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## IMPORTANCE OF MINERALOGICAL DATA FOR GROUNDWATER QUALITY AFFECTED BY CO<sub>2</sub> LEAKAGE

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### INTRODUCTION

Recently, geological storage of CO<sub>2</sub> has been extensively investigated. The impact of leakage from CO<sub>2</sub> storage reservoirs on groundwater quality is one of the concerns. Dissolution of CO<sub>2</sub> in groundwater results in a decrease in pH. Such acidic condition can affect the dissolution and sorption mechanisms of many minerals (Jaffe and Wang, 2004). Some heavy-metal-bearing minerals dissolve under acidic conditions. For example, galena (PbS) can dissolve and increase significantly Pb concentrations and diminish groundwater quality. If calcite is present in the rock, it can buffer the pH and decrease galena dissolution. Therefore, mineralogical composition and distribution in caprock, overlying aquifers, and along the leakage paths are important data that should be obtained from site characterization. Insight into which minerals and compounds are most important for groundwater quality can be obtained from reactive geochemical transport simulations. Here we present results of simulations using the code TOUGHREACT, whose physical and chemical process capabilities have been discussed by Xu et al. (2006). The simulator can be applied to one-, two-, or three-dimensional porous and fractured media with physical and chemical heterogeneity, and can accommodate any number of chemical species present in liquid, gas and solid phases.

### PROBLEM SETUP

A 1-D system of 100 m length was used for studying water quality evolution along the flow path. The system was divided into 50 uniform grid blocks. We started from a Gulf Coast Frio sandstone, and with the mineralogical composition given in Table 1. Calcite and anhydrite are assumed to react at equilibrium. Other mineral reactions proceed under kinetic conditions. A general kinetic rate law accounting for multiple mechanisms was used. The boundary can be on the storage reservoir or on the leakage path. A separate CO<sub>2</sub> phase could exist in the CO<sub>2</sub> source zone. For purpose of water quality studies, we assumed CO<sub>2</sub> (a partial pressure of 100 bar), H<sub>2</sub>S (1 bar) and SO<sub>2</sub> (10<sup>-4</sup> bar) dissolve into 1 M NaCl brine. The resulting water with a pH of about 3, a dissolved inorganic carbon concentration of 1.54 mol/kg, and a dissolved sulfur of 0.15 mol/kg, was

injected into the system. The water chemistry is assumed unchanged with time. A total of five simulations were performed using different combinations of pore velocity and mineralogical composition. Two pore water velocities were used, the higher case 10 and the lower case 0.1 m/yr. The first simulation used the higher velocity and mineral composition of Table 1 (base-case). Simulations 2 and 3 used a zero calcite abundance and double the calcite at Table 1. Simulation 4 used a lower velocity of 0.1 m/yr. Simulation 5 assumed Pb and Zn bearing minerals, galena and sphalerite, present in the rock with 1% volume fraction each. Changes in mineral abundances of calcite, galena and sphalerite are adjusted with abundance of quartz. An injected CO<sub>2</sub> stream often may contain other constituents such as NO<sub>x</sub> and mercury. The rock adsorption capabilities on the flow path are important for the heavy-metal transport. These are beyond of the scope of this paper.

**Table 1.** List of initial mineral volume fractions and possible secondary mineral phases (Gulf Coast Frio sandstone) used for reactive transport simulations.

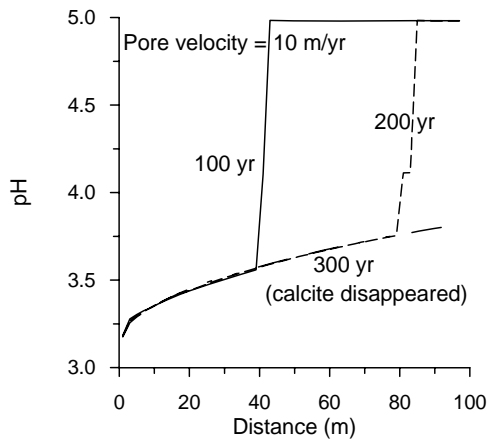
Mineral	Vol.% Of solid	A (cm <sup>2</sup> /g)
<b>Primary:</b>		
Quartz	57.888	9.8
Kaolinite	2.015	151.6
Calcite	1.929	
Illite	0.954	151.6
Oligoclase	19.795	9.8
K-feldspar	8.179	9.8
Na-smectite	3.897	151.6
Chlorite	4.556	9.8
Hematite	0.497	12.9
<b>Secondary:</b>		
Anhydrite		
Magnesite		9.8
Dolomite		9.8
Low-albite		9.8
Siderite		9.8
Ankerite		9.8
Dawsonite		9.8
Ca-smectite		151.6
Alunite		9.8
Pyrite		12.9

