Reactive transport modeling of stable carbon isotope fractionation during carbon sequestration

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Stable carbon isotopes can be of great usefulness in the characterization and monitoring of CO_2 sequestration sites. Carbon isotopes can be used to track the migration of the CO_2 plume and identify leakage sources. Moreover, they provide unique information about the chemical reactions that take place in the CO_2-water-rock system. However, there are few tools that allow modelers to incorporate stable isotope information into the flow and transport codes used in evaluating CO_2 sequestration problems. In this study we present a numerical tool for modeling the transport of stable carbon isotopes in multiphase reactive systems relevant to geologic carbon sequestration. The code is an extension of the reactive transport code TOUGHREACT. The transport module of TOUGHREACT was modified to include isotopic species containing the element carbon (CO_2, CO_3^{2-}, HCO_3^-,…) as separate species. This way, it allows any process of transport or reactivity influencing a given species to inherently influence its isotopic ratio. The chemical module and database is expanded to include isotopic exchange and fractionation between gas phase and brine.

Three ideal systems have been studied using the current isotope model compared with analytical models, including a batch gas mixture model, a batch water + gas model, and a 1D flow and transport model. The performance of the code is also illustrated using field data from the CO2 injection project carried out at Pembina Cardium, Alberta, Canada. Results show that the flow and transport model shows a much better fit of the field data in terms of the relationship between $\delta^{13}C(g)$ and mole fraction of CO_2 in the gas phase, compare to the gas mixture model used in Johnson *et al.* (2009). Both the field data and the two-phase flow and transport model show that the carbon isotope signature arrives at the monitoring well earlier than expected from a gas mixture model.

[1] Johnson, G., Raistrick, M., Mayer, B., Shevalier, M., Taylor, S., Nightingale, M., Hutcheon, I., 2009. The use of stable isotope measurements for monitoring and verification of CO2 storage. Energy Procedia 1, 2315-2322.