Example Problem CO2-5

Mineral Trapping in a Glauconitic Sandstone Aquifer (GeoSeq # 5)

Abstract: *This problem addresses geochemical effects of CO_2 injection into a glauconitic sandstone aquifer, and analyzes the impact of CO_2 immobilization through carbonate precipitation. This problem is based on Problem 5 of the code intercomparison problems developed under the GeoSeq Project (Pruess et al. 2002). Batch reaction modeling of the geochemical evolution of this aquifer is performed in the presence of CO_2 at high pressure. The problem is based on (Gunter et al. 1997), who modeled water-rock reactions when CO_2 is injected into a glauconitic sandstone aquifer in the Alberta Sedimentary Basin, Canada.*

Problem Description

This problem addresses geochemical effects of CO_2 injection into a glauconitic sandstone aquifer, and analyzes the impact of CO_2 immobilization through carbonate precipitation. Batch reaction modeling of the geochemical evolution of this aquifer is performed in the presence of CO_2 at high pressure.

The chemical reactions caused by CO_2 injection begin with the dissolution of CO2 in water to form weak carbonic acid:

$$CO_2(g) + H_2O = CO_2(aq) \tag{1}$$

This is followed by dissociation of carbonic acid to form the bicarbonate ion:

$$CO_2(aq) = H^+ + HCO_3^- \tag{2}$$

The increased acidity causes dissolution of primary host rock minerals, which in turn causes complexing of dissolved cations with the bicarbonate ion such as

$$Ca^{2+} + HCO_3^- = CaHCO_3^+ \tag{3}$$

The dissolved bicarbonate species react with divalent cations to precipitate carbonates. Formation of calcium, magnesium, and ferrous carbonates are expected to be the primary mechanism by which CO_2 is immobilized (Gunter et al. 1997).

$$HCO_3^- + Ca^{2+} = CaCO_3(s) + H^+ \quad (4)$$
$$HCO_3^- + Mg^{2+} = MgCO_3(s) + H^+ \quad (5)$$
$$HCO_3^- + Fe^{2+} = FeCO_3(s) + H^+ \quad (6)$$

The glauconitic sandstone aquifer (Alberta Sedimentary Basin, Canada) is a medium- to fine-grained litharenite. The average mineral composition is shown in Table 1. The average porosity is 12%. A representative glauconite chemical composition and thermodynamic properties were estimated from descriptions of the mineralogical compositions of glauconite and its paragenesis as reported in the published literature (Xu et al. 2001). Oligoclase was incorporated as a solid solution of plagioclase, and the thermodynamic properties of oligoclase were calculated from calorimetric studies of plagioclase solid solutions reported in the literature. Furthermore, organic matter was assumed to be present in the glauconitic sandstone, and was represented by the generic composition, CH_2O. Goethite (FeOOH) was added as a possible secondary mineral phase.

Table 1. List of initial mineral volume fractions, potential secondary mineral phases, and their kinetic properties

Mineral	Composition	Volume, %	Surface Area, cm^2/g	k_{25}, $mol/m^2\,s$	E_a, kJ/mol
Quartz	SiO_2	71.28	3.77E+01	1.26E-14	87.5
Glauconite	$K_{1.5}Mg_{0.5}Fe_{2.5}Fe_{0.5}AlSi_{7.5}O_{20}(OH)_4$	4.4	3.64E+02	1.00E-14	58.62
Illite	$K_{0.6}Mg_{0.25}Al_{1.8}(Al_{0.5}Si_{3.5}O_{10})(OH)_2$	2.64	3.64E+03	1.00E-14	58.62
Organic	CH_2O	2.64	1.00E+02	1.00E-13	0
Kaolinite	$Al_2Si_2O_5(OH)_4$	1.76	3.86E+03	1.00E-13	62.76
K-feldspar	$KAlSi_3O8$	1.76	3.91E+01	1.00E-12	67.83
Calcite	$CaCO_3$	0.88	3.69E+01	1.60E-09	41.87
Dolomite	$CaMg(CO_3)_2$	0.88	3.50E+01	6.00E-10	41.87
Oligoclase	$CaNa_4Al_6Si_{14}O_{40}$	0.88	3.62E+01	1.00E-12	67.83
Siderite	$FeCO_3$	0.88	2.54E+01	6.00E-10	41.87

Albite-low	$NaAlSi_3O_8$	0	9.54E-01	1.00E-12	67.83
Smectite-Ca	$Ca_{0.145}Mg_{0.26}Al_{1.77}Si_{3.97}O_{10}(OH)_2$	0	1.14E+02	1.00E-14	58.62
Smectite-Na	$Na_{0.29}Mg_{0.26}Al_{1.77}Si_{3.97}O_{10}(OH)_2$	0	1.00E+02	1.00E-14	58.62
Goethite	FeOOH	0	5.85E+01	1.00E-14	58.62

Currently there are four reaction rate models available with the STOMP simulator: 1) Steefel-Lasagna Dissolution-Precipitation (a.k.a Transition-State Theory or TST), 2) Smith-Atkins Forward-Backward, 3) Valocchi Monod, and 4) Valocchi Sorption. This example uses the TST rate equation (Lasaga 1984; Steefel and Lasaga 1994), which is expressed as

$$R_k = A_m k \left[1 - \frac{Q}{K_{eq}} \right] \tag{7}$$

where m is mineral index, R_k is the dissolution/precipitation rate (positive values indicate dissolution, and negative values precipitation), A_m is the specific reactive surface area, k is the rate constant (moles per unit mineral surface area and unit time) which is temperature dependent, K_{eq} is the equilibrium constant for the mineral-water reaction written for the destruction of one mole of mineral m, and Q is ion activity product. The temperature dependence of the reaction rate constant can be expressed reasonably well via an Arrhenius equation (Lasaga 1984; Steefel and Lasaga 1994). Since many rate constants are reported at 25°C, it is convenient to approximate rate constant dependency as a function of temperature,

$$k = k_{25} \exp\left[\frac{-E_a}{R} \left(\frac{1}{T} - \frac{1}{298.15} \right) \right] \tag{8}$$

where E_a is the activation energy, k_{25} is the rate constant at 25°C, R is gas constant, and T is absolute temperature.

To run a reactive transport problem, there are a few additions to the solution control card. First, the qualifier w/ECKEChem must be added after the mode description on the third line. The default minimum concentration for aqueous species is 1×10^{-30}. To specify a number smaller than that, the optional qualifier "w/ minimum concentration" can be added after that. Then the minimum concentration, down to a value of 1×10^{-110}, may be specified on the last line of the solution control card. To solve the equilibrium equations using the logarithm of the species concentrations, add the qualifier "w/log". This qualifier may help certain problems converge. Also, if a problem fails to converge on the first time step, the qualifier "w/guess" may help.

```
~Solution Control Card
Normal,
H2O-NaCl-CO2 w/ ECKEChem w/minimum concentration w/log w/constant surface area,
1,
0,s,100000,yr,1.e-3,s,10,yr,1.01,16,1.e-06,
99999,
Variable Aqueous Diffusion,
Variable Gas Diffusion,
0,
1.d-70,
```

The data from Table 1 must be entered into specific cards in the STOMP input file. The density and molecular weight of each mineral species are listed in the *Solid Species Card*. The species name must be unique and distinct from aqueous and gas species names (e.g., FeCO3(s), FeCO3_solid, solid FeCO3, FeCO3s).

```
~Solid Species Card
14,
Albite_low,2.62,g/cm^3,262.223,kg/kmol,
Calcite,2.71,g/cm^3,100.087,kg/kmol,
Dolomite,2.86,g/cm^3,184.401,kg/kmol,
Glauconite,2.75,g/cm^3,830.030,kg/kmol,
Goethite,4.27,g/cm^3,88.854,kg/kmol,
Illite,2.75,g/cm^3,383.901,kg/kmol,
K-Feldspar,2.56,g/cm^3,278.332,kg/kmol,
Kaolinite,2.59,g/cm^3,258.160,kg/kmol,
Oligoclase,2.64,g/cm^3,1327.100,kg/kmol,
Organic_matter,1.00,g/cm^3,30.026,kg/kmol,
Quartz,2.65,g/cm^3,60.084,kg/kmol,
Siderite,3.94,g/cm^3,115.856,kg/kmol,
Smectite-Ca,2.20,g/cm^3,366.043,kg/kmol,
Smectite-Na,2.50,g/cm^3,367.017,kg/kmol,
```