## RESULTS

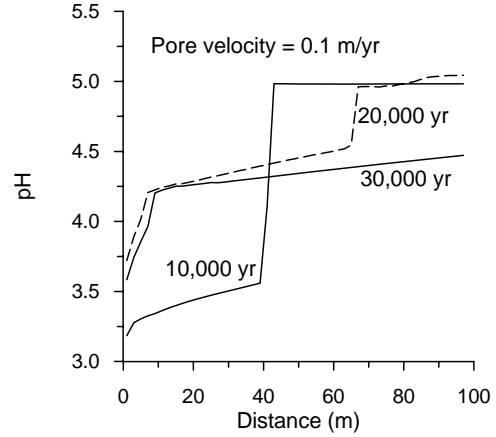
Dissolution of calcite makes the pH increase from 3 to about 5 (Figure 1). The calcite dissolution is typically quite rapid, assumed at equilibrium, relative to the time frame being modeled. Therefore, a step increase in pH is observed. After 100 years, the front of calcite dissolution moves 40 m. After 240 years, calcite dissolves completely and a steady-state pH and concentration profile is formed, which is buffered by other mineral reactions. pH increases from 3 to about 3.8 at 100 m distance. A zero calcite abundance results in a pH profile similar to the curve at 300 yr. The double calcite simulation cause the dissolution and pH front slow by a factor of 2.

Results for a lower pore velocity of 0.1 m/yr, are shown in Figure 2. After 24,000 years, a steady state buffered by other mineral reactions is formed. pH is higher than the base case (4.4 over 3.8 at the outlet).

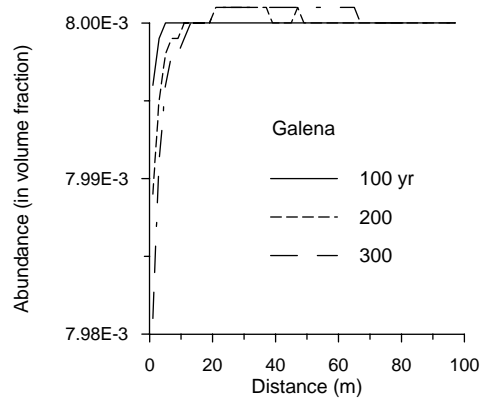
Galena and sphalerite dissolve in lower pH regions (Figure 3). Consequently, Pb concentration increases to about  $4 \times 10^{-6}$  mol/l (much higher than the action level of  $7.25 \times 10^{-8}$  mol/l reported by Wang and Jaffe (2004)), and Zn concentration increases to about  $3 \times 10^{-4}$  mol/l). Galena dissolution essentially occurs within 20 m of the CO<sub>2</sub> source. The simulation suggests that galena dissolution will not be a problem at distance greater than 20 m from the injection point. Therefore, data on mineral distribution along the flow path is important in addition to the mineral composition.



**Figure 1.** pH distribution at three different times for a pore velocity of 10 m/yr.



**Figure 2.** pH distribution at three different times for a lower pore velocity of 0.1 m/yr.



**Figure 3.** Abundance of galena (in volume fraction) at three different times for a pore velocity of 10 m/yr.

## CONCLUSIONS

Mineralogical composition and distribution in the CO<sub>2</sub> leakage pathway and in overlying aquifers are important data for water quality evolution, and therefore should be an important part of CO<sub>2</sub> site characterization. If carbonate minerals such as calcite are present along the leakage pathway, they can buffer the pH to about 5. Other minerals can also buffer the pH but to lesser degree. Acidic conditions affect significantly the dissolution and sorption mechanisms of many minerals. For example, if galena is present in the low pH regions its dissolution causes Pb concentration to increase to about  $4 \times 10^{-6}$  mol/l, which is much higher than the action level of  $7.25 \times 10^{-8}$  mol/l (Wang and Jaffe, 2004).

### **ACKNOWLEDGMENT**

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### **REFERENCES**

Wang, S., and Jaffe, P.R., Dissolution of a mineral phase in potable aquifers due to CO<sub>2</sub> releases from deep formations: effect of dissolution kinetics, Energy Conversion and Management, v. 45, 2833-2848, 2004.

Xu, T., E.L. Sonnenthal, N. Spycher, and K. Pruess, TOUGHREACT: A simulation program for non-isothermal multiphase reactive geochemical transport in variably saturated geologic media, Computer & Geoscience, v 32/2, 145-165, 2006.