO4:2H2O
H2(g)	-37.69	-40.82	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
Halite	-21.72	-20.15	1.57	NaCl
O2(g)	-9.52	-12.38	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca-Montmorillonite	0.00	-45.76	-45.76	1.000e+001	1.000e+001	-2.061e-006

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

Elements	Molality	Moles
Al	4.802e-006	4.802e-006
C	4.154e-006	4.154e-006
Ca	2.206e-006	2.206e-006
Cl	8.124e-016	8.124e-016
K	2.601e-016	2.601e-016
Mg	3.308e-016	3.308e-016
N	1.329e-014	1.329e-014
Na	8.832e-006	8.832e-006
S	2.785e-015	2.785e-015
Si	7.563e-006	7.563e-006

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

```
                                    pH  =   6.617      Charge balance
                                    pe  =  12.232      Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  1.255e-005
                    Mass of water (kg)  =  1.000e+000
              Total alkalinity (eq/kg)  =  1.890e-005
                    Total CO2 (mol/kg)  =  4.154e-006
                   Temperature (deg C)  =  20.000
                Electrical balance (eq) =  8.749e-006
Percent error, 100*(Cat-|An|)/(Cat+|An|) =  42.54
                             Iterations =   9
                                Total H = 1.110124e+002
                                Total O = 5.550625e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.427e-007	2.417e-007	-6.615	-6.617	-0.002
OH-	2.821e-008	2.809e-008	-7.550	-7.551	-0.002
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Al	4.802e-006				
Al(OH)4-	3.246e-006	3.233e-006	-5.489	-5.490	-0.002
Al(OH)2+	1.061e-006	1.057e-006	-5.974	-5.976	-0.002
Al(OH)3	4.405e-007	4.405e-007	-6.356	-6.356	0.000
AlOH+2	5.195e-008	5.110e-008	-7.284	-7.292	-0.007
Al+3	1.792e-009	1.727e-009	-8.747	-8.763	-0.016
AlSO4+	1.406e-020	1.400e-020	-19.852	-19.854	-0.002
AlHSO4+2	2.928e-028	2.880e-028	-27.533	-27.541	-0.007
Al(SO4)2-	1.189e-033	1.184e-033	-32.925	-32.927	-0.002
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-131.527	-131.527	0.000
C(4)	4.154e-006				
HCO3-	2.629e-006	2.618e-006	-5.580	-5.582	-0.002
CO2	1.524e-006	1.524e-006	-5.817	-5.817	0.000
CO3-2	4.638e-010	4.563e-010	-9.334	-9.341	-0.007
CaHCO3+	6.687e-011	6.659e-011	-10.175	-10.177	-0.002
NaHCO3	1.295e-011	1.295e-011	-10.888	-10.888	0.000
CaCO3	1.519e-012	1.519e-012	-11.819	-11.819	0.000
NaCO3-	5.806e-014	5.782e-014	-13.236	-13.238	-0.002
MgHCO3+	9.816e-021	9.776e-021	-20.008	-20.010	-0.002
MgCO3	1.312e-022	1.312e-022	-21.882	-21.882	0.000
Ca	2.206e-006				
Ca+2	2.206e-006	2.170e-006	-5.656	-5.664	-0.007
CaHCO3+	6.687e-011	6.659e-011	-10.175	-10.177	-0.002
CaCO3	1.519e-012	1.519e-012	-11.819	-11.819	0.000
CaOH+	1.496e-012	1.490e-012	-11.825	-11.827	-0.002
CaSO4	1.131e-018	1.131e-018	-17.947	-17.947	0.000
CaHSO4+	1.515e-024	1.509e-024	-23.820	-23.821	-0.002
Cl	8.124e-016				
Cl-	8.124e-016	8.091e-016	-15.090	-15.092	-0.002
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.825	-40.825	0.000
K	2.601e-016				
K+	2.601e-016	2.590e-016	-15.585	-15.587	-0.002
KOH	3.717e-024	3.717e-024	-23.430	-23.430	0.000
KSO4-	4.580e-030	4.561e-030	-29.339	-29.341	-0.002
Mg	3.308e-016				
Mg+2	3.308e-016	3.254e-016	-15.480	-15.488	-0.007
MgHCO3+	9.816e-021	9.776e-021	-20.008	-20.010	-0.002
MgOH+	3.101e-021	3.089e-021	-20.508	-20.510	-0.002
MgCO3	1.312e-022	1.312e-022	-21.882	-21.882	0.000
MgSO4	1.833e-028	1.833e-028	-27.737	-27.737	0.000
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-56.482	-56.483	-0.002
NH3	0.000e+000	0.000e+000	-59.267	-59.267	0.000
NH4SO4-	0.000e+000	0.000e+000	-69.934	-69.936	-0.002
N(0)	6.446e-019				
N2	3.223e-019	3.223e-019	-18.492	-18.492	0.000
N(3)	3.498e-023				
NO2-	3.498e-023	3.484e-023	-22.456	-22.458	-0.002
N(5)	1.329e-014				
NO3-	1.329e-014	1.323e-014	-13.876	-13.878	-0.002
Na	8.832e-006				
Na+	8.832e-006	8.796e-006	-5.054	-5.056	-0.002
NaHCO3	1.295e-011	1.295e-011	-10.888	-10.888	0.000
NaOH	2.405e-013	2.405e-013	-12.619	-12.619	0.000
NaCO3-	5.806e-014	5.782e-014	-13.236	-13.238	-0.002
NaSO4-	1.174e-019	1.169e-019	-18.930	-18.932	-0.002
O(0)	8.500e-013				
O2	4.250e-013	4.250e-013	-12.372	-12.372	0.000

```
S(-2)            0.000e+000
   H2S                   0.000e+000  0.000e+000  -137.171  -137.171     0.000
   HS-                   0.000e+000  0.000e+000  -137.563  -137.564    -0.002
   S-2                   0.000e+000  0.000e+000  -144.010  -144.017    -0.007
S(6)             2.785e-015
   SO4-2                 2.784e-015  2.738e-015   -14.555   -14.562    -0.007
   CaSO4                 1.131e-018  1.131e-018   -17.947   -17.947     0.000
   NaSO4-                1.174e-019  1.169e-019   -18.930   -18.932    -0.002
   HSO4-                 5.806e-020  5.782e-020   -19.236   -19.238    -0.002
   AlSO4+                1.406e-020  1.400e-020   -19.852   -19.854    -0.002
   CaHSO4+               1.515e-024  1.509e-024   -23.820   -23.821    -0.002
   AlHSO4+2              2.928e-028  2.880e-028   -27.533   -27.541    -0.007
   MgSO4                 1.833e-028  1.833e-028   -27.737   -27.737     0.000
   KSO4-                 4.580e-030  4.561e-030   -29.339   -29.341    -0.002
   Al(SO4)2-             1.189e-033  1.184e-033   -32.925   -32.927    -0.002
   NH4SO4-               0.000e+000  0.000e+000   -69.934   -69.936    -0.002
Si               7.563e-006
   H4SiO4                7.559e-006  7.559e-006    -5.122    -5.122     0.000
   H3SiO4-               3.869e-009  3.854e-009    -8.412    -8.414    -0.002
   H2SiO4-2              7.884e-016  7.756e-016   -15.103   -15.110    -0.007

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

      Phase               SI log IAP  log KT

      Al(OH)3(a)       -0.04   11.09   11.13  Al(OH)3
      Albite           -7.58  -25.91  -18.33  NaAlSi3O8
      Alunite         -30.53  -31.30   -0.77  KAl3(SO4)2(OH)6
      Anhydrite       -15.88  -20.23   -4.34  CaSO4
      Anorthite        -7.03  -26.89  -19.86  CaAl2Si2O8
      Aragonite        -6.70  -15.00   -8.31  CaCO3
      Ca-Montmorillonite   0.00  -45.76  -45.76  Ca0.165Al2.33Si3.67O10(OH)2
      Calcite          -6.55  -15.00   -8.45  CaCO3
      CH4(g)         -128.71 -131.53   -2.82  CH4
      Chalcedony       -1.51   -5.12   -3.61  SiO2
      Chlorite(14A)   -74.73   -4.46   70.27  Mg5Al2Si3O10(OH)8
      Chrysotile      -49.84  -17.01   32.83  Mg3Si2O5(OH)4
      CO2(g)           -4.41   -5.82   -1.41  CO2
      Dolomite        -22.86  -39.83  -16.97  CaMg(CO3)2
      Gibbsite          2.69   11.09    8.40  Al(OH)3
      Gypsum          -15.64  -20.23   -4.58  CaSO4:2H2O
      H2(g)           -37.70  -40.82   -3.13  H2
      H2O(g)           -1.64   -0.00    1.64  H2O
      H2S(g)         -136.23 -137.17   -0.94  H2S
      Halite          -21.72  -20.15    1.57  NaCl
      Illite          -10.77  -51.72  -40.95  K0.6Mg0.25Al2.3Si3.5O10(OH)2
      K-feldspar      -15.48  -36.44  -20.96  KAlSi3O8
      K-mica           -4.52    8.93   13.45  KAl3Si3O10(OH)2
      Kaolinite         4.06   11.93    7.88  Al2Si2O5(OH)4
      N2(g)           -15.25  -18.49   -3.24  N2
      NH3(g)          -61.14  -59.27    1.87  NH3
      O2(g)            -9.52  -12.37   -2.85  O2
      Quartz           -1.07   -5.12   -4.06  SiO2
      Sepiolite       -35.77  -19.87   15.89  Mg2Si3O7.5OH:3H2O
      Sepiolite(d)    -38.53  -19.87   18.66  Mg2Si3O7.5OH:3H2O
      SiO2(a)          -2.37   -5.12   -2.75  SiO2
      Sulfur         -104.48  -99.47    5.00  S
      Talc            -49.23  -27.25   21.98  Mg3Si4O10(OH)2

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 2.
------------------------------------
```

```
-----------
End of run.
-----------
```

Run 6

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\50-50mix\mix NaOH and calcite GW.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\50-50mix\mix NaOH and calcite GW.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 2 NaOH
          temp      20
          pH        14
          pe        4
          redox     pe
          units     mmol/kgw
          density   1
          Na        24.9 Mol/kgw
          water    1 # kg
      SOLUTION 1 GW @ eqb w/ Calcite
          temp      20
          pH        7.301
          pe        -1.841
          redox     pe
          units     mmol/kgw
          density   1
          Ca        0.001789
          C         0.003961
          water    1 # kg
      SAVE solution 1-2
      MIX 1 Mix NaOH and GW @ equ w/ calcite
          1    0.5
          2    0.5
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     GW @ eqb w/ Calcite

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

      Elements           Molality       Moles

      C                 3.961e-006  3.961e-006
      Ca                1.789e-006  1.789e-006

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

                                       pH  =   7.301
                                       pe  =  -1.841
                          Activity of water  =   1.000
                             Ionic strength  =  5.444e-006
                         Mass of water (kg)  =  1.000e+000
```

```
                 Total alkalinity (eq/kg)  =  3.626e-006
                       Total CO2 (mol/kg)  =  3.961e-006
                     Temperature (deg C)   =  20.000
                  Electrical balance (eq)  = -4.751e-008
  Percent error, 100*(Cat-|An|)/(Cat+|An|) =  -0.65
                              Iterations   =   3
                                 Total H   = 1.110124e+002
                                 Total O   = 5.550623e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.361e-007	1.358e-007	-6.866	-6.867	-0.001
H+	5.014e-008	5.000e-008	-7.300	-7.301	-0.001
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	1.058e-025				
CH4	1.058e-025	1.058e-025	-24.975	-24.975	0.000
C(4)	3.961e-006				
HCO3-	3.533e-006	3.524e-006	-5.452	-5.453	-0.001
CO2	4.245e-007	4.245e-007	-6.372	-6.372	0.000
CO3-2	3.000e-009	2.968e-009	-8.523	-8.528	-0.005
CaHCO3+	7.328e-011	7.309e-011	-10.135	-10.136	-0.001
CaCO3	8.056e-012	8.056e-012	-11.094	-11.094	0.000
Ca	1.789e-006				
Ca+2	1.789e-006	1.770e-006	-5.747	-5.752	-0.005
CaHCO3+	7.328e-011	7.309e-011	-10.135	-10.136	-0.001
CaCO3	8.056e-012	8.056e-012	-11.094	-11.094	0.000
CaOH+	5.889e-012	5.873e-012	-11.230	-11.231	-0.001
H(0)	1.791e-014				
H2	8.953e-015	8.953e-015	-14.048	-14.048	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-65.925	-65.925	0.000

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

Phase	SI	log IAP	log KT	
Aragonite	-5.97	-14.28	-8.31	CaCO3
Calcite	-5.83	-14.28	-8.45	CaCO3
CH4(g)	-22.16	-24.98	-2.82	CH4
CO2(g)	-4.97	-6.37	-1.41	CO2
H2(g)	-10.92	-14.05	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.07	-65.93	-2.85	O2

Initial solution 2. NaOH

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

Elements	Molality	Moles
Na	2.490e+001	2.490e+001

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

```
                                pH  =  14.000
                                pe  =   4.000
                  Activity of water  =   0.562
                     Ionic strength  = 1.184e+001
                 Mass of water (kg)  = 1.000e+000
           Total alkalinity (eq/kg)  = 2.931e+000
              Total carbon (mol/kg)  = 0.000e+000
                 Total CO2 (mol/kg)  = 0.000e+000
               Temperature (deg C)   = 20.000
            Electrical balance (eq)  = 2.197e+001
```

```
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  92.76
                                Iterations  =   6
                                   Total H  = 1.139431e+002
                                   Total O  = 5.843693e+001

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

                                                Log       Log         Log
   Species                  Molality    Activity  Molality  Activity    Gamma

   OH-                    8.574e-001  3.816e-001    -0.067    -0.418   -0.352
   H+                     1.432e-014  1.000e-014   -13.844   -14.000   -0.156
   H2O                    5.551e+001  5.621e-001     1.744    -0.250    0.000
H(0)              0.000e+000
   H2                     0.000e+000  7.447e-040   -40.312   -39.128    1.184
Na                2.490e+001
   Na+                    2.283e+001  8.532e+001     1.358     1.931    0.573
   NaOH                   2.073e+000  3.169e+001     0.317     1.501    1.184
O(0)              7.102e-018
   O2                     3.551e-018  5.427e-017   -17.450   -16.265    1.184

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

      Phase               SI log IAP  log KT

      H2(g)           -36.00  -39.13   -3.13  H2
      H2O(g)           -1.89   -0.25    1.64  H2O
      O2(g)           -13.41  -16.27   -2.85  O2

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

Reaction step 1.

