

A basic study on the mineral trapping process of CO₂ through numerical simulations

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The underground storage of CO₂ consists of four processes (structural, physical, dissolution and mineral-trapping processes). In this study, the mineral trapping process of CO₂ was investigated through numerical simulations on equilibrium and kinetic models.

(1) Numerical experiment on an equilibrium model

Groundwater and sandstone were interacted at 50 deg.C in order to produce an initial fluid/mineral system with a 0.4 porosity. The chemical compositions of groundwater and sandstone were cited from Okuyama et al. (2007) and Togashi et al. (2000), respectively. The carbon (-10 wt%) was added to the sandstone in order to internally control environmental factors. The simulation was performed using the GWB software (Bethke, 1996).

The experimental results were as follows. (i) The chemical composition of groundwater was not influenced on the experimental result because of its lesser amounts of dissolved species than those in the rock. (ii) A small addition of carbon in the sandstone resulted in an alkali pH of initial fluid/mineral system, and a large addition of carbon in the sandstone resulted in a neutral pH of initial fluid/mineral system with some carbonate minerals. (iii) Predominant mineral-alteration processes during CO₂ injection were plagioclase through smectite to kaolinite, smectite to dolomite or siderite, and albite to dawsonite. K-feldspar had no relation to these processes. (iv) A total amount of CO₂ fixed in the system was determined to be about 0.2 vol.%. Then, when carbonate minerals were present in the initial fluid/mineral system, the amount of CO₂ fixed during the CO₂ injection relatively decreased. (v) The total amounts of CO₂ fixed in the system largely varied, when the secondary carbonate mineral assemblages were changed (i.e., calcite+dolomite+siderite+dawsonite:150-180kg/m³, calcite only:less than 50kg/m³).

(2) Numerical experiment on a kinetic model

Seawater saturated with CO₂ was numerically interacted with sandstone at 50deg.C and 100 bars using the software TOUGHREACT with ECO2 module (Xu et al., 2006). The chemical composition of seawater and sandstone were cited from Kitano (1995) and Togashi et al. (2000), respectively, and the kinetic parameters were picked up from Palandri and Kharaha (2004). The mineral grains forming the sandstone were assumed to be spherical with diameters of 0.5 mm and reaction surfaces of 450cm²/g.

The experimental results for 1,000 years were as follows. (i) The pH of fluid started to increase toward alkaline around several tens of years, and decreased to 7-8 around 800 years. (ii) Plagioclase started to alter to dawsonite around several years, and plagioclase and dawsonite altered to albite and calcite around 400 years. (iii) The change in porosity by 1,000 years was about 0.01, and the amount of CO₂ fixed in the system was about 20 kg/m³. (iv) The fluid/mineral interaction proceeded at one order of magnitude faster, when the reaction surfaces of minerals were one order of magnitude larger.

Thus, these two types of numerical experiments suggested the potential mineral-trapping of CO₂. The followings should be more issued for a future simulation. (a) The alteration of plagioclase to carbonate minerals is the most important reaction process for the CO₂ storage. (b) The amount of CO₂ fixed in the system can increase with increasing carbonate mineral assemblages in the equilibrium model, but in the kinetic model, it should be judged whether the carbonate minerals were intermediate or final products (especially for dawsonite). (c) The reaction model is quite sensitive to the reaction surfaces of minerals. (d) It is ambiguous whether an initial fluid/mineral system without any change in the given initial fluid composition can be numerically produced, because the natural fluid/mineral system might not attain the fluid/mineral equilibrium state.