The specific surface area and volume fraction of each mineral are listed in the *Lithology Card*:

```
~Lithology Card
```

```
Aquifer,14,
Albite_low,9.54E-01,cm^2/g,0.,
Calcite,3.69E+01,cm^2/g,0.0088,
Dolomite,3.50E+01,cm^2/g,0.0088,
Glauconite,3.64E+02,cm^2/g,0.044,
Goethite,5.85E+01,cm^2/g,0.,
Illite,3.64E+03,cm^2/g,0.0264,
K-Feldspar,3.91E+01,cm^2/g,0.0176,
Kaolinite,3.86E+03,cm^2/g,0.0176,
Oligoclase,3.62E+01,cm^2/g,0.0088,
Organic_matter,1.00E+02,cm^2/g,0.0264,
Quartz,3.77E+01,cm^2/g,0.7128,
Siderite,2.54E+01,cm^2/g,0.0088,
Smectite-Ca,1.14E+02,cm^2/g,0.,
Smectite-Na,1.00E+02,cm^2/g,0.,
```

The TST rate parameters and equilibrium coefficients for each mineral are listed in the *Kinetic Reactions Card*, along with all aqueous species involved in the dissolution/precipitation reaction. Most equilibrium coefficients for minerals were taken from the EQ3/6 v8.0 database (Wolery and Jarek 2003) with the exception of organic matter, which is assumed to degrade at the forward rate.

```
~Kinetic Reactions Card
14,
KnRc-26,TST,Albite_low,3,Al+++,1,Na+,1,SiO2(aq),3,2,Albite_low,1,H+,4,
1.0e-12,mol/m^2 s,67.83,kJ/mol,25,C,
,1.7907,,,,
KnRc-27,TST,Calcite,2,Ca++,1,HCO3-,1,2,Calcite,1,H+,1,
1.6e-09,mol/m^2 s,41.87,kJ/mol,25,C,
,1.42,,,,
KnRc-28,TST,Dolomite,3,Ca++,1,Mg++,1,HCO3-,2,2,Dolomite,1,H+,2,
6.0e-10,mol/m^2 s,41.87,kJ/mol,25,C,
,1.5279,,,,
KnRc-
29,TST,Glauconite,6,Fe++,2.5,Fe+++,0.5,Mg++,0.5,K+,1.5,Al+++,1,SiO2(aq),7.5,2,Glauconite,1,H+,
12,
1.0e-14,mol/m^2 s,58.62,kJ/mol,25,C,
,3.1421,,,,
KnRc-30,TST,Goethite,1,Fe+++,1,2,Goethite,1,H+,3,
1.0e-13,mol/m^2 s,58.62,kJ/mol,25,C,
,-0.424,,,,
KnRc-31,TST,Illite,4,Mg++,0.25,K+,0.6,Al+++,2.3,SiO2(aq),3.5,2,Illite,1,H+,8,
1.0e-14,mol/m^2 s,58.62,kJ/mol,25,C,
,6.1421,,,,
KnRc-32,TST,K-Feldspar,3,Al+++,1,K+,1,SiO2(aq),3,2,K-Feldspar,1,H+,4,
1.0e-12,mol/m^2 s,67.83,kJ/mol,25,C,
,-0.817,,,,
KnRc-33,TST,Kaolinite,2,Al+++,2,SiO2(aq),2,2,Kaolinite,1,H+,6,
1.0e-13,mol/m^2 s,62.76,kJ/mol,25,C,
,4.3344,,,,
KnRc-34,TST,Oligoclase,4,Ca++,1,Al+++,6,SiO2(aq),14,Na+,4,2,Oligoclase,1,H+,24,
1.0e-12,mol/m^2 s,67.83,kJ/mol,25,C,
,16.7372,,,,
KnRc-35,TST,Organic_matter,3,Methane(aq),0.5,H+,0.5,HCO3-,0.5,1,Organic_matter,1,
```

```
1.0e-13,mol/m^2 s,0.0,kJ/mol,25,C,
,1.e+02,,,,
KnRc-36,TST,Quartz,1,SiO2(aq),1,1,Quartz,1,
1.2589e-14,mol/m^2 s,87.5,kJ/mol,25,C,
,-3.5434,,,,
KnRc-37,TST,Siderite,2,Fe++,1,HCO3-,1,2,Siderite,1,H+,1,
6.0e-09,mol/m^2 s,41.87,kJ/mol,25,C,
,-0.7248,,,,
KnRc-38,TST,Smectite-Ca,4,Ca++,0.1450,Mg++,0.26,Al+++,1.77,SiO2(aq),3.97,2,Smectite-
Ca,1,H+,6.12,
1.0e-13,mol/m^2 s,58.62,kJ/mol,25,C,
,-3.7022,,,,
KnRc-39,TST,Smectite-Na,4,Mg++,0.26,Na+,0.29,Al+++,1.77,SiO2(aq),3.97,2,Smectite-
Na,1,H+,6.12,
1.0e-13,mol/m^2 s,58.62,kJ/mol,25,C,
,-3.8023,,,,
```

The relevant aqueous species for this simulation were determined using EQ3/6 v8.0 (Wolery and Jarek 2003), and must be defined in the *Aqueous Species Card*. Required input includes the species name, aqueous molecular diffusion coefficient for all species, activity coefficient model option, species charge, species diameter, and species molecular weight. The species name must be unique and distinct from gas and solid species names (e.g., CO2(aq), CO2_aqueous, dissolved CO2, CO2a). Currently, the activity coefficient models include Davies, B-Dot, Pitzer and a constant coefficient option. If the constant coefficient option is chosen then the species charge, diameter, molecular weight inputs are not required. This example uses the B-dot (Helgeson 1969) activity coefficient model:

```
~Aqueous Species Card
37,1.e-9,cm^2/s,Bdot,1.0,
Al(OH)2+,1.0,4.0,A,60.996,kg/kmol,
Al+++,3.0,9.0,A,26.982,kg/kmol,
AlO2-,-1.0,4.0,A,58.980,kg/kmol,
AlOH++,2.0,4.5,A,43.989,kg/kmol,
CO(aq),0.0,3.0,A,28.010,kg/kmol,
CO2(aq),0.0,3.0,A,44.010,kg/kmol,
Ca++,2.0,6.0,A,40.078,kg/kmol,
CaCl+,1.0,4.0,A,75.531,kg/kmol,
CaCl2(aq),0.0,3.0,A,110.983,kg/kmol,
CaHCO3+,1.0,4.0,A,101.095,kg/kmol,
Cl-,-1.0,3.0,A,35.453,kg/kmol,
Ethane(aq),0.0,3.0,A,30.070,kg/kmol,
Fe(OH)2+,1.0,4.0,A,89.862,kg/kmol,
Fe(OH)3(aq),0.0,3.0,A,106.869,kg/kmol,
Fe++,2.0,6.0,A,55.847,kg/kmol,
Fe+++,3.0,9.0,A,55.847,kg/kmol,
FeCl+,1.0,4.0,A,91.300,kg/kmol,
FeCl++,2.0,4.5,A,91.300,kg/kmol,
```

```
FeCl2+,1.0,4.0,A,126.752,kg/kmol,
FeHCO3+,1.0,4.0,A,116.864,kg/kmol,
FeOH++,2.0,4.5,A,72.854,kg/kmol,
H+,1.0,9.0,A,1.008,kg/kmol,
HAlO2(aq),0.0,3.0,A,59.988,kg/kmol,
HCO3-,-1.0,4.0,A,61.017,kg/kmol,
K+,1.0,3.0,A,39.098,kg/kmol,
KCl(aq),0.0,3.0,A,74.551,kg/kmol,
Methane(aq),0.0,3.0,A,16.043,kg/kmol,
Mg++,2.0,8.0,A,24.305,kg/kmol,
MgCl+,1.0,4.0,A,59.758,kg/kmol,
MgHCO3+,1.0,4.0,A,85.322,kg/kmol,
Na+,1.0,4.0,A,22.990,kg/kmol,
NaAlO2(aq),0.0,3.0,A,81.970,kg/kmol,
NaCl(aq),0.0,3.0,A,58.442,kg/kmol,
NaHCO3(aq),0.0,3.0,A,84.007,kg/kmol,
NaHSiO3(aq),0.0,3.0,A,100.081,kg/kmol,
O2(aq),0.0,3.0,A,31.999,kg/kmol,
SiO2(aq),0.0,3.0,A,60.084,kg/kmol,
```

Geochemical models usually assume some reactions to be in equilibrium. This assumption is often justified for some reactions, especially those involving only aqueous species. Equilibrium reactions have high reaction rates and reach equilibrium quickly when transport, other reactions, or changes in physical chemical conditions disturb it. Specifically, if the rate of a reaction is much greater than the characteristic time of the problem being solved, it should be classified as an equilibrium reaction.