Using mix 1.      Mix NaOH and GW @ equ w/ calcite

Mixture 1.  Mix NaOH and GW @ equ w/ calcite

       5.000e-001 Solution 1  GW @ eqb w/ Calcite
       5.000e-001 Solution 2  NaOH

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

      Elements           Molality       Moles

      C                1.980e-006  1.981e-006
      Ca               8.945e-007  8.945e-007
      Na               1.245e+001  1.245e+001

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

                                      pH  =  13.654      Charge balance
                                      pe  =   5.465      Adjusted to redox equilibrium
                         Activity of water  =   0.780
                            Ionic strength  =  5.997e+000
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  1.465e+000
                       Total CO2 (mol/kg)   =  1.980e-006
                     Temperature (deg C)    =  20.000
                  Electrical balance (eq)   =  1.098e+001
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  91.59
                                Iterations  =  14
                                   Total H  = 1.124778e+002
                                   Total O  = 5.697158e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	5.045e-001	2.388e-001	-0.297	-0.622	-0.325
H+	3.135e-014	2.217e-014	-13.504	-13.654	-0.151
H2O	5.551e+001	7.798e-001	1.744	-0.108	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-146.282	-145.683	0.600
C(4)	1.980e-006				
NaCO3-	1.757e-006	6.237e-006	-5.755	-5.205	0.550
CO3-2	2.230e-007	2.632e-008	-6.652	-7.580	-0.928
NaHCO3	3.221e-011	1.281e-010	-10.492	-9.892	0.600
HCO3-	2.364e-011	1.385e-011	-10.626	-10.858	-0.232
CaCO3	3.437e-012	1.367e-011	-11.464	-10.864	0.600
CaHCO3+	9.385e-017	5.500e-017	-16.028	-16.260	-0.232
CO2	2.385e-019	9.489e-019	-18.622	-18.023	0.600
Ca	8.945e-007				
CaOH+	5.573e-007	1.978e-006	-6.254	-5.704	0.550
Ca+2	3.372e-007	3.388e-007	-6.472	-6.470	0.002
CaCO3	3.437e-012	1.367e-011	-11.464	-10.864	0.600
CaHCO3+	9.385e-017	5.500e-017	-16.028	-16.260	-0.232
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-41.966	-41.366	0.600
Na	1.245e+001				
Na+	1.149e+001	1.645e+001	1.060	1.216	0.156
NaOH	9.608e-001	3.822e+000	-0.017	0.582	0.600
NaCO3-	1.757e-006	6.237e-006	-5.755	-5.205	0.550
NaHCO3	3.221e-011	1.281e-010	-10.492	-9.892	0.600
O(0)	1.572e-012				
O2	7.861e-013	3.127e-012	-12.105	-11.505	0.600

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

Phase	SI	log IAP	log KT	
Aragonite	-5.74	-14.05	-8.31	CaCO3
Calcite	-5.60	-14.05	-8.45	CaCO3
CH4(g)	-142.86	-145.68	-2.82	CH4
CO2(g)	-16.62	-18.02	-1.41	CO2
H2(g)	-38.24	-41.37	-3.13	H2
H2O(g)	-1.75	-0.11	1.64	H2O
O2(g)	-8.65	-11.50	-2.85	O2

End of simulation.

Reading input data for simulation 2.

End of run.

Run 6

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\50-50mix\mix 1 eqb calcite and CO2.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\50-50mix\mix 1 eqb calcite and CO2.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 1 mix 1 eqb with calcite and CO2
          temp      20
          pH        13.654
          pe        5.465
          redox     pe
          units     mmol/kgw
          density   1
          C         1.98e-006
          Ca        8.945e-007
          Na        12.45
          water    1 # kg
      EQUILIBRIUM_PHASES 1
          Calcite   0 10
          CO2(g)    -2 10
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.     mix 1 eqb with calcite and CO2

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

      Elements           Molality       Moles

      C                1.980e-009  1.980e-009
      Ca               8.945e-010  8.945e-010
      Na               1.245e-002  1.245e-002

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

                                       pH  =  13.654
                                       pe  =   5.465
                         Activity of water  =   0.992
                            Ionic strength  =  2.219e-001
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  4.357e-001
                       Total CO2 (mol/kg)   =  1.980e-009
                      Temperature (deg C)   =  20.000
                  Electrical balance (eq)   = -4.232e-001
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   = -95.36
                                Iterations  =   5
                                   Total H  = 1.114481e+002
                                   Total O  = 5.594189e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	4.335e-001	3.037e-001	-0.363	-0.517	-0.155
H+	2.790e-014	2.218e-014	-13.554	-13.654	-0.100
H2O	5.551e+001	9.924e-001	1.744	-0.003	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-147.680	-147.658	0.022
C(4)	1.980e-009				
CO3-2	1.895e-009	5.733e-010	-8.722	-9.242	-0.519
NaCO3-	8.467e-011	6.304e-011	-10.072	-10.200	-0.128
HCO3-	4.072e-013	3.020e-013	-12.390	-12.520	-0.130
NaHCO3	1.231e-015	1.296e-015	-14.910	-14.887	0.022
CaCO3	5.688e-017	5.986e-017	-16.245	-16.223	0.022
CO2	1.545e-020	1.626e-020	-19.811	-19.789	0.022
CaHCO3+	3.248e-022	2.409e-022	-21.488	-21.618	-0.130
Ca	8.945e-010				
CaOH+	6.789e-010	5.055e-010	-9.168	-9.296	-0.128
Ca+2	2.156e-010	6.807e-011	-9.666	-10.167	-0.501
CaCO3	5.688e-017	5.986e-017	-16.245	-16.223	0.022
CaHCO3+	3.248e-022	2.409e-022	-21.488	-21.618	-0.130
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-41.388	-41.366	0.022
Na	1.245e-002				
Na+	1.031e-002	7.632e-003	-1.987	-2.117	-0.130
NaOH	2.143e-003	2.256e-003	-2.669	-2.647	0.022
NaCO3-	8.467e-011	6.304e-011	-10.072	-10.200	-0.128
NaHCO3	1.231e-015	1.296e-015	-14.910	-14.887	0.022
O(0)	9.618e-012				
O2	4.809e-012	5.061e-012	-11.318	-11.296	0.022

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

Phase	SI	log IAP	log KT	
Aragonite	-11.10	-19.41	-8.31	CaCO3
Calcite	-10.96	-19.41	-8.45	CaCO3
CH4(g)	-144.84	-147.66	-2.82	CH4
CO2(g)	-18.38	-19.79	-1.41	CO2
H2(g)	-38.24	-41.37	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-8.44	-11.30	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. mix 1 eqb with calcite and CO2
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Calcite	0.00	-8.45	-8.45	1.000e+001	1.000e+001	-6.789e-006
CO2(g)	-2.00	-3.41	-1.41	1.000e+001	9.618e+000	-3.818e-001

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

Elements	Molality	Moles

C	3.815e-001	3.818e-001
Ca	6.783e-006	6.790e-006
Na	1.244e-002	1.245e-002

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

pH	=	9.168	Charge balance
pe	=	9.952	Adjusted to redox equilibrium
Activity of water	=	0.993	
Ionic strength	=	2.731e-001	
Mass of water (kg)	=	1.001e+000	
Total alkalinity (eq/kg)	=	4.353e-001	
Total CO2 (mol/kg)	=	3.815e-001	
Temperature (deg C)	=	20.000	
Electrical balance (eq)	=	-4.232e-001	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-95.68	
Iterations	=	14	
Total H	=	1.114481e+002	
Total O	=	5.670559e+001	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.451e-005	9.925e-006	-4.838	-5.003	-0.165
H+	8.632e-010	6.795e-010	-9.064	-9.168	-0.104
H2O	5.551e+001	9.934e-001	1.744	-0.003	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-131.312	-131.284	0.027
C(4)	3.815e-001				
HCO3-	3.261e-001	2.378e-001	-0.487	-0.624	-0.137
CO3-2	5.213e-002	1.474e-002	-1.283	-1.832	-0.549
NaCO3-	2.009e-003	1.482e-003	-2.697	-2.829	-0.132
NaHCO3	8.765e-004	9.334e-004	-3.057	-3.030	0.027
CO2	3.680e-004	3.919e-004	-3.434	-3.407	0.027
CaCO3	5.072e-006	5.401e-006	-5.295	-5.268	0.027
CaHCO3+	9.132e-007	6.659e-007	-6.039	-6.177	-0.137
Ca	6.783e-006				
CaCO3	5.072e-006	5.401e-006	-5.295	-5.268	0.027
CaHCO3+	9.132e-007	6.659e-007	-6.039	-6.177	-0.137
Ca+2	7.984e-007	2.390e-007	-6.098	-6.622	-0.524
CaOH+	7.856e-011	5.797e-011	-10.105	-10.237	-0.132
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-41.395	-41.368	0.027
Na	1.244e-002				
Na+	9.553e-003	6.981e-003	-2.020	-2.156	-0.136
NaCO3-	2.009e-003	1.482e-003	-2.697	-2.829	-0.132
NaHCO3	8.765e-004	9.334e-004	-3.057	-3.030	0.027
NaOH	6.332e-008	6.742e-008	-7.198	-7.171	0.027
O(0)	9.613e-012				
O2	4.806e-012	5.118e-012	-11.318	-11.291	0.027

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

Phase	SI	log IAP	log KT	
Aragonite	-0.15	-8.45	-8.31	CaCO3
Calcite	0.00	-8.45	-8.45	CaCO3
CH4(g)	-128.47	-131.28	-2.82	CH4
CO2(g)	-2.00	-3.41	-1.41	CO2
H2(g)	-38.24	-41.37	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-8.44	-11.29	-2.85	O2

End of simulation.

```
------------------

-------------------------------------
Reading input data for simulation 2.
-------------------------------------

-----------
End of run.
-----------
```

Run 6 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\50-50mix\mix 2 eqb montmorillonite.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\50-50mix\mix 2 eqb montmorillonite.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 1 mix 2 eqb montmorillonite
          temp      20
          pH        9.168
          pe        9.954
          redox     pe
          units     mmol/kgw
          density   1
          C         0.3815
          Ca        6.783e-006
          Na        0.01244
          water    1 # kg
      EQUILIBRIUM_PHASES 1
          Ca-Montmorillonite 0 10
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     mix 2 eqb montmorillonite

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

      Elements           Molality       Moles

      C                 3.815e-004  3.815e-004
      Ca                6.783e-009  6.783e-009
      Na                1.244e-005  1.244e-005

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

                                       pH  =   9.168
                                       pe  =   9.954
                         Activity of water  =   1.000
                            Ionic strength  =  2.368e-004
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  4.145e-004
                       Total CO2 (mol/kg)   =  3.815e-004
                      Temperature (deg C)   =  20.000
                  Electrical balance (eq)   = -4.020e-004
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -94.17
                                Iterations  =   4
                                   Total H  = 1.110128e+002
                                   Total O  = 5.550737e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.017e-005	9.996e-006	-4.993	-5.000	-0.008
H+	6.909e-010	6.792e-010	-9.161	-9.168	-0.007
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-134.140	-134.140	0.000
C(4)	3.815e-004				
HCO3-	3.576e-004	3.514e-004	-3.447	-3.454	-0.008
CO3-2	2.336e-005	2.179e-005	-4.632	-4.662	-0.030
CO2	5.749e-007	5.750e-007	-6.240	-6.240	0.000
NaCO3-	3.903e-009	3.835e-009	-8.409	-8.416	-0.008
NaHCO3	2.414e-009	2.414e-009	-8.617	-8.617	0.000
CaCO3	2.042e-010	2.042e-010	-9.690	-9.690	0.000
CaHCO3+	2.561e-011	2.516e-011	-10.592	-10.599	-0.008
Ca	6.783e-009				
Ca+2	6.552e-009	6.110e-009	-8.184	-8.214	-0.030
CaCO3	2.042e-010	2.042e-010	-9.690	-9.690	0.000
CaHCO3+	2.561e-011	2.516e-011	-10.592	-10.599	-0.008
CaOH+	1.519e-012	1.493e-012	-11.818	-11.826	-0.008
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-41.372	-41.372	0.000
Na	1.244e-005				
Na+	1.243e-005	1.222e-005	-4.905	-4.913	-0.008
NaCO3-	3.903e-009	3.835e-009	-8.409	-8.416	-0.008
NaHCO3	2.414e-009	2.414e-009	-8.617	-8.617	0.000
NaOH	1.188e-010	1.188e-010	-9.925	-9.925	0.000
O(0)	1.057e-011				
O2	5.283e-012	5.283e-012	-11.277	-11.277	0.000

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

Phase	SI	log IAP	log KT	
Aragonite	-4.57	-12.88	-8.31	CaCO3
Calcite	-4.42	-12.88	-8.45	CaCO3
CH4(g)	-131.32	-134.14	-2.82	CH4
CO2(g)	-4.83	-6.24	-1.41	CO2
H2(g)	-38.24	-41.37	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-8.42	-11.28	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. mix 2 eqb montmorillonite
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca-Montmorillonite	0.00	-45.76	-45.76	1.000e+001	1.000e+001	-9.610e-006

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

Elements	Molality	Moles
Al	2.239e-005	2.239e-005
C	3.815e-004	3.815e-004

Ca	1.592e-006	1.592e-006
Na	1.244e-005	1.244e-005
Si	3.527e-005	3.527e-005

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

pH	=	8.746	Charge balance
pe	=	10.376	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	2.273e-004	
Mass of water (kg)	=	1.000e+000	
Total alkalinity (eq/kg)	=	4.848e-004	
Total CO2 (mol/kg)	=	3.815e-004	
Temperature (deg C)	=	20.000	
Electrical balance (eq)	=	-4.020e-004	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-92.81	
Iterations	=	9	
Total H	=	1.110128e+002	
Total O	=	5.550749e+001	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	3.852e-006	3.786e-006	-5.414	-5.422	-0.007
H+	1.824e-009	1.793e-009	-8.739	-8.746	-0.007
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Al	2.239e-005				
Al(OH)4-	2.237e-005	2.199e-005	-4.650	-4.658	-0.007
Al(OH)3	2.223e-008	2.223e-008	-7.653	-7.653	0.000
Al(OH)2+	4.028e-010	3.959e-010	-9.395	-9.402	-0.007
AlOH+2	1.521e-013	1.420e-013	-12.818	-12.848	-0.030
Al+3	4.143e-017	3.562e-017	-16.383	-16.448	-0.066
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-133.702	-133.702	0.000
C(4)	3.815e-004				
HCO3-	3.707e-004	3.645e-004	-3.431	-3.438	-0.007
CO3-2	9.164e-006	8.559e-006	-5.038	-5.068	-0.030
CO2	1.574e-006	1.575e-006	-5.803	-5.803	0.000
CaCO3	1.921e-008	1.921e-008	-7.717	-7.717	0.000
CaHCO3+	6.358e-009	6.250e-009	-8.197	-8.204	-0.007
NaHCO3	2.505e-009	2.505e-009	-8.601	-8.601	0.000
NaCO3-	1.534e-009	1.508e-009	-8.814	-8.822	-0.007
Ca	1.592e-006				
Ca+2	1.567e-006	1.463e-006	-5.805	-5.835	-0.030
CaCO3	1.921e-008	1.921e-008	-7.717	-7.717	0.000
CaHCO3+	6.358e-009	6.250e-009	-8.197	-8.204	-0.007
CaOH+	1.378e-010	1.354e-010	-9.861	-9.868	-0.007
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-41.372	-41.372	0.000
Na	1.244e-005				
Na+	1.244e-005	1.222e-005	-4.905	-4.913	-0.007
NaHCO3	2.505e-009	2.505e-009	-8.601	-8.601	0.000
NaCO3-	1.534e-009	1.508e-009	-8.814	-8.822	-0.007
NaOH	4.504e-011	4.504e-011	-10.346	-10.346	0.000
O(0)	1.057e-011				
O2	5.283e-012	5.283e-012	-11.277	-11.277	0.000
Si	3.527e-005				
H4SiO4	3.297e-005	3.297e-005	-4.482	-4.482	0.000
H3SiO4-	2.304e-006	2.265e-006	-5.637	-5.645	-0.007
H2SiO4-2	6.580e-011	6.143e-011	-10.182	-10.212	-0.030

