Reactive transport modelling of mineral trapping of CO_2, revised by water sampling data at Nagaoka CO_2 storage site

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Carbon dioxide capture and storage (CCS) in saline aquifer is one of the global warming countermeasure technologies. A part of injected CO_2 will be stored by reacting with formation water and reservoir rock forming minerals over many years, which is more stable for CO_2 trapping. Conducting reactive transport simulation is needed to evaluate CO_2 mineralization. However, some geochemical input data for kinetic mineral dissolution/precipitaion calculation has high uncertainty. We have attempted to revise the geochemical data by matching the geochemical simulation results with sampled formation water composition, to make more realistic model for long term CO_2 behavior prediction . A series of trial runs would be needed to gain a good match, and so we used 1-D radial model for simulation-time saving. If a field-scale model is used, we have to consider lots of geological uncertainties simultaneously, which should make the study too complicated and time consuming.

Formation water was sampled twice after CO_2 injection from the observation well OB-2 at the depth of 1118m at the Nagaoka site. The concentration changes of HCO_3^-, Ca, and Si from the first run to the second run was chosen for matching data, because only calcite is a carbonate mineral in the initial mineral composition referring to Mito et al. [1]. 1-D radial model was constructed with TOUGHREACT, based on the previous study. Since the reservoir pressure is already stable, CO_2 dissolved water moves mainly by the gravity effect, which can't be expressed in 1-D radial model. Instead, the diffusion coefficient was adjusted by considering HCO_3^- concentration. We selected reactive surface area (RSA) for varying geochemical parameter, and the initial data was based on the experimental results using reservoir rock powder. Finally, RSA value was modified to 0.015 times of the initial model, then a good matching result was obtained. This result is reasonable because the sandstone of Nagaoka site has some conglomerate, and thus should have the narrower contact area with formation water than expected. Subsequently, we performed long term CO_2 behavior simulation with this matched model.

[1] Mito, S., et al (2013) Applied Geochemistry 30, p.33-40

Hydrogen isotope exchange between insoluble organic matter and water in chondrite parent bodies

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The high deuterium enrichment in insoluble organic matter (IOM) in chondrites has largely been attributed to small molecule chemistry prior to IOM, specifically ion-molecule reactions at low temperature interstellar medium (ISM) [1]. The hydrogen isotope (D/H) ratio of IOM tends to decrease as alteration proceeds [2]. While water in carbonaceous chondrites is more depleted in D [3]. Thus, the decrease in D/H ratio of IOM could be attributed to the hydrogen isotope exchange between D-enriched IOM precursor and D-depleted water, which could have occurred during and/or after the formation of IOM.

Cody et al. [4] proposed that IOM in chondrites may have formed through the polymerization of interstellar formaldehyde after the planetesimal accretion, in the presence of liquid water. Our recent study successfully enhanced production of IOM analog materials from formaldehyde in the presence of ammonia [5]. Using this formaldehyde polymer as an IOM analog we have conducted kinetic hydrogen isotope exchange experiments, starting with (1) deuterated formaldehyde polymer and normal water, and (2) normal formaldehyde polymer and deuterated water, both as a function of temperature. The three-dimensional diffusion rate control model was found to fit well the changes in the D/H ratio with time. The apparent activation energies and the frequency factors were obtained by the apparent rate constants for each temperature with the Arrhenius equation. Using these kinetic expressions, hydrogen isotope exchange profiles were estimated for time and temperature behavior, based on the assumption that the kinetic rate low is valid over all temperatures. We will discuss the δD variation observed in various chondrites, and the IOM grain size effects, based on our hydrogen isotope exchange kinetics.

[1] Robert & Epstein (1982) GCA 46, 81-95. [2] Herd et al (2011) Science 332, 1304-1307. [3] Alexander et al (2012) Science 337, 721-723. [4] Cody et al (2011) PNAS 108, 19171-19176. [5] Kebukawa et al ApJ under review.