Aqueous species are associated with the defined equilibrium reactions via the *Equilibrium Equations Card*. Required inputs include the number of species in the equilibrium equation (including the equilibrium species), species names, equilibrium reaction name, and the species exponents. The equilibrium species is distinguished from the other species in the equilibrium equation by being the first species listed for the equilibrium equation. For example, Equations (1), (2) and (3) are equilibrium reactions; Equation (3) is labeled below as EqRc-8:

```
~Equilibrium Equations Card
26,
3,Al(OH)2+,Al+++,1,H+,-2,EqRc-1,1.0,
3,AlO2-,Al+++,1,H+,-4,EqRc-2,1.0,
3,AlOH++,Al+++,1,H+,-1,EqRc-3,1.0,
3,CO(aq),CO2(aq),1,O2(aq),-5.e-01,EqRc-4,1.0,
3,HCO3-,CO2(aq),1,H+,-1,EqRc-5,1.0,
3,CaCl+,Ca++,1,Cl-,1,EqRc-6,1.0,
3,CaCl2(aq),Ca++,1,Cl-,2,EqRc-7,1.0,
4,CaHCO3+,CO2(aq),1,Ca++,1,H+,-1,EqRc-8,1.0,
```

```
3,Ethane(aq),CO2(aq),2,O2(aq),-3.5,EqRc-9,1.0,
4,Fe(OH)2+,Fe++,1,H+,-1,O2(aq),2.5e-01,EqRc-10,1.0,
4,Fe(OH)3(aq),Fe++,1,H+,-2,O2(aq),2.5e-01,EqRc-11,1.0,
4,Fe+++,Fe++,1,H+,1,O2(aq),2.5e-01,EqRc-12,1.0,
3,FeCl+,Cl-,1,Fe++,1,EqRc-13,1.0,
5,FeCl++,Cl-,1,Fe++,1,H+,1,O2(aq),2.5e-01,EqRc-14,1.0,
5,FeCl2+,Cl-,2,Fe++,1,H+,1,O2(aq),2.5e-01,EqRc-15,1.0,
4,FeHCO3+,CO2(aq),1,Fe++,1,H+,-1,EqRc-16,1.0,
3,FeOH++,Fe++,1,O2(aq),2.5e-01,EqRc-17,1.0,
3,HAlO2(aq),Al+++,1,H+,-3,EqRc-18,1.0,
3,KCl(aq),Cl-,1,K+,1,EqRc-19,1.0,
3,Methane(aq),CO2(aq),1,O2(aq),-2,EqRc-20,1.0,
3,MgCl+,Cl-,1,Mg++,1,EqRc-21,1.0,
4,MgHCO3+,CO2(aq),1,H+,-1,Mg++,1,EqRc-22,1.0,
4,NaAlO2(aq),Al+++,1,H+,-4,Na+,1,EqRc-23,1.0,
3,NaCl(aq),Cl-,1,Na+,1,EqRc-24,1.0,
4,NaHCO3(aq),CO2(aq),1,H+,-1,Na+,1,EqRc-25,1.0,
4,NaHSiO3(aq),H+,-1,Na+,1,SiO2(aq),1,EqRc-26,1.0,
```

The *Equilibrium Reactions Card* specifies the equilibrium reaction constants to be considered in the simulation. This card is only used to specify the parameters used in the temperature dependent equations for equilibrium constants. Required inputs include the equilibrium reaction name and equation coefficients for the temperature dependent equilibrium constant. The equilibrium reaction name must be unique and distinct from kinetic reaction names (e.g., EqRc-1, E1, Equil-Reac-1, er-1). This example uses equilibrium coefficients, calculated at 54°C using the EQ3/6 v8.0 database (Wolery and Jarek 2003).

```
~Equilibrium Reactions Card
26,
EqRc-1,0.0,-9.040,0.0,0.0,0.0,1/mol,
EqRc-2,0.0,-20.084,0.0,0.0,0.0,1/mol,
EqRc-3,0.0,-4.157,0.0,0.0,0.0,1/mol,
EqRc-4,0.0,-42.049,0.0,0.0,0.0,1/mol,
EqRc-5,0.0,-6.265,0.0,0.0,0.0,1/mol,
EqRc-6,0.0,-0.616,0.0,0.0,0.0,1/mol,
EqRc-7,0.0,-0.649,0.0,0.0,0.0,1/mol,
EqRc-8,0.0,-5.136,0.0,0.0,0.0,1/mol,
EqRc-9,0.0,-232.518,0.0,0.0,0.0,1/mol,
EqRc-10,0.0,-2.525,0.0,0.0,0.0,1/mol,
EqRc-11,0.0,-8.855,0.0,0.0,0.0,1/mol,
EqRc-12,0.0,3.145,0.0,0.0,0.0,1/mol,
EqRc-13,0.0,-0.066,0.0,0.0,0.0,1/mol,
EqRc-14,0.0,2.961,0.0,0.0,0.0,1/mol,
EqRc-15,0.0,5.275,0.0,0.0,0.0,1/mol,
EqRc-16,0.0,-3.545,0.0,0.0,0.0,1/mol,
EqRc-17,0.0,0.955,0.0,0.0,0.0,1/mol,
EqRc-18,0.0,-14.154,0.0,0.0,0.0,1/mol,
EqRc-19,0.0,-1.262,0.0,0.0,0.0,1/mol,
EqRc-20,0.0,-127.710,0.0,0.0,0.0,1/mol,
EqRc-21,0.0,-0.081,0.0,0.0,0.0,1/mol,
EqRc-22,0.0,-5.134,0.0,0.0,0.0,1/mol,
```

```
EqRc-23,0.0,-20.649,0.0,0.0,0.0,1/mol,
EqRc-24,0.0,-0.676,0.0,0.0,0.0,1/mol,
EqRc-25,0.0,-6.331,0.0,0.0,0.0,1/mol,
EqRc-26,0.0,-8.098,0.0,0.0,0.0,1/mol,
```

Equation 1, which defines the dissolution of supercritical or gas phase CO_2 in brine, does not have to be explicitly defined in the *Equilibrium Equations Card*, as it is calculated according to Henry's Law with a correction for salinity in the equation of state module for STOMP.

The aqueous CO_2 mass fraction calculated in the coupled flow and transport may be associated with the aqueous species CO_2(aq) via the *Species Link Card*. This card associates reactive species with components in the coupled flow and transport equations and defines which species name defines the system pH. Currently the following coupled flow and transport components can be associated: aqueous water, gas water, aqueous CO_2, gas CO_2, aqueous salt, and solid salt. Required inputs include the number of reactive species links, species names, and linked components (i.e., Aqueous pH, Aqueous Water, Gas Water, Aqueous CO_2, Gas CO_2).

```
~Species Link Card
2,
H+,pH,
Total_CO2(aq),Aqueous CO2,
```

The final input card needed to define the reaction network is the *Conservation Equations Card*. This card specifies the conservation equations to be considered in the simulation. Conservation equations have the following general form:

$$\frac{d\sum\left(a_i C_i\right)}{dt} = 0 \qquad (9)$$

where C_i is the concentration of species i (expressed as aqueous molar concentration), and ai is the stochiometric coefficient of species i, and a_i is the component species concentration (expressed as aqueous molar concentration). Required inputs include the component species name, number of species in the conservation equation, species names, and species stochiometric coefficients.