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

Phase	SI	log IAP	log KT

```
Al(OH)3(a)          -1.34    9.79   11.13  Al(OH)3
Albite              -4.69  -23.02  -18.33  NaAlSi3O8
Anorthite           -4.26  -24.11  -19.86  CaAl2Si2O8
Aragonite           -2.60  -10.90   -8.31  CaCO3
Ca-Montmorillonite   0.00  -45.76  -45.76  Ca0.165Al2.33Si3.67O10(OH)2
Calcite             -2.45  -10.90   -8.45  CaCO3
CH4(g)            -130.88 -133.70   -2.82  CH4
Chalcedony          -0.87   -4.48   -3.61  SiO2
CO2(g)              -4.40   -5.80   -1.41  CO2
Gibbsite             1.40    9.79    8.40  Al(OH)3
H2(g)              -38.24  -41.37   -3.13  H2
H2O(g)              -1.64   -0.00    1.64  H2O
Kaolinite            2.74   10.62    7.88  Al2Si2O5(OH)4
O2(g)               -8.42  -11.28   -2.85  O2
Quartz              -0.43   -4.48   -4.06  SiO2
SiO2(a)             -1.73   -4.48   -2.75  SiO2

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 2.
------------------------------------

-----------
End of run.
-----------
```

Run 7

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\75-25mix\mix NaOH and calcite GW.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\75-25mix\mix NaOH and calcite GW.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 2 NaOH
          temp      20
          pH        14
          pe        4
          redox     pe
          units     mmol/kgw
          density   1
          Na        24.9 Mol/kgw
          water    1 # kg
      SOLUTION 1 GW @ eqb w/ Calcite
          temp      20
          pH        7.301
          pe        -1.841
          redox     pe
          units     mmol/kgw
          density   1
          Ca        0.001789
          C         0.003961
          water    1 # kg
      SAVE solution 1-2
      MIX 1 Mix NaOH and GW @ equ w/ calcite
          1    0.75
          2    0.25
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     GW @ eqb w/ Calcite

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

      Elements           Molality       Moles

      C                3.961e-006  3.961e-006
      Ca               1.789e-006  1.789e-006

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

                                       pH  =   7.301
                                       pe  =  -1.841
                          Activity of water  =   1.000
                             Ionic strength  =  5.444e-006
                         Mass of water (kg)  =  1.000e+000
```

```
                 Total alkalinity (eq/kg)  =  3.626e-006
                       Total CO2 (mol/kg)  =  3.961e-006
                     Temperature (deg C)   =  20.000
                  Electrical balance (eq)  = -4.751e-008
  Percent error, 100*(Cat-|An|)/(Cat+|An|) =  -0.65
                              Iterations  =   3
                                 Total H  = 1.110124e+002
                                 Total O  = 5.550623e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.361e-007	1.358e-007	-6.866	-6.867	-0.001
H+	5.014e-008	5.000e-008	-7.300	-7.301	-0.001
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	1.058e-025				
CH4	1.058e-025	1.058e-025	-24.975	-24.975	0.000
C(4)	3.961e-006				
HCO3-	3.533e-006	3.524e-006	-5.452	-5.453	-0.001
CO2	4.245e-007	4.245e-007	-6.372	-6.372	0.000
CO3-2	3.000e-009	2.968e-009	-8.523	-8.528	-0.005
CaHCO3+	7.328e-011	7.309e-011	-10.135	-10.136	-0.001
CaCO3	8.056e-012	8.056e-012	-11.094	-11.094	0.000
Ca	1.789e-006				
Ca+2	1.789e-006	1.770e-006	-5.747	-5.752	-0.005
CaHCO3+	7.328e-011	7.309e-011	-10.135	-10.136	-0.001
CaCO3	8.056e-012	8.056e-012	-11.094	-11.094	0.000
CaOH+	5.889e-012	5.873e-012	-11.230	-11.231	-0.001
H(0)	1.791e-014				
H2	8.953e-015	8.953e-015	-14.048	-14.048	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-65.925	-65.925	0.000

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

Phase	SI	log IAP	log KT	
Aragonite	-5.97	-14.28	-8.31	CaCO3
Calcite	-5.83	-14.28	-8.45	CaCO3
CH4(g)	-22.16	-24.98	-2.82	CH4
CO2(g)	-4.97	-6.37	-1.41	CO2
H2(g)	-10.92	-14.05	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.07	-65.93	-2.85	O2

Initial solution 2. NaOH

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

Elements	Molality	Moles
Na	2.490e+001	2.490e+001

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

```
                                  pH  =  14.000
                                  pe  =   4.000
                   Activity of water  =   0.562
                      Ionic strength  =  1.184e+001
                  Mass of water (kg)  =  1.000e+000
        Total alkalinity (eq/kg)      =  2.931e+000
           Total carbon (mol/kg)      =  0.000e+000
              Total CO2 (mol/kg)      =  0.000e+000
            Temperature (deg C)       =  20.000
         Electrical balance (eq)      =  2.197e+001
```

```
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  92.76
                              Iterations  =   6
                                 Total H  = 1.139431e+002
                                 Total O  = 5.843693e+001

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

                                                   Log       Log         Log
   Species                 Molality    Activity  Molality  Activity     Gamma

   OH-                   8.574e-001  3.816e-001    -0.067    -0.418    -0.352
   H+                    1.432e-014  1.000e-014   -13.844   -14.000    -0.156
   H2O                   5.551e+001  5.621e-001     1.744    -0.250     0.000
H(0)             0.000e+000
   H2                    0.000e+000  7.447e-040   -40.312   -39.128     1.184
Na               2.490e+001
   Na+                   2.283e+001  8.532e+001     1.358     1.931     0.573
   NaOH                  2.073e+000  3.169e+001     0.317     1.501     1.184
O(0)             7.102e-018
   O2                    3.551e-018  5.427e-017   -17.450   -16.265     1.184

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

      Phase               SI log IAP  log KT

      H2(g)           -36.00  -39.13   -3.13  H2
      H2O(g)           -1.89   -0.25    1.64  H2O
      O2(g)           -13.41  -16.27   -2.85  O2

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

Reaction step 1.

Using mix 1.      Mix NaOH and GW @ equ w/ calcite

Mixture 1.  Mix NaOH and GW @ equ w/ calcite

       7.500e-001 Solution 1  GW @ eqb w/ Calcite
       2.500e-001 Solution 2  NaOH

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

      Elements           Molality       Moles

      C                2.971e-006  2.971e-006
      Ca               1.342e-006  1.342e-006
      Na               6.225e+000  6.225e+000

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

                                      pH  =  13.429      Charge balance
                                      pe  =  -8.061      Adjusted to redox equilibrium
                         Activity of water  =   0.889
                            Ionic strength  =  3.065e+000
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  7.327e-001
                       Total CO2 (mol/kg)   =  2.971e-006
                     Temperature (deg C)    =  20.000
                  Electrical balance (eq)   =  5.492e+000
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  89.60
                              Iterations  =  12
                                 Total H  = 1.117451e+002
                                 Total O  = 5.623890e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	3.188e-001	1.620e-001	-0.496	-0.791	-0.294
H+	5.184e-014	3.725e-014	-13.285	-13.429	-0.144
H2O	5.551e+001	8.888e-001	1.744	-0.051	0.000
C(-4)	3.587e-036				
CH4	3.587e-036	7.264e-036	-35.445	-35.139	0.307
C(4)	2.971e-006				
NaCO3-	2.623e-006	3.646e-006	-5.581	-5.438	0.143
CO3-2	3.475e-007	4.759e-008	-6.459	-7.322	-0.863
HCO3-	6.919e-011	4.209e-011	-10.160	-10.376	-0.216
NaHCO3	6.214e-011	1.258e-010	-10.207	-9.900	0.307
CaCO3	8.932e-012	1.809e-011	-11.049	-10.743	0.307
CaHCO3+	2.010e-016	1.223e-016	-15.697	-15.913	-0.216
CO2	2.098e-018	4.250e-018	-17.678	-17.372	0.307
Ca	1.342e-006				
CaOH+	7.062e-007	9.814e-007	-6.151	-6.008	0.143
Ca+2	6.356e-007	2.479e-007	-6.197	-6.606	-0.409
CaCO3	8.932e-012	1.809e-011	-11.049	-10.743	0.307
CaHCO3+	2.010e-016	1.223e-016	-15.697	-15.913	-0.216
H(0)	1.349e-014				
H2	6.744e-015	1.366e-014	-14.171	-13.865	0.307
Na	6.225e+000				
Na+	5.811e+000	5.317e+000	0.764	0.726	-0.039
NaOH	4.138e-001	8.382e-001	-0.383	-0.077	0.307
NaCO3-	2.623e-006	3.646e-006	-5.581	-5.438	0.143
NaHCO3	6.214e-011	1.258e-010	-10.207	-9.900	0.307
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.701	-66.394	0.307

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

Phase	SI	log IAP	log KT	
Aragonite	-5.62	-13.93	-8.31	CaCO3
Calcite	-5.47	-13.93	-8.45	CaCO3
CH4(g)	-32.32	-35.14	-2.82	CH4
CO2(g)	-15.96	-17.37	-1.41	CO2
H2(g)	-10.74	-13.86	-3.13	H2
H2O(g)	-1.69	-0.05	1.64	H2O
O2(g)	-63.54	-66.39	-2.85	O2

End of simulation.

Reading input data for simulation 2.

End of run.

Run 7 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\75-25mix\mix 1 eqb w calcite and co2.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\75-25mix\mix 1 eqb w calcite and co2.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          Calcite   0 10
          CO2(g)    -2 10
      SOLUTION 1 Mix 1
          temp      20
          pH        13.429
          pe        -8.061
          redox     pe
          units     mmol/kgw
          density   1
          C         2.971e-006
          Ca        1.342e-006
          Na        6.225
          water    1 # kg
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.     Mix 1

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

      Elements           Molality       Moles

      C                2.971e-009  2.971e-009
      Ca               1.342e-009  1.342e-009
      Na               6.225e-003  6.225e-003

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

                                       pH  =  13.429
                                       pe  =  -8.061
                         Activity of water  =   0.996
                            Ionic strength  =  1.243e-001
                       Mass of water (kg)   =  1.000e+000
                  Total alkalinity (eq/kg)  =  2.438e-001
                       Total CO2 (mol/kg)   =  2.971e-009
                      Temperature (deg C)   =  20.000
                  Electrical balance (eq)   = -2.376e-001
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -95.58
                                 Iterations =   5
                                    Total H = 1.112563e+002
                                    Total O = 5.575005e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	2.431e-001	1.815e-001	-0.614	-0.741	-0.127
H+	4.553e-014	3.724e-014	-13.342	-13.429	-0.087
H2O	5.551e+001	9.958e-001	1.744	-0.002	0.000
C(-4)	1.114e-037				
CH4	1.114e-037	1.146e-037	-36.953	-36.941	0.012
C(4)	2.971e-009				
CO3-2	2.886e-009	1.051e-009	-8.540	-8.978	-0.439
NaCO3-	8.330e-011	6.425e-011	-10.079	-10.192	-0.113
HCO3-	1.196e-012	9.294e-013	-11.922	-12.032	-0.110
NaHCO3	2.155e-015	2.217e-015	-14.667	-14.654	0.012
CaCO3	2.487e-016	2.559e-016	-15.604	-15.592	0.012
CO2	8.137e-020	8.374e-020	-19.090	-19.077	0.012
CaHCO3+	2.226e-021	1.729e-021	-20.652	-20.762	-0.110
Ca	1.342e-009				
CaOH+	9.136e-010	7.046e-010	-9.039	-9.152	-0.113
Ca+2	4.284e-010	1.588e-010	-9.368	-9.799	-0.431
CaCO3	2.487e-016	2.559e-016	-15.604	-15.592	0.012
CaHCO3+	2.226e-021	1.729e-021	-20.652	-20.762	-0.110
H(0)	2.658e-014				
H2	1.329e-014	1.368e-014	-13.876	-13.864	0.012
Na	6.225e-003				
Na+	5.497e-003	4.242e-003	-2.260	-2.372	-0.112
NaOH	7.283e-004	7.495e-004	-3.138	-3.125	0.012
NaCO3-	8.330e-011	6.425e-011	-10.079	-10.192	-0.113
NaHCO3	2.155e-015	2.217e-015	-14.667	-14.654	0.012
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.309	-66.297	0.012

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

Phase	SI	log IAP	log KT	
Aragonite	-10.47	-18.78	-8.31	CaCO3
Calcite	-10.32	-18.78	-8.45	CaCO3
CH4(g)	-34.12	-36.94	-2.82	CH4
CO2(g)	-17.67	-19.08	-1.41	CO2
H2(g)	-10.74	-13.86	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.44	-66.30	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Mix 1
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Calcite	0.00	-8.45	-8.45	1.000e+001	1.000e+001	-8.064e-006
CO2(g)	-2.00	-3.41	-1.41	1.000e+001	9.775e+000	-2.251e-001

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

Elements	Molality	Moles

C	2.251e-001	2.252e-001
Ca	8.063e-006	8.066e-006
Na	6.223e-003	6.225e-003

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

pH	=	8.988	Charge balance
pe	=	-3.641	Adjusted to redox equilibrium
Activity of water	=	0.996	
Ionic strength	=	1.427e-001	
Mass of water (kg)	=	1.000e+000	
Total alkalinity (eq/kg)	=	2.438e-001	
Total CO2 (mol/kg)	=	2.251e-001	
Temperature (deg C)	=	20.000	
Electrical balance (eq)	=	-2.376e-001	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-95.67	
Iterations	=	13	
Total H	=	1.112563e+002	
Total O	=	5.620038e+001	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	8.947e-006	6.585e-006	-5.048	-5.181	-0.133
H+	1.264e-009	1.027e-009	-8.898	-8.988	-0.090
H2O	5.551e+001	9.961e-001	1.744	-0.002	0.000
C(-4)	7.645e-022				
CH4	7.645e-022	7.901e-022	-21.117	-21.102	0.014
C(4)	2.251e-001				
HCO3-	2.053e-001	1.578e-001	-0.688	-0.802	-0.114
CO3-2	1.855e-002	6.469e-003	-1.732	-2.189	-0.458
NaCO3-	5.005e-004	3.824e-004	-3.301	-3.417	-0.117
CO2	3.792e-004	3.919e-004	-3.421	-3.407	0.014
NaHCO3	3.522e-004	3.639e-004	-3.453	-3.439	0.014
CaCO3	5.226e-006	5.401e-006	-5.282	-5.268	0.014
CaHCO3+	1.310e-006	1.006e-006	-5.883	-5.997	-0.114
Ca	8.063e-006				
CaCO3	5.226e-006	5.401e-006	-5.282	-5.268	0.014
Ca+2	1.527e-006	5.443e-007	-5.816	-6.264	-0.448
CaHCO3+	1.310e-006	1.006e-006	-5.883	-5.997	-0.114
CaOH+	1.147e-010	8.762e-011	-9.941	-10.057	-0.117
H(0)	2.917e-014				
H2	1.458e-014	1.507e-014	-13.836	-13.822	0.014
Na	6.223e-003				
Na+	5.370e-003	4.103e-003	-2.270	-2.387	-0.117
NaCO3-	5.005e-004	3.824e-004	-3.301	-3.417	-0.117
NaHCO3	3.522e-004	3.639e-004	-3.453	-3.439	0.014
NaOH	2.544e-008	2.629e-008	-7.594	-7.580	0.014
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.395	-66.381	0.014

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

Phase	SI	log IAP	log KT	
Aragonite	-0.15	-8.45	-8.31	CaCO3
Calcite	0.00	-8.45	-8.45	CaCO3
CH4(g)	-18.28	-21.10	-2.82	CH4
CO2(g)	-2.00	-3.41	-1.41	CO2
H2(g)	-10.69	-13.82	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.53	-66.38	-2.85	O2

End of simulation.

