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Stable isotope reactive transport modeling in water-rock interactions during CO_2 injection

Juan J. Hidalgo (1), Vincent Lagneau (2), Pierre Agrinier (1,3)

(1) Institut de Physique du Globe de Paris, Paris, France (hidalgo@ipgp.fr), (2) Mines Paristech, Paris, France, (3) Université Denis Diderot, Paris, France

Stable isotopes can be of great usefulness in the characterization and monitoring of CO_2 sequestration sites. Stable 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 on the CO_2-water-rock system. However, there is a lack of appropriate tools that help modelers to incorporate stable isotope information into the flow and transport models used in CO_2 sequestration problems.

In this work, we present a numerical tool for modeling the transport of stable isotopes in groundwater reactive systems. The code is an extension of the groundwater single-phase flow and reactive transport code HYTEC [2]. HYTEC's transport module was modified to include element isotopes as separate species. This way, it is able to track isotope composition of the system by computing the mixing between the background water and the injected solution accounting for the dependency of diffusion on the isotope mass. The chemical module and database have been expanded to included isotopic exchange with minerals and the isotope fractionation associated with chemical reactions and mineral dissolution or precipitation.

The performance of the code is illustrated through a series of column synthetic models. The code is also used to model the aqueous phase CO_2 injection test carried out at the Lamont-Doherty Earth Observatory site (Palisades, New York, USA) [1].

References

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