The component species name must begin with "Total_" followed with the species name of a reactive species in the conservation equation (e.g., Total_CO2, Total_H2CO3, Total_H+). This name specification is critical in that it links the named species with the conservation equation, making the concentration for that species the primary unknown for the conservation equation.

```
~Conservation Equations Card
11,
Total_Al+++,14,Al+++,1,Al(OH)2+,1,AlO2-
        ,1,AlOH++,1,Albite_low,1,Glauconite,1,HAlO2(aq),1,Illite,2.3,K-
        Feldspar,1,Kaolinite,2,NaAlO2(aq),1,Oligoclase,6,Smectite-Ca,1.77,Smectite-Na,1.77,
Total_CO2(aq),13,CO2(aq),1,CO(aq),1,CaHCO3+,1,Calcite,1,Dolomite,2,Ethane(aq),2,FeHCO3+,1,
        HCO3-,1,Methane(aq),1,MgHCO3+,1,NaHCO3(aq),1,Organic_matter,1,Siderite,1,
Total_Ca++,8,Ca++,1,CaCl+,1,CaCl2(aq),1,CaHCO3+,1,Calcite,1,Dolomite,1,Oligoclase,1,Smectite
        -Ca,1.45e-01,
Total_Cl-,9,Cl-,1,CaCl+,1,CaCl2(aq),2,FeCl+,1,FeCl++,1,FeCl2+,2,KCl(aq),1,MgCl+,1,NaCl(aq),1,
Total_Fe++,12,Fe++,1,Fe(OH)2+,1,Fe(OH)3(aq),1,Fe+++,1,FeCl+,1,FeCl++,1,FeCl2+,1,FeHCO3+,1,
        FeOH++,1,Glauconite,3,Goethite,1,Siderite,1,
Total_H+,29,H+,1,Al(OH)2+,-2,AlO2-,-4,AlOH++,-1,Albite_low,-4,CaHCO3+,-1,Calcite,-
        2,Dolomite,-4,Fe(OH)2+,-1,Fe(OH)3(aq),-2,Fe+++,1,FeCl++,1,FeCl2+,1,FeHCO3+,-
        1,Glauconite,-1.15e+01,Goethite,-2,HAlO2(aq),-3,HCO3-,-1,Illite,-8,K-Feldspar,-
        4,Kaolinite,-6,MgHCO3+,-1,NaAlO2(aq),-4,NaHCO3(aq),-1,NaHSiO3(aq),-1,Oligoclase,-
        2.4e+01,Siderite,-2,Smectite-Ca,-6.12,Smectite-Na,-6.12,
Total_K+,5,K+,1,Glauconite,1.5,Illite,6.e-01,K-Feldspar,1,KCl(aq),1,
Total_Mg++,8,Mg++,1,Dolomite,1,Glauconite,5.e-01,Illite,2.5e-01,MgCl+,1,MgHCO3+,1,Smectite-
        Ca,2.6e-01,Smectite-Na,2.6e-01,
Total_Na+,8,Na+,1,Albite_low,1,NaAlO2(aq),1,NaCl(aq),1,NaHCO3(aq),1,NaHSiO3(aq),1,Oligocl
        ase,4,Smectite-Na,2.9e-01,
Total_O2(aq),13,O2(aq),1,CO(aq),-5.e-01,Ethane(aq),-3.5,Fe(OH)2+,2.5e-01,Fe(OH)3(aq),2.5e-
        01,Fe+++,2.5e-01,FeCl++,2.5e-01,FeCl2+,2.5e-01,FeOH++,2.5e-01,Glauconite,1.25e-
        01,Goethite,2.5e-01,Methane(aq),-2,Organic_matter,-1,
Total_SiO2(aq),11,SiO2(aq),1,Albite_low,3,Glauconite,7.5,Illite,3.5,K-
        Feldspar,3,Kaolinite,2,NaHSiO3(aq),1,Oligoclase,1.4e+01,Quartz,1,Smectite-
        Ca,3.97,Smectite-Na,3.97,
```

The geochemical simulations consider 1 m^3 water-saturated medium. The simulation is assumed to start immediately after injection of CO_2. The CO_2 injection pressure was set at 260 bar. The formation pressure was calculated assuming a depth of 1500 meters and a hydrostatic gradient of 0.0992 bar/m. The initial water chemistry used in the simulation is a pure 1.0 M solution of sodium chloride reacting with the primary minerals listed in Table 1 at a temperature of 54 ˚C, a pH of 7, and an Eh of -0.1. The dissolved oxygen content calculated by EQ3/6 v8.0 (Wolery and Jarek 2003) for these initial conditions is 10^{-57}. Any aqueous species not specified in the *Initial Conditions Card* are assumed to be less than 10^{-30}.

~Initial Conditions Card
Gas Pressure,Aqueous Pressure,
7,
Gas Pressure,260,bar,,,,,,,1,1,1,1,1,1,
Aqueous Pressure,148.80475,bar,,,,,,,1,1,1,1,1,1,
Temperature,54.0,C,,,,,,,1,1,1,1,1,1,
Salt Mass Fraction,0.1,,,,,,,,1,1,1,1,1,1,
Species Aqueous Volumetric,Cl-,1.00e+00,mol/liter,,,,,,,1,1,1,1,1,1,
Species Aqueous Volumetric,pH,7.0,,,,,,,,1,1,1,1,1,1,
Species Aqueous Volumetric,Na+,1.00e+00,mol/liter,,,,,,,1,1,1,1,1,1,

Results

The reactant minerals dissolve progressively into the formation water, modifying the water composition and leading to precipitation of product phases, with sequestration of CO_2 within precipitated carbonates. The pH increases with time as primary minerals dissolve and consume H^+; dissolved oxygen concentrations remain low with time due to degradation of organic matter that consumes oxygen (Figure 1). Due to the precipitation of dolomite and siderite, and moderated by the dissolution of calcite, the total amount of CO_2 sequestered as carbonate minerals in 100,000 years is 20 kg per m^3 of formation (Figure 2). The precipitation of carbonate minerals is driven by the dissolution of primary silicate minerals illite, glauconite, and oligoclase (Figure 3). The dissolution of illite provides Mg^{2+} for the formation of dolomite, glauconite provides Mg^{2+} and Fe^{2+} for the formation of siderite and dolomite, and oligoclase provides Ca^{2+} for the formation of dolomite.