```
------------------

-------------------------------------
Reading input data for simulation 2.
-------------------------------------

-----------
End of run.
-----------
```

Run 7 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\75-25mix\mix 2 eqb w montmorillonite.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\75-25mix\mix 2 eqb w montmorillonite.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 1 mix 2 eqb w montmorillonite
          temp      20
          pH        8.988
          pe        -3.641
          redox     pe
          units     mmol/kgw
          density   1
          C         0.2251
          Ca        8.063e-006
          Na        0.006223
          water    1 # kg
      EQUILIBRIUM_PHASES 1
          Ca-Montmorillonite 0 10
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     mix 2 eqb w montmorillonite

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

      Elements           Molality       Moles

      C                2.251e-004  2.251e-004
      Ca               8.063e-009  8.063e-009
      Na               6.223e-006  6.223e-006

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

                                       pH  =   8.988
                                       pe  =  -3.641
                         Activity of water  =   1.000
                            Ionic strength  =  1.325e-004
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  2.404e-004
                       Total CO2 (mol/kg)   =  2.251e-004
                     Temperature (deg C)    =  20.000
                  Electrical balance (eq)   = -2.342e-004
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   = -94.94
                                Iterations  =   3
                                   Total H  = 1.110127e+002
                                   Total O  = 5.550690e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.692e-006	6.604e-006	-5.174	-5.180	-0.006
H+	1.041e-009	1.028e-009	-8.982	-8.988	-0.006
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	1.052e-024				
CH4	1.052e-024	1.052e-024	-23.978	-23.978	0.000
C(4)	2.251e-004				
HCO3-	2.154e-004	2.126e-004	-3.667	-3.672	-0.006
CO3-2	9.178e-006	8.709e-006	-5.037	-5.060	-0.023
CO2	5.265e-007	5.265e-007	-6.279	-6.279	0.000
NaCO3-	7.807e-010	7.705e-010	-9.108	-9.113	-0.006
NaHCO3	7.340e-010	7.340e-010	-9.134	-9.134	0.000
CaCO3	1.007e-010	1.007e-010	-9.997	-9.997	0.000
CaHCO3+	1.902e-011	1.878e-011	-10.721	-10.726	-0.006
Ca	8.063e-009				
Ca+2	7.942e-009	7.536e-009	-8.100	-8.123	-0.023
CaCO3	1.007e-010	1.007e-010	-9.997	-9.997	0.000
CaHCO3+	1.902e-011	1.878e-011	-10.721	-10.726	-0.006
CaOH+	1.233e-012	1.217e-012	-11.909	-11.915	-0.006
H(0)	3.013e-014				
H2	1.507e-014	1.507e-014	-13.822	-13.822	0.000
Na	6.223e-006				
Na+	6.221e-006	6.140e-006	-5.206	-5.212	-0.006
NaCO3-	7.807e-010	7.705e-010	-9.108	-9.113	-0.006
NaHCO3	7.340e-010	7.340e-010	-9.134	-9.134	0.000
NaOH	3.946e-011	3.946e-011	-10.404	-10.404	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.377	-66.377	0.000

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

Phase	SI	log IAP	log KT	
Aragonite	-4.88	-13.18	-8.31	CaCO3
Calcite	-4.73	-13.18	-8.45	CaCO3
CH4(g)	-21.16	-23.98	-2.82	CH4
CO2(g)	-4.87	-6.28	-1.41	CO2
H2(g)	-10.69	-13.82	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.52	-66.38	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. mix 2 eqb w montmorillonite
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca-Montmorillonite	0.00	-45.76	-45.76	1.000e+001	1.000e+001	-6.846e-006

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

Elements	Molality	Moles
Al	1.595e-005	1.595e-005
C	2.251e-004	2.251e-004

Ca	1.138e-006	1.138e-006
Na	6.223e-006	6.223e-006
Si	2.513e-005	2.513e-005

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

```
                                    pH  =   8.328      Charge balance
                                    pe  =  -2.984      Adjusted to redox equilibrium
                       Activity of water  =   1.000
                          Ionic strength  =  1.288e-004
                     Mass of water (kg)   =  1.000e+000
                Total alkalinity (eq/kg)  =  2.906e-004
                     Total CO2 (mol/kg)   =  2.251e-004
                   Temperature (deg C)    =  20.000
                 Electrical balance (eq)  = -2.342e-004
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -93.24
                            Iterations    =   9
                               Total H    = 1.110127e+002
                               Total O    = 5.550698e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.462e-006	1.444e-006	-5.835	-5.841	-0.006
H+	4.764e-009	4.703e-009	-8.322	-8.328	-0.006
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Al	1.595e-005				
Al(OH)4-	1.591e-005	1.570e-005	-4.798	-4.804	-0.006
Al(OH)3	4.164e-008	4.164e-008	-7.380	-7.380	0.000
Al(OH)2+	1.970e-009	1.945e-009	-8.706	-8.711	-0.006
AlOH+2	1.927e-012	1.829e-012	-11.715	-11.738	-0.023
Al+3	1.350e-015	1.203e-015	-14.870	-14.920	-0.050
C(-4)	5.255e-024				
CH4	5.255e-024	5.255e-024	-23.279	-23.279	0.000
C(4)	2.251e-004				
HCO3-	2.206e-004	2.177e-004	-3.656	-3.662	-0.006
CO2	2.467e-006	2.467e-006	-5.608	-5.608	0.000
CO3-2	2.053e-006	1.950e-006	-5.688	-5.710	-0.022
CaCO3	3.213e-009	3.213e-009	-8.493	-8.493	0.000
CaHCO3+	2.778e-009	2.742e-009	-8.556	-8.562	-0.006
NaHCO3	7.520e-010	7.520e-010	-9.124	-9.124	0.000
NaCO3-	1.748e-010	1.725e-010	-9.757	-9.763	-0.006
Ca	1.138e-006				
Ca+2	1.132e-006	1.075e-006	-5.946	-5.969	-0.022
CaCO3	3.213e-009	3.213e-009	-8.493	-8.493	0.000
CaHCO3+	2.778e-009	2.742e-009	-8.556	-8.562	-0.006
CaOH+	3.841e-011	3.792e-011	-10.416	-10.421	-0.006
H(0)	3.062e-014				
H2	1.531e-014	1.531e-014	-13.815	-13.815	0.000
Na	6.223e-006				
Na+	6.222e-006	6.142e-006	-5.206	-5.212	-0.006
NaHCO3	7.520e-010	7.520e-010	-9.124	-9.124	0.000
NaCO3-	1.748e-010	1.725e-010	-9.757	-9.763	-0.006
NaOH	8.628e-012	8.628e-012	-11.064	-11.064	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.391	-66.391	0.000
Si	2.513e-005				
H4SiO4	2.448e-005	2.448e-005	-4.611	-4.611	0.000
H3SiO4-	6.496e-007	6.412e-007	-6.187	-6.193	-0.006
H2SiO4-2	6.985e-012	6.631e-012	-11.156	-11.178	-0.023

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

Phase	SI	log IAP	log KT

```
Al(OH)3(a)        -1.07   10.06   11.13  Al(OH)3
Albite            -5.52  -23.85  -18.33  NaAlSi3O8
Anorthite         -4.94  -24.80  -19.86  CaAl2Si2O8
Aragonite         -3.37  -11.68   -8.31  CaCO3
Ca-Montmorillonite   0.00  -45.76  -45.76  Ca0.165Al2.33Si3.67O10(OH)2
Calcite           -3.23  -11.68   -8.45  CaCO3
CH4(g)           -20.46  -23.28   -2.82  CH4
Chalcedony        -1.00   -4.61   -3.61  SiO2
CO2(g)            -4.20   -5.61   -1.41  CO2
Gibbsite           1.67   10.06    8.40  Al(OH)3
H2(g)            -10.69  -13.82   -3.13  H2
H2O(g)            -1.64   -0.00    1.64  H2O
Kaolinite          3.03   10.90    7.88  Al2Si2O5(OH)4
O2(g)            -63.54  -66.39   -2.85  O2
Quartz            -0.56   -4.61   -4.06  SiO2
SiO2(a)           -1.86   -4.61   -2.75  SiO2

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 2.
-----------------------------------

-----------
End of run.
-----------
```

Run 8

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\123109\mix NaOH and calcite GW.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\123109\mix NaOH and calcite GW.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 2 NaOH
          temp      20
          pH        14
          pe        4
          redox     pe
          units     mmol/kgw
          density   1
          Na        24.9 Mol/kgw
          water    1 # kg
      SOLUTION 1 GW @ eqb w/ Calcite
          temp      20
          pH        7.301
          pe        -1.841
          redox     pe
          units     mmol/kgw
          density   1
          Ca        0.001789
          C         0.003961
          water    1 # kg
      SAVE solution 1-2
      MIX 1 Mix NaOH and GW @ equ w/ calcite
          1    0.9
          2    0.1
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     GW @ eqb w/ Calcite

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

      Elements           Molality       Moles

      C                3.961e-006  3.961e-006
      Ca               1.789e-006  1.789e-006

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

                                     pH  =   7.301
                                     pe  =  -1.841
                        Activity of water  =   1.000
                           Ionic strength  =  5.444e-006
                       Mass of water (kg)  =  1.000e+000
```

```
                 Total alkalinity (eq/kg)  =  3.626e-006
                       Total CO2 (mol/kg)  =  3.961e-006
                     Temperature (deg C)   =  20.000
                  Electrical balance (eq)  = -4.751e-008
  Percent error, 100*(Cat-|An|)/(Cat+|An|) =  -0.65
                              Iterations   =   3
                                 Total H   = 1.110124e+002
                                 Total O   = 5.550623e+001

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

                                                   Log       Log        Log
   Species                  Molality    Activity  Molality  Activity   Gamma

   OH-                     1.361e-007  1.358e-007   -6.866    -6.867   -0.001
   H+                      5.014e-008  5.000e-008   -7.300    -7.301   -0.001
   H2O                     5.551e+001  1.000e+000    1.744    -0.000    0.000
C(-4)            1.058e-025
   CH4                     1.058e-025  1.058e-025  -24.975   -24.975    0.000
C(4)             3.961e-006
   HCO3-                   3.533e-006  3.524e-006   -5.452    -5.453   -0.001
   CO2                     4.245e-007  4.245e-007   -6.372    -6.372    0.000
   CO3-2                   3.000e-009  2.968e-009   -8.523    -8.528   -0.005
   CaHCO3+                 7.328e-011  7.309e-011  -10.135   -10.136   -0.001
   CaCO3                   8.056e-012  8.056e-012  -11.094   -11.094    0.000
Ca               1.789e-006
   Ca+2                    1.789e-006  1.770e-006   -5.747    -5.752   -0.005
   CaHCO3+                 7.328e-011  7.309e-011  -10.135   -10.136   -0.001
   CaCO3                   8.056e-012  8.056e-012  -11.094   -11.094    0.000
   CaOH+                   5.889e-012  5.873e-012  -11.230   -11.231   -0.001
H(0)             1.791e-014
   H2                      8.953e-015  8.953e-015  -14.048   -14.048    0.000
O(0)             0.000e+000
   O2                      0.000e+000  0.000e+000  -65.925   -65.925    0.000

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

     Phase              SI log IAP  log KT

     Aragonite       -5.97  -14.28   -8.31  CaCO3
     Calcite         -5.83  -14.28   -8.45  CaCO3
     CH4(g)         -22.16  -24.98   -2.82  CH4
     CO2(g)          -4.97   -6.37   -1.41  CO2
     H2(g)          -10.92  -14.05   -3.13  H2
     H2O(g)          -1.64   -0.00    1.64  H2O
     O2(g)          -63.07  -65.93   -2.85  O2

Initial solution 2.     NaOH

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

     Elements          Molality       Moles

     Na              2.490e+001  2.490e+001

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

                                     pH  =  14.000
                                     pe  =   4.000
                       Activity of water  =   0.562
                          Ionic strength  =  1.184e+001
                     Mass of water (kg)   =  1.000e+000
               Total alkalinity (eq/kg)   =  2.931e+000
                  Total carbon (mol/kg)   =  0.000e+000
                     Total CO2 (mol/kg)   =  0.000e+000
                   Temperature (deg C)    =  20.000
                Electrical balance (eq)   =  2.197e+001
```

```
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  92.76
                                Iterations  =   6
                                   Total H  = 1.139431e+002
                                   Total O  = 5.843693e+001

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

                                                   Log       Log         Log
   Species                 Molality    Activity  Molality  Activity     Gamma

   OH-                   8.574e-001  3.816e-001    -0.067    -0.418    -0.352
   H+                    1.432e-014  1.000e-014   -13.844   -14.000    -0.156
   H2O                   5.551e+001  5.621e-001     1.744    -0.250     0.000
H(0)             0.000e+000
   H2                    0.000e+000  7.447e-040   -40.312   -39.128     1.184
Na               2.490e+001
   Na+                   2.283e+001  8.532e+001     1.358     1.931     0.573
   NaOH                  2.073e+000  3.169e+001     0.317     1.501     1.184
O(0)             7.102e-018
   O2                    3.551e-018  5.427e-017   -17.450   -16.265     1.184

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

      Phase               SI log IAP  log KT

      H2(g)           -36.00  -39.13   -3.13  H2
      H2O(g)           -1.89   -0.25    1.64  H2O
      O2(g)           -13.41  -16.27   -2.85  O2

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

Reaction step 1.

Using mix 1.      Mix NaOH and GW @ equ w/ calcite

Mixture 1.  Mix NaOH and GW @ equ w/ calcite

       9.000e-001 Solution 1  GW @ eqb w/ Calcite
       1.000e-001 Solution 2  NaOH

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

      Elements           Molality       Moles

      C                3.565e-006  3.565e-006
      Ca               1.610e-006  1.610e-006
      Na               2.490e+000  2.490e+000

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

                                     pH  =  13.173      Charge balance
                                     pe  =  -7.872      Adjusted to redox equilibrium
                        Activity of water  =   0.955
                           Ionic strength  =  1.270e+000
                       Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  =  2.931e-001
                       Total CO2 (mol/kg)  =  3.565e-006
                     Temperature (deg C)   =  20.000
                  Electrical balance (eq)  =  2.197e+000
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  86.52
                                Iterations  =  11
                                   Total H  = 1.113055e+002
                                   Total O  = 5.579930e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.712e-001	9.661e-002	-0.767	-1.015	-0.248
H+	9.086e-014	6.709e-014	-13.042	-13.173	-0.132
H2O	5.551e+001	9.548e-001	1.744	-0.020	0.000
C(-4)	1.033e-034				
CH4	1.033e-034	1.384e-034	-33.986	-33.859	0.127
C(4)	3.565e-006				
NaCO3-	2.986e-006	2.511e-006	-5.525	-5.600	-0.075
CO3-2	5.783e-007	1.003e-007	-6.238	-6.998	-0.761
HCO3-	2.477e-010	1.599e-010	-9.606	-9.796	-0.190
NaHCO3	1.166e-010	1.561e-010	-9.933	-9.806	0.127
CaCO3	2.759e-011	3.696e-011	-10.559	-10.432	0.127
CaHCO3+	6.971e-016	4.499e-016	-15.157	-15.347	-0.190
CO2	2.020e-017	2.706e-017	-16.695	-16.568	0.127
Ca	1.610e-006				
Ca+2	9.357e-007	2.401e-007	-6.029	-6.620	-0.591
CaOH+	6.744e-007	5.672e-007	-6.171	-6.246	-0.075
CaCO3	2.759e-011	3.696e-011	-10.559	-10.432	0.127
CaHCO3+	6.971e-016	4.499e-016	-15.157	-15.347	-0.190
H(0)	2.780e-014				
H2	1.390e-014	1.862e-014	-13.857	-13.730	0.127
Na	2.490e+000				
Na+	2.368e+000	1.737e+000	0.374	0.240	-0.135
NaOH	1.219e-001	1.633e-001	-0.914	-0.787	0.127
NaCO3-	2.986e-006	2.511e-006	-5.525	-5.600	-0.075
NaHCO3	1.166e-010	1.561e-010	-9.933	-9.806	0.127
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.728	-66.601	0.127

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

Phase	SI	log IAP	log KT	
Aragonite	-5.31	-13.62	-8.31	CaCO3
Calcite	-5.16	-13.62	-8.45	CaCO3
CH4(g)	-31.04	-33.86	-2.82	CH4
CO2(g)	-15.16	-16.57	-1.41	CO2
H2(g)	-10.60	-13.73	-3.13	H2
H2O(g)	-1.66	-0.02	1.64	H2O
O2(g)	-63.75	-66.60	-2.85	O2

End of simulation.

