

## TOUGHREACT SIMULATION STUDIES FOR MINERAL TRAPPING FOLLOWING CO<sub>2</sub> DISPOSAL IN DEEP SALINE AQUIFERS

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### RESEARCH OBJECTIVES

A reactive fluid flow and geochemical transport numerical model TOUGHREACT has been developed for evaluating long-term CO<sub>2</sub> disposal in deep geologic formations. The model is needed because alteration of the aluminosilicate minerals in the predominant host rock is very slow and not amenable to laboratory experiment under ambient deep-formation conditions. Using this model, we performed: (1) batch geochemical modeling analysis with three rock types (glauconitic sandstone from the Canada Alberta Sedimentary Basin, a sediment from the United States Gulf Coast, and a dunite); (2) reactive transport simulations of a 1-D radial-well region under CO<sub>2</sub> injection conditions to analyze CO<sub>2</sub> immobilization through carbonate precipitation in Gulf Coast sandstone of the Frio formation (Texas); and (3) reactive transport simulations of CO<sub>2</sub> sequestration in bedded sandstone-shale sequences.

### APPROACH

TOUGHREACT was developed by introducing reactive chemistry into the framework of the existing multiphase fluid and heat flow code TOUGH2. The code 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, or solid phases. A wide range of subsurface thermal-physical-chemical processes is considered, including (1) redox processes that could be important in deep subsurface environments; (2) the presence of organic matter; (3) the kinetics of chemical interactions between the host rock minerals and the aqueous phase; and (4) CO<sub>2</sub> solubility dependence on pressure, temperature, and salinity of the system.

### ACCOMPLISHMENTS

We evaluated the geochemical evolution under both natural background and CO<sub>2</sub> injection conditions. Changes in porosity were monitored during the simulations. Under favorable conditions, the amount of CO<sub>2</sub> that may be sequestered by precipitation of secondary carbonates is comparable to (and can be larger than) the effect of CO<sub>2</sub> dissolution in pore waters. The addition of CO<sub>2</sub> mass as secondary carbonates (Figure 1) to the solid matrix decreases porosity, and a small porosity decrease can result in a significant decrease in permeability. The mass-transfer pattern of aqueous chemical components

under high CO<sub>2</sub> pressure conditions is different from that under natural conditions—most CO<sub>2</sub> sequestration occurs in the sandstone. Simulation results of mineral alteration under natural conditions agree well with field observations. The limited information currently available for the mineralogy of high-pressure CO<sub>2</sub> reservoirs is also generally consistent with our simulation. More details are given in Xu et al. (2003a, b, c).

### RELATED PUBLICATIONS

- Xu, T, J. A. Apps, and K. Pruess, Numerical simulation to study mineral trapping for CO<sub>2</sub> disposal in deep aquifers. *Applied Geochemistry*, 2003 (in press).
- Xu, T, J.A. Apps, and K. Pruess, Reactive geochemical transport simulation to study mineral trapping for CO<sub>2</sub> disposal in deep arenaceous formations. *Journal of Geophysical Research*, 108 (B2), 2071, doi:10.1029/2002JB001979, 2003.
- Xu, T, J.A. Apps, and K. Pruess, Mass transfer, mineral alteration, and CO<sub>2</sub> sequestration in a sandstone-shale system. *Chemical Geology*, 2003 (submitted).

### ACKNOWLEDGMENTS

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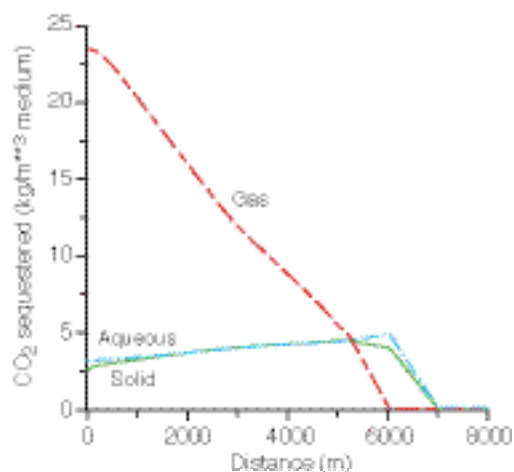


Figure 1. Cumulative CO<sub>2</sub> sequestration in different phases after 10,000 years