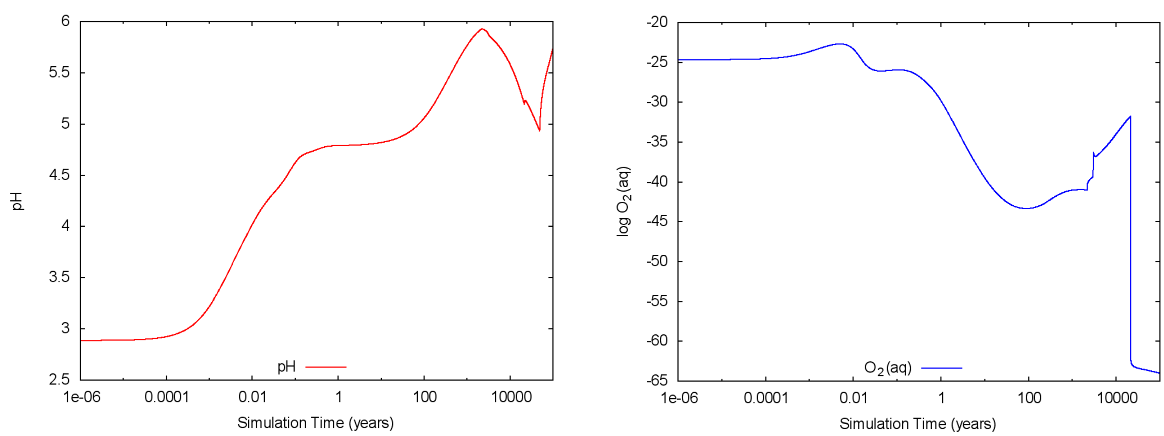

Figure 1. Change in pH and dissolved oxygen vs. time

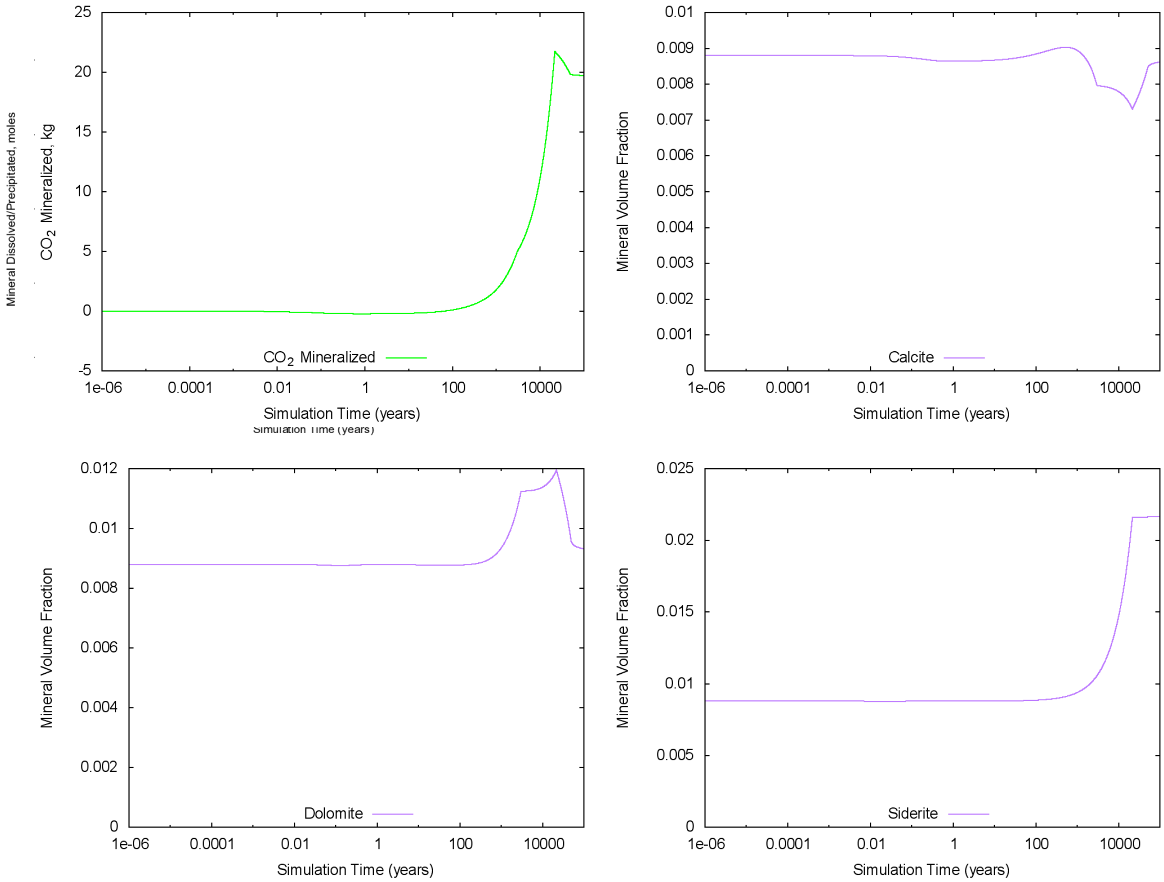

Figure 2. Change in carbonate minerals vs. time

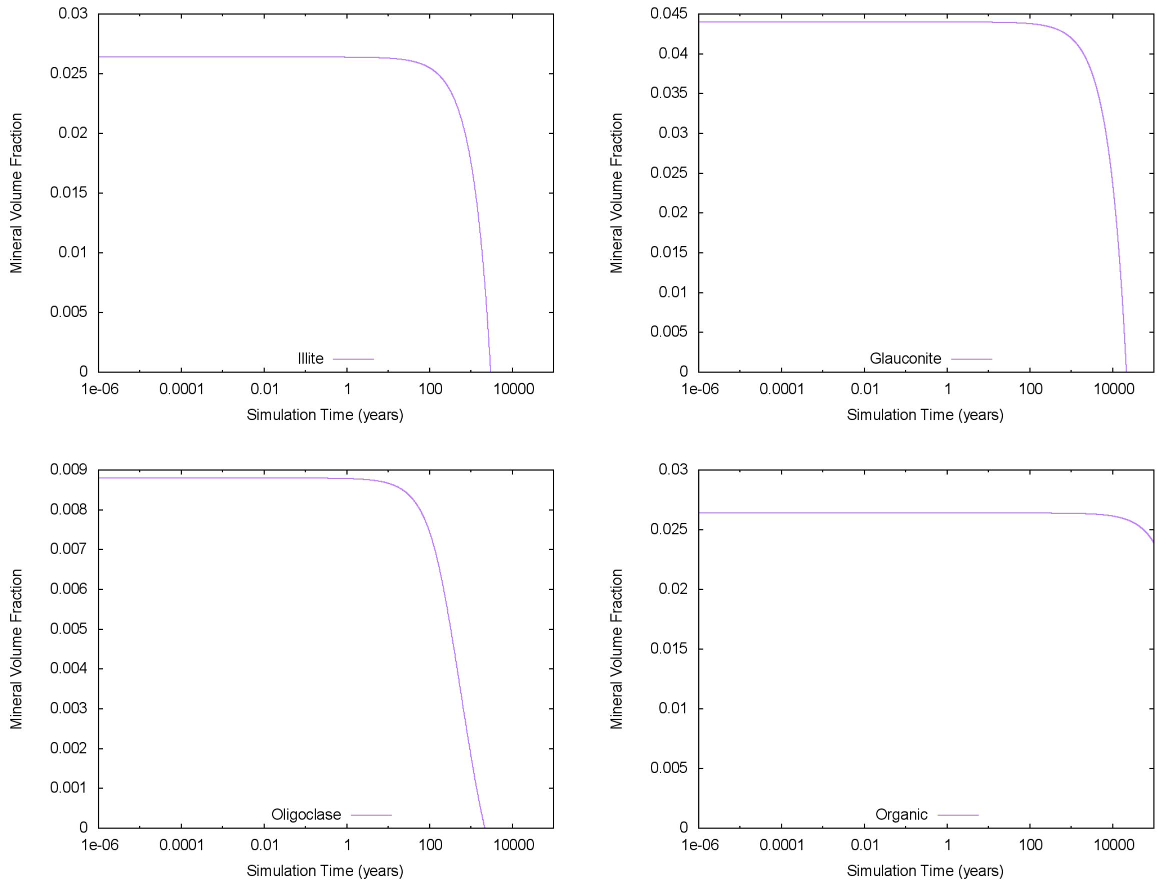

Figure 3. Dissolution of primary minerals vs. time

References

Gunter WD, B Wiwchar, and EH Perkins. 1997. “Aquifer disposal of CO_2-rich greenhouse gases: Extension of the time scale of experiment for CO_2-sequestering reactions by geochemical modelling.” *Mineralogy and Petrology*, 59(1-2):121-140.

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Xu T, JA Apps, and K Pruess. 2001. Analysis of Mineral Trapping for CO_2 Disposal in Deep Aquifers. LBNL-46992, Lawrence Berkeley National Laboratory, Berkeley, California.

Exercises

Tip: save a backup copy of your original input file before making any of these modifications.

1. Double the dissolution rate constant for glauconite and calculate the difference in the amount of CO_2 sequestered as carbonate.
2. Vary the temperature of the formation by ±5°C. What is the effect on the amount of CO_2 sequestered as carbonate? Explain.
3. What effect does varying the siderite kinetic reaction rate by an order of magnitude have on CO_2 sequestration rates? Explain.
4. Goethite was added as a secondary mineral because it was suggested that it would precipitate and compete with siderite for iron, which could reduce the amount of CO_2 sequestered. Remove goethite from the reaction network to see whether or not this is the case (hint: you can do this by changing one line of the input file). If not, explain why.