Reading input data for simulation 2.

End of run.

Run 8 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\123109\mix 1 eqb w calcite and co2.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\123109\mix 1 eqb w calcite and co2.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-------------------------------------
Reading input data for simulation 1.
-------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          Calcite   0 10
          CO2(g)    -2 10
      SOLUTION 1 Mix 1
          temp      20
          pH        13.173
          pe        -7.872
          redox     pe
          units     mmol/kgw
          density   1
          C         3.565e-006
          Ca        1.61e-006
          Na        2.49
          water    1 # kg
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.     Mix 1

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

      Elements           Molality       Moles

      C                3.565e-009  3.565e-009
      Ca               1.610e-009  1.610e-009
      Na               2.490e-003  2.490e-003

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

                                       pH  =  13.173
                                       pe  =  -7.872
                         Activity of water  =   0.998
                            Ionic strength  =  6.458e-002
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  1.270e-001
                       Total CO2 (mol/kg)   =  3.565e-009
                     Temperature (deg C)    =  20.000
                  Electrical balance (eq)   = -1.245e-001
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   = -96.42
                                Iterations  =   5
                                   Total H  = 1.111395e+002
                                   Total O  = 5.563324e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.268e-001	1.009e-001	-0.897	-0.996	-0.099
H+	7.950e-014	6.714e-014	-13.100	-13.173	-0.073
H2O	5.551e+001	9.978e-001	1.744	-0.001	0.000
C(-4)	1.852e-036				
CH4	1.852e-036	1.880e-036	-35.732	-35.726	0.006
C(4)	3.565e-009				
CO3-2	3.510e-009	1.553e-009	-8.455	-8.809	-0.354
NaCO3-	5.179e-011	4.185e-011	-10.286	-10.378	-0.093
HCO3-	3.036e-012	2.476e-012	-11.518	-11.606	-0.089
NaHCO3	2.566e-015	2.604e-015	-14.591	-14.584	0.006
CaCO3	7.127e-016	7.234e-016	-15.147	-15.141	0.006
CO2	3.954e-019	4.013e-019	-18.403	-18.396	0.006
CaHCO3+	1.081e-020	8.812e-021	-19.966	-20.055	-0.089
Ca	1.610e-009				
CaOH+	9.270e-010	7.491e-010	-9.033	-9.125	-0.093
Ca+2	6.830e-010	3.037e-010	-9.166	-9.518	-0.352
CaCO3	7.127e-016	7.234e-016	-15.147	-15.141	0.006
CaHCO3+	1.081e-020	8.812e-021	-19.966	-20.055	-0.089
H(0)	3.669e-014				
H2	1.835e-014	1.862e-014	-13.736	-13.730	0.006
Na	2.490e-003				
Na+	2.309e-003	1.871e-003	-2.637	-2.728	-0.091
NaOH	1.810e-004	1.837e-004	-3.742	-3.736	0.006
NaCO3-	5.179e-011	4.185e-011	-10.286	-10.378	-0.093
NaHCO3	2.566e-015	2.604e-015	-14.591	-14.584	0.006
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.569	-66.563	0.006

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

Phase	SI	log IAP	log KT	
Aragonite	-10.02	-18.33	-8.31	CaCO3
Calcite	-9.87	-18.33	-8.45	CaCO3
CH4(g)	-32.91	-35.73	-2.82	CH4
CO2(g)	-16.99	-18.40	-1.41	CO2
H2(g)	-10.60	-13.73	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.71	-66.56	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Mix 1
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Calcite	0.00	-8.45	-8.45	1.000e+001	1.000e+001	-1.091e-005
CO2(g)	-2.00	-3.41	-1.41	1.000e+001	9.878e+000	-1.220e-001

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

Elements	Molality	Moles

C	1.220e-001	1.220e-001
Ca	1.091e-005	1.091e-005
Na	2.490e-003	2.490e-003

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

pH	=	8.764	Charge balance
pe	=	-3.392	Adjusted to redox equilibrium
Activity of water	=	0.998	
Ionic strength	=	6.991e-002	
Mass of water (kg)	=	1.000e+000	
Total alkalinity (eq/kg)	=	1.270e-001	
Total CO2 (mol/kg)	=	1.220e-001	
Temperature (deg C)	=	20.000	
Electrical balance (eq)	=	-1.245e-001	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-96.40	
Iterations	=	15	
Total H	=	1.111395e+002	
Total O	=	5.587729e+001	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	4.977e-006	3.931e-006	-5.303	-5.406	-0.102
H+	2.049e-009	1.724e-009	-8.689	-8.764	-0.075
H2O	5.551e+001	9.979e-001	1.744	-0.001	0.000
C(-4)	4.944e-022				
CH4	4.944e-022	5.024e-022	-21.306	-21.299	0.007
C(4)	1.220e-001				
HCO3-	1.161e-001	9.417e-002	-0.935	-1.026	-0.091
CO3-2	5.320e-003	2.301e-003	-2.274	-2.638	-0.364
CO2	3.856e-004	3.919e-004	-3.414	-3.407	0.007
NaHCO3	9.719e-005	9.877e-005	-4.012	-4.005	0.007
NaCO3-	7.696e-005	6.184e-005	-4.114	-4.209	-0.095
CaCO3	5.315e-006	5.401e-006	-5.275	-5.268	0.007
CaHCO3+	2.083e-006	1.689e-006	-5.681	-5.772	-0.091
Ca	1.091e-005				
CaCO3	5.315e-006	5.401e-006	-5.275	-5.268	0.007
Ca+2	3.516e-006	1.530e-006	-5.454	-5.815	-0.361
CaHCO3+	2.083e-006	1.689e-006	-5.681	-5.772	-0.091
CaOH+	1.830e-010	1.470e-010	-9.738	-9.833	-0.095
H(0)	2.651e-014				
H2	1.325e-014	1.347e-014	-13.878	-13.871	0.007
Na	2.490e-003				
Na+	2.316e-003	1.865e-003	-2.635	-2.729	-0.094
NaHCO3	9.719e-005	9.877e-005	-4.012	-4.005	0.007
NaCO3-	7.696e-005	6.184e-005	-4.114	-4.209	-0.095
NaOH	7.021e-009	7.135e-009	-8.154	-8.147	0.007
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.289	-66.282	0.007

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

Phase	SI	log IAP	log KT	
Aragonite	-0.15	-8.45	-8.31	CaCO3
Calcite	0.00	-8.45	-8.45	CaCO3
CH4(g)	-18.48	-21.30	-2.82	CH4
CO2(g)	-2.00	-3.41	-1.41	CO2
H2(g)	-10.74	-13.87	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.43	-66.28	-2.85	O2

End of simulation.

```
------------------

-------------------------------------
Reading input data for simulation 2.
-------------------------------------

-----------
End of run.
-----------
```

Run 8 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\123109\mix 2 eqb w montmorillonite.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\123109\mix 2 eqb w montmorillonite.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 1 mix 2 eqb w montmorillonite
          temp      20
          pH        8.764
          pe        -3.392
          redox     pe
          units     mmol/kgw
          density   1
          C         0.122
          Ca        1.091e-005
          Na        0.00249
          water    1 # kg
      EQUILIBRIUM_PHASES 1
          Ca-Montmorillonite 0 10
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     mix 2 eqb w montmorillonite

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

      Elements           Molality       Moles

      C                1.220e-004  1.220e-004
      Ca               1.091e-008  1.091e-008
      Na               2.490e-006  2.490e-006

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

                                       pH  =   8.764
                                       pe  =  -3.392
                        Activity of water  =   1.000
                           Ionic strength  =  6.849e-005
                       Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  =  1.285e-004
                       Total CO2 (mol/kg)  =  1.220e-004
                     Temperature (deg C)   =  20.000
                  Electrical balance (eq)  = -1.260e-004
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -96.16
                                Iterations  =   4
                                   Total H  = 1.110126e+002
                                   Total O  = 5.550659e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	3.981e-006	3.943e-006	-5.400	-5.404	-0.004
H+	1.738e-009	1.722e-009	-8.760	-8.764	-0.004
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	6.141e-025				
CH4	6.141e-025	6.141e-025	-24.212	-24.212	0.000
C(4)	1.220e-004				
HCO3-	1.185e-004	1.174e-004	-3.926	-3.930	-0.004
CO3-2	2.983e-006	2.872e-006	-5.525	-5.542	-0.016
CO2	4.870e-007	4.871e-007	-6.312	-6.312	0.000
NaHCO3	1.628e-010	1.628e-010	-9.788	-9.788	0.000
NaCO3-	1.030e-010	1.020e-010	-9.987	-9.991	-0.004
CaCO3	4.600e-011	4.600e-011	-10.337	-10.337	0.000
CaHCO3+	1.451e-011	1.437e-011	-10.838	-10.842	-0.004
Ca	1.091e-008				
Ca+2	1.085e-008	1.044e-008	-7.965	-7.981	-0.016
CaCO3	4.600e-011	4.600e-011	-10.337	-10.337	0.000
CaHCO3+	1.451e-011	1.437e-011	-10.838	-10.842	-0.004
CaOH+	1.016e-012	1.007e-012	-11.993	-11.997	-0.004
H(0)	2.685e-014				
H2	1.343e-014	1.343e-014	-13.872	-13.872	0.000
Na	2.490e-006				
Na+	2.490e-006	2.466e-006	-5.604	-5.608	-0.004
NaHCO3	1.628e-010	1.628e-010	-9.788	-9.788	0.000
NaCO3-	1.030e-010	1.020e-010	-9.987	-9.991	-0.004
NaOH	9.463e-012	9.463e-012	-11.024	-11.024	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.277	-66.277	0.000

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

Phase	SI	log IAP	log KT	
Aragonite	-5.22	-13.52	-8.31	CaCO3
Calcite	-5.07	-13.52	-8.45	CaCO3
CH4(g)	-21.39	-24.21	-2.82	CH4
CO2(g)	-4.91	-6.31	-1.41	CO2
H2(g)	-10.74	-13.87	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.42	-66.28	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. mix 2 eqb w montmorillonite
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca-Montmorillonite	0.00	-45.76	-45.76	1.000e+001	1.000e+001	-4.759e-006

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

Elements	Molality	Moles
Al	1.109e-005	1.109e-005
C	1.220e-004	1.220e-004

Ca	7.962e-007	7.962e-007
Na	2.490e-006	2.490e-006
Si	1.747e-005	1.747e-005

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

pH	=	7.854	Charge balance
pe	=	-2.379	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	6.825e-005	
Mass of water (kg)	=	1.000e+000	
Total alkalinity (eq/kg)	=	1.633e-004	
Total CO2 (mol/kg)	=	1.220e-004	
Temperature (deg C)	=	20.000	
Electrical balance (eq)	=	-1.260e-004	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-93.88	
Iterations	=	8	
Total H	=	1.110126e+002	
Total O	=	5.550664e+001	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	4.900e-007	4.854e-007	-6.310	-6.314	-0.004
H+	1.412e-008	1.399e-008	-7.850	-7.854	-0.004
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Al	1.109e-005				
Al(OH)4-	1.099e-005	1.089e-005	-4.959	-4.963	-0.004
Al(OH)3	8.587e-008	8.587e-008	-7.066	-7.066	0.000
Al(OH)2+	1.204e-008	1.193e-008	-7.919	-7.923	-0.004
AlOH+2	3.466e-011	3.337e-011	-10.460	-10.477	-0.017
Al+3	7.103e-014	6.528e-014	-13.149	-13.185	-0.037
C(-4)	7.428e-025				
CH4	7.428e-025	7.428e-025	-24.129	-24.129	0.000
C(4)	1.220e-004				
HCO3-	1.177e-004	1.166e-004	-3.929	-3.933	-0.004
CO2	3.929e-006	3.929e-006	-5.406	-5.406	0.000
CO3-2	3.646e-007	3.511e-007	-6.438	-6.455	-0.016
CaHCO3+	1.056e-009	1.046e-009	-8.977	-8.981	-0.004
CaCO3	4.120e-010	4.120e-010	-9.385	-9.385	0.000
NaHCO3	1.617e-010	1.617e-010	-9.791	-9.791	0.000
NaCO3-	1.259e-011	1.247e-011	-10.900	-10.904	-0.004
Ca	7.962e-007				
Ca+2	7.947e-007	7.652e-007	-6.100	-6.116	-0.016
CaHCO3+	1.056e-009	1.046e-009	-8.977	-8.981	-0.004
CaCO3	4.120e-010	4.120e-010	-9.385	-9.385	0.000
CaOH+	9.166e-012	9.079e-012	-11.038	-11.042	-0.004
H(0)	1.671e-014				
H2	8.355e-015	8.356e-015	-14.078	-14.078	0.000
Na	2.490e-006				
Na+	2.490e-006	2.466e-006	-5.604	-5.608	-0.004
NaHCO3	1.617e-010	1.617e-010	-9.791	-9.791	0.000
NaCO3-	1.259e-011	1.247e-011	-10.900	-10.904	-0.004
NaOH	1.165e-012	1.165e-012	-11.934	-11.934	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-65.865	-65.865	0.000
Si	1.747e-005				
H4SiO4	1.731e-005	1.731e-005	-4.762	-4.762	0.000
H3SiO4-	1.540e-007	1.525e-007	-6.813	-6.817	-0.004
H2SiO4-2	5.508e-013	5.303e-013	-12.259	-12.275	-0.017

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

Phase	SI	log IAP	log KT

```
Al(OH)3(a)          -0.75   10.38   11.13  Al(OH)3
Albite              -6.53  -24.86  -18.33  NaAlSi3O8
Anorthite           -5.71  -25.57  -19.86  CaAl2Si2O8
Aragonite           -4.26  -12.57   -8.31  CaCO3
Ca-Montmorillonite   0.00  -45.76  -45.76  Ca0.165Al2.33Si3.67O10(OH)2
Calcite             -4.12  -12.57   -8.45  CaCO3
CH4(g)             -21.31  -24.13   -2.82  CH4
Chalcedony          -1.15   -4.76   -3.61  SiO2
CO2(g)              -4.00   -5.41   -1.41  CO2
Gibbsite             1.98   10.38    8.40  Al(OH)3
H2(g)              -10.95  -14.08   -3.13  H2
H2O(g)              -1.64   -0.00    1.64  H2O
Kaolinite            3.36   11.23    7.88  Al2Si2O5(OH)4
O2(g)              -63.01  -65.87   -2.85  O2
Quartz              -0.71   -4.76   -4.06  SiO2
SiO2(a)             -2.01   -4.76   -2.75  SiO2

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 2.
------------------------------------

-----------
End of run.
-----------
```

Run 9

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\95-5 mix\mix 5%NaOH and 95%calcite GW.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\95-5 mix\mix 5%NaOH and 95%calcite GW.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
------------------------------------
Reading input data for simulation 1.
------------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 2 NaOH
          temp      20
          pH        14
          pe        4
          redox     pe
          units     mmol/kgw
          density   1
          Na        24.9 Mol/kgw
          water    1 # kg
      SOLUTION 1 GW @ eqb w/ Calcite
          temp      20
          pH        7.301
          pe        -1.841
          redox     pe
          units     mmol/kgw
          density   1
          Ca        0.001789
          C         0.003961
          water    1 # kg
      SAVE solution 1-2
      MIX 1 Mix NaOH and GW @ equ w/ calcite
          1    0.95
          2    0.05
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     GW @ eqb w/ Calcite

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

      Elements           Molality       Moles

      C                3.961e-006  3.961e-006
      Ca               1.789e-006  1.789e-006

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

                                       pH  =   7.301
                                       pe  =  -1.841
                         Activity of water  =   1.000
                            Ionic strength  =  5.444e-006
                        Mass of water (kg)  =  1.000e+000
```

```
                 Total alkalinity (eq/kg)  =  3.626e-006
                       Total CO2 (mol/kg)  =  3.961e-006
                     Temperature (deg C)   =  20.000
                  Electrical balance (eq)  = -4.751e-008
  Percent error, 100*(Cat-|An|)/(Cat+|An|) =  -0.65
                              Iterations  =   3
                                 Total H  = 1.110124e+002
                                 Total O  = 5.550623e+001

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

                                                   Log       Log         Log
   Species                 Molality    Activity  Molality  Activity     Gamma

   OH-                   1.361e-007  1.358e-007    -6.866    -6.867    -0.001
   H+                    5.014e-008  5.000e-008    -7.300    -7.301    -0.001
   H2O                   5.551e+001  1.000e+000     1.744    -0.000     0.000
C(-4)            1.058e-025
   CH4                   1.058e-025  1.058e-025   -24.975   -24.975     0.000
C(4)             3.961e-006
   HCO3-                 3.533e-006  3.524e-006    -5.452    -5.453    -0.001
   CO2                   4.245e-007  4.245e-007    -6.372    -6.372     0.000
   CO3-2                 3.000e-009  2.968e-009    -8.523    -8.528    -0.005
   CaHCO3+               7.328e-011  7.309e-011   -10.135   -10.136    -0.001
   CaCO3                 8.056e-012  8.056e-012   -11.094   -11.094     0.000
Ca               1.789e-006
   Ca+2                  1.789e-006  1.770e-006    -5.747    -5.752    -0.005
   CaHCO3+               7.328e-011  7.309e-011   -10.135   -10.136    -0.001
   CaCO3                 8.056e-012  8.056e-012   -11.094   -11.094     0.000
   CaOH+                 5.889e-012  5.873e-012   -11.230   -11.231    -0.001
H(0)             1.791e-014
   H2                    8.953e-015  8.953e-015   -14.048   -14.048     0.000
O(0)             0.000e+000
   O2                    0.000e+000  0.000e+000   -65.925   -65.925     0.000

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

      Phase               SI log IAP  log KT

      Aragonite        -5.97  -14.28   -8.31  CaCO3
      Calcite          -5.83  -14.28   -8.45  CaCO3
      CH4(g)          -22.16  -24.98   -2.82  CH4
      CO2(g)           -4.97   -6.37   -1.41  CO2
      H2(g)           -10.92  -14.05   -3.13  H2
      H2O(g)           -1.64   -0.00    1.64  H2O
      O2(g)           -63.07  -65.93   -2.85  O2

Initial solution 2.     NaOH

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

      Elements           Molality       Moles

      Na               2.490e+001  2.490e+001

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

                                     pH  =  14.000
                                     pe  =   4.000
                         Activity of water  =   0.562
                            Ionic strength  =  1.184e+001
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  2.931e+000
                    Total carbon (mol/kg)   =  0.000e+000
                       Total CO2 (mol/kg)   =  0.000e+000
                     Temperature (deg C)    =  20.000
                  Electrical balance (eq)   =  2.197e+001
```

```
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  92.76
                                Iterations  =   6
                                   Total H  = 1.139431e+002
                                   Total O  = 5.843693e+001

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

                                                   Log       Log         Log
   Species                 Molality    Activity  Molality  Activity     Gamma

   OH-                   8.574e-001  3.816e-001    -0.067    -0.418    -0.352
   H+                    1.432e-014  1.000e-014   -13.844   -14.000    -0.156
   H2O                   5.551e+001  5.621e-001     1.744    -0.250     0.000
H(0)             0.000e+000
   H2                    0.000e+000  7.447e-040   -40.312   -39.128     1.184
Na               2.490e+001
   Na+                   2.283e+001  8.532e+001     1.358     1.931     0.573
   NaOH                  2.073e+000  3.169e+001     0.317     1.501     1.184
O(0)             7.102e-018
   O2                    3.551e-018  5.427e-017   -17.450   -16.265     1.184

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

      Phase               SI log IAP  log KT

      H2(g)           -36.00  -39.13   -3.13  H2
      H2O(g)           -1.89   -0.25    1.64  H2O
      O2(g)           -13.41  -16.27   -2.85  O2

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

Reaction step 1.

Using mix 1.      Mix NaOH and GW @ equ w/ calcite

Mixture 1.  Mix NaOH and GW @ equ w/ calcite

       9.500e-001 Solution 1  GW @ eqb w/ Calcite
       5.000e-002 Solution 2  NaOH

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

      Elements           Molality       Moles

      C                3.763e-006  3.763e-006
      Ca               1.700e-006  1.700e-006
      Na               1.245e+000  1.245e+000

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

                                      pH  =  12.975      Charge balance
                                      pe  =  -7.646      Adjusted to redox equilibrium
                         Activity of water  =   0.977
                            Ionic strength  =  6.511e-001
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  1.465e-001
                       Total CO2 (mol/kg)   =  3.763e-006
                     Temperature (deg C)    =  20.000
                  Electrical balance (eq)   =  1.098e+000
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  84.35
                                Iterations  =  11
                                   Total H  = 1.111590e+002
                                   Total O  = 5.565276e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.019e-001	6.259e-002	-0.992	-1.204	-0.212
H+	1.399e-013	1.060e-013	-12.854	-12.975	-0.121
H2O	5.551e+001	9.771e-001	1.744	-0.010	0.000
C(-4)	2.951e-034				
CH4	2.951e-034	3.428e-034	-33.530	-33.465	0.065
C(4)	3.763e-006				
NaCO3-	2.926e-006	2.184e-006	-5.534	-5.661	-0.127
CO3-2	8.364e-007	1.781e-007	-6.078	-6.749	-0.672
HCO3-	6.599e-010	4.483e-010	-9.181	-9.348	-0.168
NaHCO3	1.847e-010	2.146e-010	-9.734	-9.668	0.065
CaCO3	6.679e-011	7.759e-011	-10.175	-10.110	0.065
CaHCO3+	2.197e-015	1.492e-015	-14.658	-14.826	-0.168
CO2	1.008e-016	1.172e-016	-15.996	-15.931	0.065
Ca	1.700e-006				
Ca+2	1.117e-006	2.840e-007	-5.952	-6.547	-0.595
CaOH+	5.820e-007	4.345e-007	-6.235	-6.362	-0.127
CaCO3	6.679e-011	7.759e-011	-10.175	-10.110	0.065
CaHCO3+	2.197e-015	1.492e-015	-14.658	-14.826	-0.168
H(0)	2.820e-014				
H2	1.410e-014	1.638e-014	-13.851	-13.786	0.065
Na	1.245e+000				
Na+	1.200e+000	8.512e-001	0.079	-0.070	-0.149
NaOH	4.462e-002	5.184e-002	-1.350	-1.285	0.065
NaCO3-	2.926e-006	2.184e-006	-5.534	-5.661	-0.127
NaHCO3	1.847e-010	2.146e-010	-9.734	-9.668	0.065
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.535	-66.470	0.065

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

Phase	SI	log IAP	log KT	
Aragonite	-4.99	-13.30	-8.31	CaCO3
Calcite	-4.84	-13.30	-8.45	CaCO3
CH4(g)	-30.65	-33.46	-2.82	CH4
CO2(g)	-14.52	-15.93	-1.41	CO2
H2(g)	-10.66	-13.79	-3.13	H2
H2O(g)	-1.65	-0.01	1.64	H2O
O2(g)	-63.62	-66.47	-2.85	O2

End of simulation.

Reading input data for simulation 2.

End of run.

Run 9 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\95-5 mix\mix 1 eqb w calcite and co2.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\95-5 mix\mix 1 eqb w calcite and co2.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          Calcite   0 10
          CO2(g)    -2 10
      SOLUTION 1 Mix 1
          temp      20
          pH        12.975
          pe        -7.646
          redox     pe
          units     mmol/kgw
          density   1
          C         3.763e-006
          Ca        1.7e-006
          Na        1.245
          water    1 # kg
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     Mix 1

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

      Elements           Molality       Moles

      C                3.763e-009  3.763e-009
      Ca               1.700e-009  1.700e-009
      Na               1.245e-003  1.245e-003

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

                                       pH  =  12.975
                                       pe  =  -7.646
                         Activity of water  =   0.999
                            Ionic strength  =  3.920e-002
                       Mass of water (kg)   =  1.000e+000
                 Total alkalinity (eq/kg)   =  7.728e-002
                       Total CO2 (mol/kg)   =  3.763e-009
                      Temperature (deg C)   =  20.000
                  Electrical balance (eq)   = -7.604e-002
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   = -96.98
                                Iterations  =   5
                                   Total H  = 1.110897e+002
                                   Total O  = 5.558350e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	7.722e-002	6.401e-002	-1.112	-1.194	-0.082
H+	1.225e-013	1.059e-013	-12.912	-12.975	-0.063
H2O	5.551e+001	9.987e-001	1.744	-0.001	0.000
C(-4)	3.348e-036				
CH4	3.348e-036	3.378e-036	-35.475	-35.471	0.004
C(4)	3.763e-009				
CO3-2	3.725e-009	1.883e-009	-8.429	-8.725	-0.296
NaCO3-	3.220e-011	2.693e-011	-10.492	-10.570	-0.078
HCO3-	5.617e-012	4.736e-012	-11.250	-11.325	-0.074
NaHCO3	2.620e-015	2.644e-015	-14.582	-14.578	0.004
CaCO3	1.265e-015	1.277e-015	-14.898	-14.894	0.004
CO2	1.199e-018	1.210e-018	-17.921	-17.917	0.004
CaHCO3+	2.910e-020	2.454e-020	-19.536	-19.610	-0.074
Ca	1.700e-009				
Ca+2	8.731e-010	4.420e-010	-9.059	-9.355	-0.296
CaOH+	8.269e-010	6.917e-010	-9.083	-9.160	-0.078
CaCO3	1.265e-015	1.277e-015	-14.898	-14.894	0.004
CaHCO3+	2.910e-020	2.454e-020	-19.536	-19.610	-0.074
H(0)	3.244e-014				
H2	1.622e-014	1.637e-014	-13.790	-13.786	0.004
Na	1.245e-003				
Na+	1.184e-003	9.926e-004	-2.927	-3.003	-0.076
NaOH	6.127e-005	6.183e-005	-4.213	-4.209	0.004
NaCO3-	3.220e-011	2.693e-011	-10.492	-10.570	-0.078
NaHCO3	2.620e-015	2.644e-015	-14.582	-14.578	0.004
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.454	-66.450	0.004

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

Phase	SI	log IAP	log KT	
Aragonite	-9.77	-18.08	-8.31	CaCO3
Calcite	-9.63	-18.08	-8.45	CaCO3
CH4(g)	-32.65	-35.47	-2.82	CH4
CO2(g)	-16.51	-17.92	-1.41	CO2
H2(g)	-10.66	-13.79	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.60	-66.45	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Mix 1
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Calcite	0.00	-8.45	-8.45	1.000e+001	1.000e+001	-1.558e-005
CO2(g)	-2.00	-3.41	-1.41	1.000e+001	9.924e+000	-7.569e-002

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

Elements	Molality	Moles

C	7.570e-002	7.571e-002
Ca	1.558e-005	1.558e-005
Na	1.245e-003	1.245e-003

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

pH	=	8.579	Charge balance
pe	=	9.781	Adjusted to redox equilibrium
Activity of water	=	0.999	
Ionic strength	=	4.121e-002	
Mass of water (kg)	=	1.000e+000	
Total alkalinity (eq/kg)	=	7.731e-002	
Total CO2 (mol/kg)	=	7.570e-002	
Temperature (deg C)	=	20.000	
Electrical balance (eq)	=	-7.604e-002	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-96.91	
Iterations	=	23	
Total H	=	1.110897e+002	
Total O	=	5.573493e+001	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	3.114e-006	2.571e-006	-5.507	-5.590	-0.083
H+	3.057e-009	2.637e-009	-8.515	-8.579	-0.064
H2O	5.551e+001	9.987e-001	1.744	-0.001	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-125.216	-125.212	0.004
C(4)	7.570e-002				
HCO3-	7.329e-002	6.160e-002	-1.135	-1.210	-0.075
CO3-2	1.971e-003	9.838e-004	-2.705	-3.007	-0.302
CO2	3.882e-004	3.919e-004	-3.411	-3.407	0.004
NaHCO3	3.423e-005	3.456e-005	-4.466	-4.461	0.004
NaCO3-	1.696e-005	1.414e-005	-4.771	-4.849	-0.079
CaCO3	5.350e-006	5.401e-006	-5.272	-5.268	0.004
CaHCO3+	3.074e-006	2.584e-006	-5.512	-5.588	-0.075
Ca	1.558e-005				
Ca+2	7.159e-006	3.579e-006	-5.145	-5.446	-0.301
CaCO3	5.350e-006	5.401e-006	-5.272	-5.268	0.004
CaHCO3+	3.074e-006	2.584e-006	-5.512	-5.588	-0.075
CaOH+	2.698e-010	2.250e-010	-9.569	-9.648	-0.079
H(0)	2.807e-040				
H2	1.403e-040	1.417e-040	-39.853	-39.849	0.004
Na	1.245e-003				
Na+	1.194e-003	9.977e-004	-2.923	-3.001	-0.078
NaHCO3	3.423e-005	3.456e-005	-4.466	-4.461	0.004
NaCO3-	1.696e-005	1.414e-005	-4.771	-4.849	-0.079
NaOH	2.473e-009	2.496e-009	-8.607	-8.603	0.004
O(0)	9.378e-015				
O2	4.689e-015	4.734e-015	-14.329	-14.325	0.004

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

Phase	SI	log IAP	log KT	
Aragonite	-0.15	-8.45	-8.31	CaCO3
Calcite	0.00	-8.45	-8.45	CaCO3
CH4(g)	-122.39	-125.21	-2.82	CH4
CO2(g)	-2.00	-3.41	-1.41	CO2
H2(g)	-36.72	-39.85	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-11.47	-14.32	-2.85	O2

End of simulation.

```
------------------

-------------------------------------
Reading input data for simulation 2.
-------------------------------------

-----------
End of run.
-----------
```