Input File

```
~Simulation Title Card
3.2,
STOMP Example Problem CO2-5,
DH Bacon,
Pacific Northwest Laboratory,
15 Jun 2010,
07:19 PM PDT,
3,
This problem addresses geochemical effects of CO2 injection into a glauconitic
sandstone aquifer, and analyzes the impact of CO2 immobilization through
carbonate precipitation.

~Solution Control Card
Normal,
H2O-NaCl-CO2 w/ ECKEChem w/minimum concentration w/log w/constant surface area,
1,
0,s,100000,yr,1.e-3,s,10,yr,1.01,16,1.e-06,
99999,
Variable Aqueous Diffusion,
Variable Gas Diffusion,
0,
1.d-70,

~Grid Card
Uniform Cartesian,
1,1,1,
1.0,m,
1.0,m,
1.0,m,

~Rock/Soil Zonation Card
1,
Aquifer,1,1,1,1,1,1,

~Solute/Porous Media Interaction Card
Aquifer,,,,,

~Mechanical Properties Card
Aquifer,2650,kg/m^3,0.12,0.12,Compressibility,4.5e-10,1/Pa,100.0,bar,Millington and Quirk,

~Hydraulic Properties Card
Aquifer,1.e-10,m^2,1.e-10,m^2,1.e-10,m^2,0.8,0.8,

~Saturation Function Card
Aquifer,Brooks and Corey,54.0,cm,4.033,0.8,,

~Aqueous Relative Permeability Card
Aquifer,Mualem,,

~Gas Relative Permeability Card
Aquifer,Mualem,,

~Salt Transport Card
Aquifer,0.2,m,0.2,m,

~Aqueous Species Card
```

37,1.e-9,cm^2/s,Bdot,1.0,
Al(OH)2+,1.0,4.0,A,60.996,kg/kmol,
Al+++,3.0,9.0,A,26.982,kg/kmol,
AlO2-,-1.0,4.0,A,58.980,kg/kmol,
AlOH++,2.0,4.5,A,43.989,kg/kmol,
CO(aq),0.0,3.0,A,28.010,kg/kmol,
CO2(aq),0.0,3.0,A,44.010,kg/kmol,
Ca++,2.0,6.0,A,40.078,kg/kmol,
CaCl+,1.0,4.0,A,75.531,kg/kmol,
CaCl2(aq),0.0,3.0,A,110.983,kg/kmol,
CaHCO3+,1.0,4.0,A,101.095,kg/kmol,
Cl-,-1.0,3.0,A,35.453,kg/kmol,
Ethane(aq),0.0,3.0,A,30.070,kg/kmol,
Fe(OH)2+,1.0,4.0,A,89.862,kg/kmol,
Fe(OH)3(aq),0.0,3.0,A,106.869,kg/kmol,
Fe++,2.0,6.0,A,55.847,kg/kmol,
Fe+++,3.0,9.0,A,55.847,kg/kmol,
FeCl+,1.0,4.0,A,91.300,kg/kmol,
FeCl++,2.0,4.5,A,91.300,kg/kmol,
FeCl2+,1.0,4.0,A,126.752,kg/kmol,
FeHCO3+,1.0,4.0,A,116.864,kg/kmol,
FeOH++,2.0,4.5,A,72.854,kg/kmol,
H+,1.0,9.0,A,1.008,kg/kmol,
HAlO2(aq),0.0,3.0,A,59.988,kg/kmol,
HCO3-,-1.0,4.0,A,61.017,kg/kmol,
K+,1.0,3.0,A,39.098,kg/kmol,
KCl(aq),0.0,3.0,A,74.551,kg/kmol,
Methane(aq),0.0,3.0,A,16.043,kg/kmol,
Mg++,2.0,8.0,A,24.305,kg/kmol,
MgCl+,1.0,4.0,A,59.758,kg/kmol,
MgHCO3+,1.0,4.0,A,85.322,kg/kmol,
Na+,1.0,4.0,A,22.990,kg/kmol,
NaAlO2(aq),0.0,3.0,A,81.970,kg/kmol,
NaCl(aq),0.0,3.0,A,58.442,kg/kmol,
NaHCO3(aq),0.0,3.0,A,84.007,kg/kmol,
NaHSiO3(aq),0.0,3.0,A,100.081,kg/kmol,
O2(aq),0.0,3.0,A,31.999,kg/kmol,
SiO2(aq),0.0,3.0,A,60.084,kg/kmol,

~Solid Species Card
14,
Albite_low,2.62,g/cm^3,262.223,kg/kmol,
Calcite,2.71,g/cm^3,100.087,kg/kmol,
Dolomite,2.86,g/cm^3,184.401,kg/kmol,
Glauconite,2.75,g/cm^3,830.030,kg/kmol,
Goethite,4.27,g/cm^3,88.854,kg/kmol,
Illite,2.75,g/cm^3,383.901,kg/kmol,
K-Feldspar,2.56,g/cm^3,278.332,kg/kmol,
Kaolinite,2.59,g/cm^3,258.160,kg/kmol,
Oligoclase,2.64,g/cm^3,1327.100,kg/kmol,
Organic_matter,1.00,g/cm^3,30.026,kg/kmol,
Quartz,2.65,g/cm^3,60.084,kg/kmol,
Siderite,3.94,g/cm^3,115.856,kg/kmol,
Smectite-Ca,2.20,g/cm^3,366.043,kg/kmol,
Smectite-Na,2.50,g/cm^3,367.017,kg/kmol,