Run 9 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\95-5 mix\mix 2 eqb w montmorillonite.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\95-5 mix\mix 2 eqb w montmorillonite.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 1 mix 2 eqb w montmorillonite
          temp      20
          pH        8.579
          pe        9.781
          redox     pe
          units     mmol/kgw
          density   1
          C         0.0757
          Ca        1.558e-005
          Na        0.001245
          water    1 # kg
      EQUILIBRIUM_PHASES 1
          Ca-Montmorillonite 0 10
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     mix 2 eqb w montmorillonite

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

      Elements           Molality       Moles

      C                7.570e-005  7.570e-005
      Ca               1.558e-008  1.558e-008
      Na               1.245e-006  1.245e-006

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

                                       pH  =   8.579
                                       pe  =   9.781
                        Activity of water  =   1.000
                           Ionic strength  =  4.138e-005
                       Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  =  7.903e-005
                       Total CO2 (mol/kg)  =  7.570e-005
                     Temperature (deg C)   =  20.000
                  Electrical balance (eq)  = -7.776e-005
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -96.82
                                Iterations  =   4
                                   Total H  = 1.110125e+002
                                   Total O  = 5.550645e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	2.594e-006	2.575e-006	-5.586	-5.589	-0.003
H+	2.656e-009	2.636e-009	-8.576	-8.579	-0.003
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-128.134	-128.134	0.000
C(4)	7.570e-005				
HCO3-	7.402e-005	7.348e-005	-4.131	-4.134	-0.003
CO3-2	1.209e-006	1.174e-006	-5.918	-5.930	-0.013
CO2	4.667e-007	4.667e-007	-6.331	-6.331	0.000
NaHCO3	5.106e-011	5.106e-011	-10.292	-10.292	0.000
CaCO3	2.716e-011	2.716e-011	-10.566	-10.566	0.000
NaCO3-	2.105e-011	2.090e-011	-10.677	-10.680	-0.003
CaHCO3+	1.309e-011	1.299e-011	-10.883	-10.886	-0.003
Ca	1.558e-008				
Ca+2	1.554e-008	1.509e-008	-7.809	-7.821	-0.013
CaCO3	2.716e-011	2.716e-011	-10.566	-10.566	0.000
CaHCO3+	1.309e-011	1.299e-011	-10.883	-10.886	-0.003
CaOH+	9.567e-013	9.496e-013	-12.019	-12.022	-0.003
H(0)	2.838e-040				
H2	1.419e-040	1.419e-040	-39.848	-39.848	0.000
Na	1.245e-006				
Na+	1.245e-006	1.236e-006	-5.905	-5.908	-0.003
NaHCO3	5.106e-011	5.106e-011	-10.292	-10.292	0.000
NaCO3-	2.105e-011	2.090e-011	-10.677	-10.680	-0.003
NaOH	3.097e-012	3.097e-012	-11.509	-11.509	0.000
O(0)	9.460e-015				
O2	4.730e-015	4.730e-015	-14.325	-14.325	0.000

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

Phase	SI	log IAP	log KT	
Aragonite	-5.45	-13.75	-8.31	CaCO3
Calcite	-5.30	-13.75	-8.45	CaCO3
CH4(g)	-125.32	-128.13	-2.82	CH4
CO2(g)	-4.92	-6.33	-1.41	CO2
H2(g)	-36.72	-39.85	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-11.47	-14.33	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. mix 2 eqb w montmorillonite
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca-Montmorillonite	0.00	-45.76	-45.76	1.000e+001	1.000e+001	-3.850e-006

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

Elements	Molality	Moles
Al	8.970e-006	8.970e-006
C	7.570e-005	7.570e-005

Ca	6.508e-007	6.508e-007
Na	1.245e-006	1.245e-006
Si	1.413e-005	1.413e-005

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

```
                                    pH  =   7.570      Charge balance
                                    pe  =  10.869      Adjusted to redox equilibrium
                     Activity of water  =   1.000
                        Ionic strength  =  4.225e-005
                   Mass of water (kg)   =  1.000e+000
             Total alkalinity (eq/kg)   =  1.072e-004
                   Total CO2 (mol/kg)   =  7.570e-005
                  Temperature (deg C)   =  20.000
                Electrical balance (eq) = -7.776e-005
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -93.71
                            Iterations  =   8
                               Total H  = 1.110125e+002
                               Total O  = 5.550649e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	2.543e-007	2.524e-007	-6.595	-6.598	-0.003
H+	2.709e-008	2.689e-008	-7.567	-7.570	-0.003
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Al	8.970e-006				
Al(OH)4-	8.802e-006	8.736e-006	-5.055	-5.059	-0.003
Al(OH)3	1.325e-007	1.325e-007	-6.878	-6.878	0.000
Al(OH)2+	3.565e-008	3.538e-008	-7.448	-7.451	-0.003
AlOH+2	1.961e-010	1.903e-010	-9.707	-9.720	-0.013
Al+3	7.654e-013	7.159e-013	-12.116	-12.145	-0.029
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-127.781	-127.781	0.000
C(4)	7.570e-005				
HCO3-	7.102e-005	7.049e-005	-4.149	-4.152	-0.003
CO2	4.567e-006	4.567e-006	-5.340	-5.340	0.000
CO3-2	1.137e-007	1.104e-007	-6.944	-6.957	-0.013
CaHCO3+	5.252e-010	5.213e-010	-9.280	-9.283	-0.003
CaCO3	1.068e-010	1.068e-010	-9.971	-9.971	0.000
NaHCO3	4.898e-011	4.898e-011	-10.310	-10.310	0.000
NaCO3-	1.980e-012	1.965e-012	-11.703	-11.707	-0.003
Ca	6.508e-007				
Ca+2	6.502e-007	6.310e-007	-6.187	-6.200	-0.013
CaHCO3+	5.252e-010	5.213e-010	-9.280	-9.283	-0.003
CaCO3	1.068e-010	1.068e-010	-9.971	-9.971	0.000
CaOH+	3.923e-012	3.894e-012	-11.406	-11.410	-0.003
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-40.007	-40.007	0.000
Na	1.245e-006				
Na+	1.245e-006	1.236e-006	-5.905	-5.908	-0.003
NaHCO3	4.898e-011	4.898e-011	-10.310	-10.310	0.000
NaCO3-	1.980e-012	1.965e-012	-11.703	-11.707	-0.003
NaOH	3.036e-013	3.036e-013	-12.518	-12.518	0.000
O(0)	1.971e-014				
O2	9.855e-015	9.855e-015	-14.006	-14.006	0.000
Si	1.413e-005				
H4SiO4	1.406e-005	1.406e-005	-4.852	-4.852	0.000
H3SiO4-	6.491e-008	6.443e-008	-7.188	-7.191	-0.003
H2SiO4-2	1.201e-013	1.165e-013	-12.921	-12.934	-0.013

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

Phase	SI	log IAP	log KT

```
Al(OH)3(a)          -0.57   10.57   11.13  Al(OH)3
Albite              -7.20  -25.52  -18.33  NaAlSi3O8
Anorthite           -6.16  -26.02  -19.86  CaAl2Si2O8
Aragonite           -4.85  -13.16   -8.31  CaCO3
Ca-Montmorillonite   0.00  -45.76  -45.76  Ca0.165Al2.33Si3.67O10(OH)2
Calcite             -4.70  -13.16   -8.45  CaCO3
CH4(g)            -124.96 -127.78   -2.82  CH4
Chalcedony          -1.24   -4.85   -3.61  SiO2
CO2(g)              -3.93   -5.34   -1.41  CO2
Gibbsite             2.17   10.57    8.40  Al(OH)3
H2(g)              -36.88  -40.01   -3.13  H2
H2O(g)              -1.64   -0.00    1.64  H2O
Kaolinite            3.55   11.43    7.88  Al2Si2O5(OH)4
O2(g)              -11.15  -14.01   -2.85  O2
Quartz              -0.80   -4.85   -4.06  SiO2
SiO2(a)             -2.10   -4.85   -2.75  SiO2

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 2.
------------------------------------

-----------
End of run.
-----------
```

Run 10

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\99-1 mix\mix 1%NaOH and 99%calcite GW.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\99-1 mix\mix 1%NaOH and 99%calcite GW.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 2 NaOH
          temp      20
          pH        14
          pe        4
          redox     pe
          units     mmol/kgw
          density   1
          Na        24.9 Mol/kgw
          water    1 # kg
      SOLUTION 1 GW @ eqb w/ Calcite
          temp      20
          pH        7.301
          pe        -1.841
          redox     pe
          units     mmol/kgw
          density   1
          Ca        0.001789
          C         0.003961
          water    1 # kg
      SAVE solution 1-2
      MIX 1 Mix NaOH and GW @ equ w/ calcite
          1    0.99
          2    0.01
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     GW @ eqb w/ Calcite

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

      Elements           Molality       Moles

      C                 3.961e-006  3.961e-006
      Ca                1.789e-006  1.789e-006

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

                                     pH  =   7.301
                                     pe  =  -1.841
                         Activity of water  =   1.000
                            Ionic strength  =  5.444e-006
                        Mass of water (kg)  =  1.000e+000
```

```
                 Total alkalinity (eq/kg)  =  3.626e-006
                       Total CO2 (mol/kg)  =  3.961e-006
                     Temperature (deg C)   =  20.000
                  Electrical balance (eq)  = -4.751e-008
  Percent error, 100*(Cat-|An|)/(Cat+|An|) =  -0.65
                              Iterations  =   3
                                 Total H  = 1.110124e+002
                                 Total O  = 5.550623e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.361e-007	1.358e-007	-6.866	-6.867	-0.001
H+	5.014e-008	5.000e-008	-7.300	-7.301	-0.001
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	1.058e-025				
CH4	1.058e-025	1.058e-025	-24.975	-24.975	0.000
C(4)	3.961e-006				
HCO3-	3.533e-006	3.524e-006	-5.452	-5.453	-0.001
CO2	4.245e-007	4.245e-007	-6.372	-6.372	0.000
CO3-2	3.000e-009	2.968e-009	-8.523	-8.528	-0.005
CaHCO3+	7.328e-011	7.309e-011	-10.135	-10.136	-0.001
CaCO3	8.056e-012	8.056e-012	-11.094	-11.094	0.000
Ca	1.789e-006				
Ca+2	1.789e-006	1.770e-006	-5.747	-5.752	-0.005
CaHCO3+	7.328e-011	7.309e-011	-10.135	-10.136	-0.001
CaCO3	8.056e-012	8.056e-012	-11.094	-11.094	0.000
CaOH+	5.889e-012	5.873e-012	-11.230	-11.231	-0.001
H(0)	1.791e-014				
H2	8.953e-015	8.953e-015	-14.048	-14.048	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-65.925	-65.925	0.000

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

Phase	SI	log IAP	log KT	
Aragonite	-5.97	-14.28	-8.31	CaCO3
Calcite	-5.83	-14.28	-8.45	CaCO3
CH4(g)	-22.16	-24.98	-2.82	CH4
CO2(g)	-4.97	-6.37	-1.41	CO2
H2(g)	-10.92	-14.05	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.07	-65.93	-2.85	O2

Initial solution 2. NaOH

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

Elements	Molality	Moles
Na	2.490e+001	2.490e+001

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

```
                                  pH  =  14.000
                                  pe  =   4.000
                   Activity of water  =   0.562
                      Ionic strength  =  1.184e+001
                  Mass of water (kg)  =  1.000e+000
          Total alkalinity (eq/kg)    =  2.931e+000
             Total carbon (mol/kg)    =  0.000e+000
                Total CO2 (mol/kg)    =  0.000e+000
              Temperature (deg C)     =  20.000
           Electrical balance (eq)    =  2.197e+001
```

```
  Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  92.76
                                Iterations  =   6
                                   Total H  = 1.139431e+002
                                   Total O  = 5.843693e+001

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

                                                   Log       Log         Log
   Species                  Molality    Activity  Molality  Activity     Gamma

   OH-                    8.574e-001  3.816e-001    -0.067    -0.418    -0.352
   H+                     1.432e-014  1.000e-014   -13.844   -14.000    -0.156
   H2O                    5.551e+001  5.621e-001     1.744    -0.250     0.000
H(0)              0.000e+000
   H2                     0.000e+000  7.447e-040   -40.312   -39.128     1.184
Na                2.490e+001
   Na+                    2.283e+001  8.532e+001     1.358     1.931     0.573
   NaOH                   2.073e+000  3.169e+001     0.317     1.501     1.184
O(0)              7.102e-018
   O2                     3.551e-018  5.427e-017   -17.450   -16.265     1.184

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

      Phase               SI log IAP  log KT

      H2(g)           -36.00  -39.13   -3.13  H2
      H2O(g)           -1.89   -0.25    1.64  H2O
      O2(g)           -13.41  -16.27   -2.85  O2

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

Reaction step 1.

Using mix 1.      Mix NaOH and GW @ equ w/ calcite

Mixture 1.  Mix NaOH and GW @ equ w/ calcite

       9.900e-001 Solution 1  GW @ eqb w/ Calcite
       1.000e-002 Solution 2  NaOH

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

      Elements           Molality       Moles

      C                3.921e-006  3.921e-006
      Ca               1.771e-006  1.771e-006
      Na               2.490e-001  2.490e-001

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

                                        pH  =  12.453      Charge balance
                                        pe  =  -7.053      Adjusted to redox equilibrium
                          Activity of water  =   0.995
                             Ionic strength  =  1.358e-001
                        Mass of water (kg)   =  1.000e+000
                  Total alkalinity (eq/kg)   =  2.931e-002
                        Total CO2 (mol/kg)   =  3.921e-006
                      Temperature (deg C)    =  20.000
                   Electrical balance (eq)   =  2.197e-001
  Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  80.92
                                Iterations  =  10
                                   Total H  = 1.110417e+002
                                   Total O  = 5.553554e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	2.590e-002	1.916e-002	-1.587	-1.718	-0.131
H+	4.331e-013	3.526e-013	-12.363	-12.453	-0.089
H2O	5.551e+001	9.953e-001	1.744	-0.002	0.000
C(-4)	3.247e-033				
CH4	3.247e-033	3.350e-033	-32.489	-32.475	0.014
C(4)	3.921e-006				
NaCO3-	2.177e-006	1.669e-006	-5.662	-5.778	-0.115
CO3-2	1.737e-006	6.151e-007	-5.760	-6.211	-0.451
HCO3-	6.677e-009	5.151e-009	-8.175	-8.288	-0.113
NaHCO3	5.287e-010	5.455e-010	-9.277	-9.263	0.014
CaCO3	4.794e-010	4.946e-010	-9.319	-9.306	0.014
CaHCO3+	4.103e-014	3.165e-014	-13.387	-13.500	-0.113
CO2	4.261e-015	4.397e-015	-14.370	-14.357	0.014
Ca	1.771e-006				
Ca+2	1.450e-006	5.243e-007	-5.839	-6.280	-0.442
CaOH+	3.203e-007	2.456e-007	-6.494	-6.610	-0.115
CaCO3	4.794e-010	4.946e-010	-9.319	-9.306	0.014
CaHCO3+	4.103e-014	3.165e-014	-13.387	-13.500	-0.113
H(0)	2.289e-014				
H2	1.145e-014	1.181e-014	-13.941	-13.928	0.014
Na	2.490e-001				
Na+	2.456e-001	1.883e-001	-0.610	-0.725	-0.115
NaOH	3.404e-003	3.512e-003	-2.468	-2.454	0.014
NaCO3-	2.177e-006	1.669e-006	-5.662	-5.778	-0.115
NaHCO3	5.287e-010	5.455e-010	-9.277	-9.263	0.014
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.183	-66.170	0.014

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

Phase	SI	log IAP	log KT	
Aragonite	-4.19	-12.49	-8.31	CaCO3
Calcite	-4.04	-12.49	-8.45	CaCO3
CH4(g)	-29.66	-32.47	-2.82	CH4
CO2(g)	-12.95	-14.36	-1.41	CO2
H2(g)	-10.80	-13.93	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.32	-66.17	-2.85	O2

End of simulation.