~Lithology Card
Aquifer,14,

```
Albite_low,9.54E-01,cm^2/g,0.,
Calcite,3.69E+01,cm^2/g,0.0088,
Dolomite,3.50E+01,cm^2/g,0.0088,
Glauconite,3.64E+02,cm^2/g,0.044,
Goethite,5.85E+01,cm^2/g,0.,
Illite,3.64E+03,cm^2/g,0.0264,
K-Feldspar,3.91E+01,cm^2/g,0.0176,
Kaolinite,3.86E+03,cm^2/g,0.0176,
Oligoclase,3.62E+01,cm^2/g,0.0088,
Organic_matter,1.00E+02,cm^2/g,0.0264,
Quartz,3.77E+01,cm^2/g,0.7128,
Siderite,2.54E+01,cm^2/g,0.0088,
Smectite-Ca,1.14E+02,cm^2/g,0.,
Smectite-Na,1.00E+02,cm^2/g,0.,

~Species Link Card
2,
H+,pH,
Total_CO2(aq),Aqueous CO2,

~Conservation Equations Card
11,
Total_Al+++,14,Al+++,1,Al(OH)2+,1,AlO2-
    ,1,AlOH++,1,Albite_low,1,Glauconite,1,HAlO2(aq),1,Illite,2.3,K-
    Feldspar,1,Kaolinite,2,NaAlO2(aq),1,Oligoclase,6,Smectite-Ca,1.77,Smectite-Na,1.77,
Total_CO2(aq),13,CO2(aq),1,CO(aq),1,CaHCO3+,1,Calcite,1,Dolomite,2,Ethane(aq),2,FeHCO3+,1,
    HCO3-,1,Methane(aq),1,MgHCO3+,1,NaHCO3(aq),1,Organic_matter,1,Siderite,1,
Total_Ca++,8,Ca++,1,CaCl+,1,CaCl2(aq),1,CaHCO3+,1,Calcite,1,Dolomite,1,Oligoclase,1,Smectite
    -Ca,1.45e-01,
Total_Cl-,9,Cl-,1,CaCl+,1,CaCl2(aq),2,FeCl+,1,FeCl++,1,FeCl2+,2,KCl(aq),1,MgCl+,1,NaCl(aq),1,
Total_Fe++,12,Fe++,1,Fe(OH)2+,1,Fe(OH)3(aq),1,Fe+++,1,FeCl+,1,FeCl++,1,FeCl2+,1,FeHCO3+,1,
    FeOH++,1,Glauconite,3,Goethite,1,Siderite,1,
Total_H+,29,H+,1,Al(OH)2+,-2,AlO2-,-4,AlOH++,-1,Albite_low,-4,CaHCO3+,-1,Calcite,-
    2,Dolomite,-4,Fe(OH)2+,-1,Fe(OH)3(aq),-2,Fe+++,1,FeCl++,1,FeCl2+,1,FeHCO3+,-
    1,Glauconite,-1.15e+01,Goethite,-2,HAlO2(aq),-3,HCO3-,-1,Illite,-8,K-Feldspar,-
    4,Kaolinite,-6,MgHCO3+,-1,NaAlO2(aq),-4,NaHCO3(aq),-1,NaHSiO3(aq),-1,Oligoclase,-
    2.4e+01,Siderite,-2,Smectite-Ca,-6.12,Smectite-Na,-6.12,
Total_K+,5,K+,1,Glauconite,1.5,Illite,6.e-01,K-Feldspar,1,KCl(aq),1,
Total_Mg++,8,Mg++,1,Dolomite,1,Glauconite,5.e-01,Illite,2.5e-01,MgCl+,1,MgHCO3+,1,Smectite-
    Ca,2.6e-01,Smectite-Na,2.6e-01,
Total_Na+,8,Na+,1,Albite_low,1,NaAlO2(aq),1,NaCl(aq),1,NaHCO3(aq),1,NaHSiO3(aq),1,Oligocl
    ase,4,Smectite-Na,2.9e-01,
Total_O2(aq),13,O2(aq),1,CO(aq),-5.e-01,Ethane(aq),-3.5,Fe(OH)2+,2.5e-01,Fe(OH)3(aq),2.5e-
    01,Fe+++,2.5e-01,FeCl++,2.5e-01,FeCl2+,2.5e-01,FeOH++,2.5e-01,Glauconite,1.25e-
    01,Goethite,2.5e-01,Methane(aq),-2,Organic_matter,-1,
Total_SiO2(aq),11,SiO2(aq),1,Albite_low,3,Glauconite,7.5,Illite,3.5,K-
    Feldspar,3,Kaolinite,2,NaHSiO3(aq),1,Oligoclase,1.4e+01,Quartz,1,Smectite-
    Ca,3.97,Smectite-Na,3.97,

~Equilibrium Reactions Card
26,
EqRc-1,0.0,-9.040,0.0,0.0,0.0,1/mol,
EqRc-2,0.0,-20.084,0.0,0.0,0.0,1/mol,
EqRc-3,0.0,-4.157,0.0,0.0,0.0,1/mol,
EqRc-4,0.0,-42.049,0.0,0.0,0.0,1/mol,
EqRc-5,0.0,-6.265,0.0,0.0,0.0,1/mol,
EqRc-6,0.0,-0.616,0.0,0.0,0.0,1/mol,
EqRc-7,0.0,-0.649,0.0,0.0,0.0,1/mol,
```

```
EqRc-8,0.0,-5.136,0.0,0.0,0.0,1/mol,
EqRc-9,0.0,-232.518,0.0,0.0,0.0,1/mol,
EqRc-10,0.0,-2.525,0.0,0.0,0.0,1/mol,
EqRc-11,0.0,-8.855,0.0,0.0,0.0,1/mol,
EqRc-12,0.0,3.145,0.0,0.0,0.0,1/mol,
EqRc-13,0.0,-0.066,0.0,0.0,0.0,1/mol,
EqRc-14,0.0,2.961,0.0,0.0,0.0,1/mol,
EqRc-15,0.0,5.275,0.0,0.0,0.0,1/mol,
EqRc-16,0.0,-3.545,0.0,0.0,0.0,1/mol,
EqRc-17,0.0,0.955,0.0,0.0,0.0,1/mol,
EqRc-18,0.0,-14.154,0.0,0.0,0.0,1/mol,
EqRc-19,0.0,-1.262,0.0,0.0,0.0,1/mol,
EqRc-20,0.0,-127.710,0.0,0.0,0.0,1/mol,
EqRc-21,0.0,-0.081,0.0,0.0,0.0,1/mol,
EqRc-22,0.0,-5.134,0.0,0.0,0.0,1/mol,
EqRc-23,0.0,-20.649,0.0,0.0,0.0,1/mol,
EqRc-24,0.0,-0.676,0.0,0.0,0.0,1/mol,
EqRc-25,0.0,-6.331,0.0,0.0,0.0,1/mol,
EqRc-26,0.0,-8.098,0.0,0.0,0.0,1/mol,

~Equilibrium Equations Card
26,
3,Al(OH)2+,Al+++,1,H+,-2,EqRc-1,1.0,
3,AlO2-,Al+++,1,H+,-4,EqRc-2,1.0,
3,AlOH++,Al+++,1,H+,-1,EqRc-3,1.0,
3,CO(aq),CO2(aq),1,O2(aq),-5.e-01,EqRc-4,1.0,
3,HCO3-,CO2(aq),1,H+,-1,EqRc-5,1.0,
3,CaCl+,Ca++,1,Cl-,1,EqRc-6,1.0,
3,CaCl2(aq),Ca++,1,Cl-,2,EqRc-7,1.0,
4,CaHCO3+,CO2(aq),1,Ca++,1,H+,-1,EqRc-8,1.0,
3,Ethane(aq),CO2(aq),2,O2(aq),-3.5,EqRc-9,1.0,
4,Fe(OH)2+,Fe++,1,H+,-1,O2(aq),2.5e-01,EqRc-10,1.0,
4,Fe(OH)3(aq),Fe++,1,H+,-2,O2(aq),2.5e-01,EqRc-11,1.0,
4,Fe+++,Fe++,1,H+,1,O2(aq),2.5e-01,EqRc-12,1.0,
3,FeCl+,Cl-,1,Fe++,1,EqRc-13,1.0,
5,FeCl++,Cl-,1,Fe++,1,H+,1,O2(aq),2.5e-01,EqRc-14,1.0,
5,FeCl2+,Cl-,2,Fe++,1,H+,1,O2(aq),2.5e-01,EqRc-15,1.0,
4,FeHCO3+,CO2(aq),1,Fe++,1,H+,-1,EqRc-16,1.0,
3,FeOH++,Fe++,1,O2(aq),2.5e-01,EqRc-17,1.0,
3,HAlO2(aq),Al+++,1,H+,-3,EqRc-18,1.0,
3,KCl(aq),Cl-,1,K+,1,EqRc-19,1.0,
3,Methane(aq),CO2(aq),1,O2(aq),-2,EqRc-20,1.0,
3,MgCl+,Cl-,1,Mg++,1,EqRc-21,1.0,
4,MgHCO3+,CO2(aq),1,H+,-1,Mg++,1,EqRc-22,1.0,
4,NaAlO2(aq),Al+++,1,H+,-4,Na+,1,EqRc-23,1.0,
3,NaCl(aq),Cl-,1,Na+,1,EqRc-24,1.0,
4,NaHCO3(aq),CO2(aq),1,H+,-1,Na+,1,EqRc-25,1.0,
4,NaHSiO3(aq),H+,-1,Na+,1,SiO2(aq),1,EqRc-26,1.0,

~Kinetic Reactions Card
14,
KnRc-26,TST,Albite_low,3,Al+++,1,Na+,1,SiO2(aq),3,2,Albite_low,1,H+,4,
1.0e-12,mol/m^2 s,67.83,kJ/mol,25,C,
,1.7907,,,,
KnRc-27,TST,Calcite,2,Ca++,1,HCO3-,1,2,Calcite,1,H+,1,
1.6e-09,mol/m^2 s,41.87,kJ/mol,25,C,
,1.42,,,,
KnRc-28,TST,Dolomite,3,Ca++,1,Mg++,1,HCO3-,2,2,Dolomite,1,H+,2,
```

```
6.0e-10,mol/m^2 s,41.87,kJ/mol,25,C,
,1.5279,,,,
KnRc-
    29,TST,Glauconite,6,Fe++,2.5,Fe+++,0.5,Mg++,0.5,K+,1.5,Al+++,1,SiO2(aq),7.5,2,Glauconi
    te,1,H+,12,
1.0e-14,mol/m^2 s,58.62,kJ/mol,25,C,
,3.1421,,,,
KnRc-30,TST,Goethite,1,Fe+++,1,2,Goethite,1,H+,3,
1.0e-13,mol/m^2 s,58.62,kJ/mol,25,C,
,-0.424,,,,
KnRc-31,TST,Illite,4,Mg++,0.25,K+,0.6,Al+++,2.3,SiO2(aq),3.5,2,Illite,1,H+,8,
1.0e-14,mol/m^2 s,58.62,kJ/mol,25,C,
,6.1421,,,,
KnRc-32,TST,K-Feldspar,3,Al+++,1,K+,1,SiO2(aq),3,2,K-Feldspar,1,H+,4,
1.0e-12,mol/m^2 s,67.83,kJ/mol,25,C,
,-0.817,,,,
KnRc-33,TST,Kaolinite,2,Al+++,2,SiO2(aq),2,2,Kaolinite,1,H+,6,
1.0e-13,mol/m^2 s,62.76,kJ/mol,25,C,
,4.3344,,,,
KnRc-34,TST,Oligoclase,4,Ca++,1,Al+++,6,SiO2(aq),14,Na+,4,2,Oligoclase,1,H+,24,
1.0e-12,mol/m^2 s,67.83,kJ/mol,25,C,
,16.7372,,,,
KnRc-35,TST,Organic_matter,3,Methane(aq),0.5,H+,0.5,HCO3-,0.5,1,Organic_matter,1,
1.0e-13,mol/m^2 s,0.0,kJ/mol,25,C,
,1.e+02,,,,
KnRc-36,TST,Quartz,1,SiO2(aq),1,1,Quartz,1,
1.2589e-14,mol/m^2 s,87.5,kJ/mol,25,C,
,-3.5434,,,,
KnRc-37,TST,Siderite,2,Fe++,1,HCO3-,1,2,Siderite,1,H+,1,
6.0e-09,mol/m^2 s,41.87,kJ/mol,25,C,
,-0.7248,,,,
KnRc-38,TST,Smectite-Ca,4,Ca++,0.1450,Mg++,0.26,Al+++,1.77,SiO2(aq),3.97,2,Smectite-
    Ca,1,H+,6.12,
1.0e-13,mol/m^2 s,58.62,kJ/mol,25,C,
,-3.7022,,,,
KnRc-39,TST,Smectite-Na,4,Mg++,0.26,Na+,0.29,Al+++,1.77,SiO2(aq),3.97,2,Smectite-
    Na,1,H+,6.12,
1.0e-13,mol/m^2 s,58.62,kJ/mol,25,C,
,-3.8023,,,,

~Kinetic Equations Card
14,
Kinetic_Albite_low,1,Albite_low,1,
1,KnRc-26,1,
Kinetic_Calcite,1,Calcite,1,
1,KnRc-27,1,
Kinetic_Dolomite,1,Dolomite,1,
1,KnRc-28,1,
Kinetic_Glauconite,1,Glauconite,1,
1,KnRc-29,1,
Kinetic_Goethite,1,Goethite,1,
1,KnRc-30,1,
Kinetic_Illite,1,Illite,1,
1,KnRc-31,1,
Kinetic_K-Feldspar,1,K-Feldspar,1,
1,KnRc-32,1,
Kinetic_Kaolinite,1,Kaolinite,1,
1,KnRc-33,1,
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Kinetic_Oligoclase,1,Oligoclase,1,
1,KnRc-34,1,
Kinetic_Organic_matter,1,Organic_matter,1,
1,KnRc-35,1,
Kinetic_Quartz,1,Quartz,1,
1,KnRc-36,1,
Kinetic_Siderite,1,Siderite,1,
1,KnRc-37,1,
Kinetic_Smectite-Ca,1,Smectite-Ca,1,
1,KnRc-38,1,
Kinetic_Smectite-Na,1,Smectite-Na,1,
1,KnRc-39,1,

~Initial Conditions Card
Gas Pressure,Aqueous Pressure,
7,
Gas Pressure,148.80475,bar,,,,,,,1,1,1,1,1,1,
Aqueous Pressure,148.80475,bar,,,,,,,1,1,1,1,1,1,
Temperature,54.0,C,,,,,,,1,1,1,1,1,1,
Salt Aqueous Concentration,58.44,kg/m^3,,,,,,,1,1,1,1,1,1,
Species Aqueous Volumetric,Cl-,1.00e+00,mol/liter,,,,,,,1,1,1,1,1,1,
Species Aqueous Volumetric,pH,7.0,,,,,,,,1,1,1,1,1,1,
Species Aqueous Volumetric,Na+,1.00e+00,mol/liter,,,,,,,1,1,1,1,1,1,

~Boundary Conditions Card
1,
Top,Aqueous Dirichlet,Gas Dirichlet,Aqueous Concentration,Aqu. Species Zero Flux,Gas Species
        Zero Flux,
0,
1,1,1,1,1,1,1,
0,s,148.80475,bar,1,260,bar,1,58.44,kg/m^3,

~Output Options Card
1,
1,1,1,
1,1,yr,m,6,6,6,
22,
Integrated CO2 Mass,kg,
Integrated Aqueous CO2 Mass,kg,
Integrated Gas CO2 Mass,kg,
Species Aqueous Concentration,H+,mol/liter,
Species Aqueous Concentration,O2(aq),mol/liter,
Species Integrated Mass,Calcite,mol,
Species Integrated Mass,Dolomite,mol,
Species Integrated Mass,Siderite,mol,
Species Volume Fraction,Albite_low,,
Species Volume Fraction,Calcite,,
Species Volume Fraction,Dolomite,,
Species Volume Fraction,Glauconite,,
Species Volume Fraction,Goethite,,
Species Volume Fraction,Illite,,
Species Volume Fraction,K-Feldspar,,
Species Volume Fraction,Kaolinite,,
Species Volume Fraction,Oligoclase,,
Species Volume Fraction,Organic_matter,,
Species Volume Fraction,Quartz,,
Species Volume Fraction,Siderite,,
Species Volume Fraction,Smectite-Ca,,
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Species Volume Fraction,Smectite-Na,,
0,
45,
Aqueous Saturation,,
Gas Saturation,,
Salt Saturation,,
Salt Aqueous Mass Fraction,,
CO2 Aqueous Mass Fraction,,
CO2 Gas Mass Fraction,,
Gas Pressure,Pa,
Diffusive Porosity,,
Species Aqueous Concentration,Al(OH)2+,mol/liter,
Species Aqueous Concentration,Al+++,mol/liter,
Species Aqueous Concentration,AlO2-,mol/liter,
Species Aqueous Concentration,AlOH++,mol/liter,
Species Aqueous Concentration,CO(aq),mol/liter,
Species Aqueous Concentration,CO2(aq),mol/liter,
Species Aqueous Concentration,Ca++,mol/liter,
Species Aqueous Concentration,CaCl+,mol/liter,
Species Aqueous Concentration,CaCl2(aq),mol/liter,
Species Aqueous Concentration,CaHCO3+,mol/liter,
Species Aqueous Concentration,Cl-,mol/liter,
Species Aqueous Concentration,Ethane(aq),mol/liter,
Species Aqueous Concentration,Fe(OH)2+,mol/liter,
Species Aqueous Concentration,Fe(OH)3(aq),mol/liter,
Species Aqueous Concentration,Fe++,mol/liter,
Species Aqueous Concentration,Fe+++,mol/liter,
Species Aqueous Concentration,FeCl+,mol/liter,
Species Aqueous Concentration,FeCl++,mol/liter,
Species Aqueous Concentration,FeCl2+,mol/liter,
Species Aqueous Concentration,FeHCO3+,mol/liter,
Species Aqueous Concentration,FeOH++,mol/liter,
Species Aqueous Concentration,H+,mol/liter,
Species Aqueous Concentration,HAlO2(aq),mol/liter,
Species Aqueous Concentration,HCO3-,mol/liter,
Species Aqueous Concentration,K+,mol/liter,
Species Aqueous Concentration,KCl(aq),mol/liter,
Species Aqueous Concentration,Methane(aq),mol/liter,
Species Aqueous Concentration,Mg++,mol/liter,
Species Aqueous Concentration,MgCl+,mol/liter,
Species Aqueous Concentration,MgHCO3+,mol/liter,
Species Aqueous Concentration,Na+,mol/liter,
Species Aqueous Concentration,NaAlO2(aq),mol/liter,
Species Aqueous Concentration,NaCl(aq),mol/liter,
Species Aqueous Concentration,NaHCO3(aq),mol/liter,
Species Aqueous Concentration,NaHSiO3(aq),mol/liter,
Species Aqueous Concentration,O2(aq),mol/liter,
Species Aqueous Concentration,SiO2(aq),mol/liter,

~Surface Flux Card
3,
Total CO2 Flux,kg/s,kg,Bottom,1,1,1,1,1,1,
Total CO2 Flux,kg/s,kg,Top,1,1,1,1,1,1,
Aqueous Mass Flux,kg/s,kg,Top,1,1,1,1,1,1,
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