Reading input data for simulation 2.

End of run.

Run 10 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\99-1 mix\mix 1 eqb w calcite and co2.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\99-1 mix\mix 1 eqb w calcite and co2.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      EQUILIBRIUM_PHASES 1
          Calcite   0 10
          CO2(g)    -2 10
      SOLUTION 1 Mix 1
          temp      20
          pH        12.45
          pe        -7.053
          redox     pe
          units     mmol/kgw
          density   1
          C         3.921e-006
          Ca        1.771e-006
          Na        0.249
          water    1 # kg
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.     Mix 1

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

      Elements           Molality       Moles

      C                 3.921e-009  3.921e-009
      Ca                1.771e-009  1.771e-009
      Na                2.490e-004  2.490e-004

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

                                       pH  =  12.450
                                       pe  =  -7.053
                        Activity of water  =   1.000
                           Ionic strength  =  1.078e-002
                       Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  =  2.131e-002
                       Total CO2 (mol/kg)  =  3.921e-009
                     Temperature (deg C)   =  20.000
                  Electrical balance (eq)  = -2.106e-002
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -97.73
                                Iterations  =   5
                                   Total H  = 1.110337e+002
                                   Total O  = 5.552753e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	2.131e-002	1.913e-002	-1.671	-1.718	-0.047
H+	3.892e-013	3.548e-013	-12.410	-12.450	-0.040
H2O	5.551e+001	9.996e-001	1.744	-0.000	0.000
C(-4)	1.479e-035				
CH4	1.479e-035	1.483e-035	-34.830	-34.829	0.001
C(4)	3.921e-009				
CO3-2	3.888e-009	2.585e-009	-8.410	-8.588	-0.177
HCO3-	2.412e-011	2.178e-011	-10.618	-10.662	-0.044
NaCO3-	9.133e-012	8.218e-012	-11.039	-11.085	-0.046
CaCO3	3.460e-015	3.469e-015	-14.461	-14.460	0.001
NaHCO3	2.695e-015	2.702e-015	-14.569	-14.568	0.001
CO2	1.858e-017	1.862e-017	-16.731	-16.730	0.001
CaHCO3+	2.473e-019	2.233e-019	-18.607	-18.651	-0.044
Ca	1.771e-009				
Ca+2	1.316e-009	8.748e-010	-8.881	-9.058	-0.177
CaOH+	4.546e-010	4.090e-010	-9.342	-9.388	-0.046
CaCO3	3.460e-015	3.469e-015	-14.461	-14.460	0.001
CaHCO3+	2.473e-019	2.233e-019	-18.607	-18.651	-0.044
H(0)	2.387e-014				
H2	1.194e-014	1.197e-014	-13.923	-13.922	0.001
Na	2.490e-004				
Na+	2.449e-004	2.206e-004	-3.611	-3.656	-0.045
NaOH	4.096e-006	4.107e-006	-5.388	-5.387	0.001
NaCO3-	9.133e-012	8.218e-012	-11.039	-11.085	-0.046
NaHCO3	2.695e-015	2.702e-015	-14.569	-14.568	0.001
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.179	-66.177	0.001

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

Phase	SI	log IAP	log KT	
Aragonite	-9.34	-17.65	-8.31	CaCO3
Calcite	-9.19	-17.65	-8.45	CaCO3
CH4(g)	-32.01	-34.83	-2.82	CH4
CO2(g)	-15.32	-16.73	-1.41	CO2
H2(g)	-10.79	-13.92	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.32	-66.18	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Mix 1
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Calcite	0.00	-8.45	-8.45	1.000e+001	1.000e+001	-7.119e-005
CO2(g)	-2.00	-3.41	-1.41	1.000e+001	9.978e+000	-2.162e-002

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

Elements	Molality	Moles

C	2.169e-002	2.170e-002
Ca	7.120e-005	7.120e-005
Na	2.490e-004	2.490e-004

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

pH	=	8.069	Charge balance
pe	=	-2.728	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	1.110e-002	
Mass of water (kg)	=	1.000e+000	
Total alkalinity (eq/kg)	=	2.145e-002	
Total CO2 (mol/kg)	=	2.169e-002	
Temperature (deg C)	=	20.000	
Electrical balance (eq)	=	-2.106e-002	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-96.62	
Iterations	=	12	
Total H	=	1.110337e+002	
Total O	=	5.557099e+001	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	8.879e-007	7.960e-007	-6.052	-6.099	-0.047
H+	9.362e-009	8.526e-009	-8.029	-8.069	-0.041
H2O	5.551e+001	9.996e-001	1.744	-0.000	0.000
C(-4)	8.736e-022				
CH4	8.736e-022	8.758e-022	-21.059	-21.058	0.001
C(4)	2.169e-002				
HCO3-	2.114e-002	1.907e-002	-1.675	-1.720	-0.045
CO2	3.909e-004	3.919e-004	-3.408	-3.407	0.001
CO3-2	1.424e-004	9.419e-005	-3.847	-4.026	-0.179
CaHCO3+	9.264e-006	8.355e-006	-5.033	-5.078	-0.045
CaCO3	5.387e-006	5.401e-006	-5.269	-5.268	0.001
NaHCO3	2.370e-006	2.376e-006	-5.625	-5.624	0.001
NaCO3-	3.347e-007	3.007e-007	-6.475	-6.522	-0.046
Ca	7.120e-005				
Ca+2	5.654e-005	3.738e-005	-4.248	-4.427	-0.180
CaHCO3+	9.264e-006	8.355e-006	-5.033	-5.078	-0.045
CaCO3	5.387e-006	5.401e-006	-5.269	-5.268	0.001
CaOH+	8.095e-010	7.274e-010	-9.092	-9.138	-0.046
H(0)	3.090e-014				
H2	1.545e-014	1.549e-014	-13.811	-13.810	0.001
Na	2.490e-004				
Na+	2.463e-004	2.216e-004	-3.609	-3.654	-0.046
NaHCO3	2.370e-006	2.376e-006	-5.625	-5.624	0.001
NaCO3-	3.347e-007	3.007e-007	-6.475	-6.522	-0.046
NaOH	1.712e-010	1.716e-010	-9.767	-9.765	0.001
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.403	-66.402	0.001

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

Phase	SI	log IAP	log KT	
Aragonite	-0.15	-8.45	-8.31	CaCO3
Calcite	0.00	-8.45	-8.45	CaCO3
CH4(g)	-18.24	-21.06	-2.82	CH4
CO2(g)	-2.00	-3.41	-1.41	CO2
H2(g)	-10.68	-13.81	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.55	-66.40	-2.85	O2

End of simulation.

```
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Reading input data for simulation 2.
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End of run.
-----------
```

Run 10 continued

```
   Input file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\99-1 mix\mix 2 eqb w montmorillonite.pqi
  Output file: C:\Documents and Settings\Jennifer\My Documents\BASF-Hannibal MO\PHREEQ
\010510\99-1 mix\mix 2 eqb w montmorillonite.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat

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

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\phreeqc.dat
      SOLUTION 1 mix 2 eqb w montmorillonite
          temp      20
          pH        8.069
          pe        -2.728
          redox     pe
          units     mmol/kgw
          density   1
          C         0.02169
          Ca        7.12e-005
          Na        0.000249
          water    1 # kg
      EQUILIBRIUM_PHASES 1
          Ca-Montmorillonite 0 10
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     mix 2 eqb w montmorillonite

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

      Elements           Molality       Moles

      C                2.169e-005  2.169e-005
      Ca               7.120e-008  7.120e-008
      Na               2.490e-007  2.490e-007

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

                                       pH  =   8.069
                                       pe  =  -2.728
                        Activity of water  =   1.000
                           Ionic strength  =  1.146e-005
                       Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  =  2.215e-005
                       Total CO2 (mol/kg)  =  2.169e-005
                     Temperature (deg C)   =  20.000
                  Electrical balance (eq)  = -2.176e-005
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -96.45
                                Iterations  =   3
                                   Total H  = 1.110125e+002
                                   Total O  = 5.550628e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	7.990e-007	7.958e-007	-6.097	-6.099	-0.002
H+	8.564e-009	8.531e-009	-8.067	-8.069	-0.002
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
C(-4)	9.664e-025				
CH4	9.664e-025	9.664e-025	-24.015	-24.015	0.000
C(4)	2.169e-005				
HCO3-	2.115e-005	2.107e-005	-4.675	-4.676	-0.002
CO2	4.330e-007	4.330e-007	-6.363	-6.363	0.000
CO3-2	1.056e-007	1.040e-007	-6.976	-6.983	-0.007
CaHCO3+	1.737e-011	1.730e-011	-10.760	-10.762	-0.002
CaCO3	1.118e-011	1.118e-011	-10.952	-10.952	0.000
NaHCO3	2.939e-012	2.939e-012	-11.532	-11.532	0.000
NaCO3-	3.731e-013	3.717e-013	-12.428	-12.430	-0.002
Ca	7.120e-008				
Ca+2	7.117e-008	7.006e-008	-7.148	-7.155	-0.007
CaHCO3+	1.737e-011	1.730e-011	-10.760	-10.762	-0.002
CaCO3	1.118e-011	1.118e-011	-10.952	-10.952	0.000
CaOH+	1.368e-012	1.363e-012	-11.864	-11.866	-0.002
H(0)	3.098e-014				
H2	1.549e-014	1.549e-014	-13.810	-13.810	0.000
Na	2.490e-007				
Na+	2.490e-007	2.480e-007	-6.604	-6.606	-0.002
NaHCO3	2.939e-012	2.939e-012	-11.532	-11.532	0.000
NaCO3-	3.731e-013	3.717e-013	-12.428	-12.430	-0.002
NaOH	1.921e-013	1.921e-013	-12.717	-12.717	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-66.401	-66.401	0.000

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

Phase	SI	log IAP	log KT	
Aragonite	-5.83	-14.14	-8.31	CaCO3
Calcite	-5.68	-14.14	-8.45	CaCO3
CH4(g)	-21.20	-24.01	-2.82	CH4
CO2(g)	-4.96	-6.36	-1.41	CO2
H2(g)	-10.68	-13.81	-3.13	H2
H2O(g)	-1.64	-0.00	1.64	H2O
O2(g)	-63.55	-66.40	-2.85	O2

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. mix 2 eqb w montmorillonite
Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage Initial	Final	Delta
Ca-Montmorillonite	0.00	-45.76	-45.76	1.000e+001	1.000e+001	-2.632e-006

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

Elements	Molality	Moles
Al	6.133e-006	6.133e-006
C	2.169e-005	2.169e-005

Ca	5.055e-007	5.055e-007
Na	2.490e-007	2.490e-007
Si	9.661e-006	9.661e-006

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

```
                                    pH  =   7.031      Charge balance
                                    pe  =  -1.314      Adjusted to redox equilibrium
                       Activity of water  =   1.000
                          Ionic strength  =  1.303e-005
                      Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  =  4.142e-005
                      Total CO2 (mol/kg)  =  2.169e-005
                    Temperature (deg C)  =  20.000
                 Electrical balance (eq)  = -2.176e-005
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -86.95
                             Iterations  =   7
                                Total H  = 1.110125e+002
                                Total O  = 5.550631e+001
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	9.342e-008	9.304e-008	-7.030	-7.031	-0.002
OH-	7.328e-008	7.297e-008	-7.135	-7.137	-0.002
H2O	5.551e+001	1.000e+000	1.744	-0.000	0.000
Al	6.133e-006				
Al(OH)4-	5.568e-006	5.544e-006	-5.254	-5.256	-0.002
Al(OH)3	2.908e-007	2.908e-007	-6.536	-6.536	0.000
Al(OH)2+	2.698e-007	2.687e-007	-6.569	-6.571	-0.002
AlOH+2	5.085e-009	5.000e-009	-8.294	-8.301	-0.007
Al+3	6.754e-011	6.507e-011	-10.170	-10.187	-0.016
C(-4)	8.644e-027				
CH4	8.644e-027	8.644e-027	-26.063	-26.063	0.000
C(4)	2.169e-005				
HCO3-	1.773e-005	1.765e-005	-4.751	-4.753	-0.002
CO2	3.956e-006	3.956e-006	-5.403	-5.403	0.000
CO3-2	8.125e-009	7.990e-009	-8.090	-8.097	-0.007
CaHCO3+	1.033e-010	1.028e-010	-9.986	-9.988	-0.002
CaCO3	6.091e-012	6.091e-012	-11.215	-11.215	0.000
NaHCO3	2.461e-012	2.461e-012	-11.609	-11.609	0.000
NaCO3-	2.867e-014	2.855e-014	-13.543	-13.544	-0.002
Ca	5.055e-007				
Ca+2	5.054e-007	4.971e-007	-6.296	-6.304	-0.007
CaHCO3+	1.033e-010	1.028e-010	-9.986	-9.988	-0.002
CaCO3	6.091e-012	6.091e-012	-11.215	-11.215	0.000
CaOH+	8.904e-013	8.867e-013	-12.050	-12.052	-0.002
H(0)	5.479e-015				
H2	2.740e-015	2.740e-015	-14.562	-14.562	0.000
Na	2.490e-007				
Na+	2.490e-007	2.480e-007	-6.604	-6.606	-0.002
NaHCO3	2.461e-012	2.461e-012	-11.609	-11.609	0.000
NaCO3-	2.867e-014	2.855e-014	-13.543	-13.544	-0.002
NaOH	1.761e-014	1.761e-014	-13.754	-13.754	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-64.897	-64.897	0.000
Si	9.661e-006				
H4SiO4	9.648e-006	9.648e-006	-5.016	-5.016	0.000
H3SiO4-	1.283e-008	1.278e-008	-7.892	-7.894	-0.002
H2SiO4-2	6.792e-015	6.679e-015	-14.168	-14.175	-0.007

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

Phase	SI	log IAP	log KT

```
Al(OH)3(a)          -0.22   10.91   11.13  Al(OH)3
Albite              -8.58  -26.91  -18.33  NaAlSi3O8
Anorthite           -6.99  -26.85  -19.86  CaAl2Si2O8
Aragonite           -6.10  -14.40   -8.31  CaCO3
Ca-Montmorillonite   0.00  -45.76  -45.76  Ca0.165Al2.33Si3.67O10(OH)2
Calcite             -5.95  -14.40   -8.45  CaCO3
CH4(g)             -23.25  -26.06   -2.82  CH4
Chalcedony          -1.41   -5.02   -3.61  SiO2
CO2(g)              -4.00   -5.40   -1.41  CO2
Gibbsite             2.51   10.91    8.40  Al(OH)3
H2(g)              -11.43  -14.56   -3.13  H2
H2O(g)              -1.64   -0.00    1.64  H2O
Kaolinite            3.91   11.78    7.88  Al2Si2O5(OH)4
O2(g)              -62.04  -64.90   -2.85  O2
Quartz              -0.96   -5.02   -4.06  SiO2
SiO2(a)             -2.26   -5.02   -2.75  SiO2

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End of simulation.
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Reading input data for simulation 2.
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End of run.
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