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The increasing place of numerical modelling in the geosciences, as in numerous fields is well known. Owing to rapid progress in computer sciences and hardware, more and more complex systems, i.e. also more and more realistic ones, can be simulated. HYTEC is a versatile coupled reactive transport code, currently used for several applications, such as groundwater pollution studies, safety assessment of nuclear waste disposals, CO_2 storage, geochemical studies or interpretation of laboratory column experiments. This work presents a newly developed functionality in HYTEC, which allows taking into account isotopic speciation and filiation.
Variations in isotopic compositions give useful information for the geosciences. They can help track the evolution of aqueous and mineral species, mixing of different origin fluids, and are helpful for dating. Then, environmental isotopes experiences and modelling complete geochemical and physical hydrology studies.

For a specific element, all isotopes have similar chemical properties, due to an identical filling of their electronic orbitals. However, the slight difference in mass causes differences in reaction rates and equilibrium constants. This can be treated directly with as many reactions as isotopes, or more usually by first gathering all the isotopes within the element reaction then correcting with a fractionation factor. Moreover, isotopes can be radioactively unstable, leading to a chain of parent and daughter decay isotopes.

We have included in the reactive transport code HYTEC a description of isotopes, derived from chemical elements. Then, the radioactive filiation and isotopic fractionation were implemented. The overall resolution algorithm is based on an operator splitting method: the main idea is to take advantage of an analytical resolution of the filiation problem, which is the toughest to handle due to very large differences in half-lives, from milliseconds to millions of years.
Between time t and $t+dt$, the algorithm can be decomposed in successive steps. First, HYTEC solves the filiation problem: the radioactive decay and filiation is computed analytically for all the isotopes. Second, HYTEC updates the total concentration for each element. Third, the chemical module updates the speciation. Fourth, a transport-chemistry iterative loop is performed: transport is calculated on the total aqueous concentration for each isotope, then isotope concentrations are collapsed for the element-based speciation resolution. Each time the speciation module is called, the fractionation resolution is performed to dispatch element-based species concentrations into isotopic species concentrations.

The isotopic filiation model was tested on an simple problem with an analytical solution: the transport of Cesium 137 through a porous media containing a sorbing surface mineral. Three processes occur at the same time: transport of the isotopes, sorption of the Cesium on the surface sites and radioactive decay of ^{137}Ce into two daughters, ^{137}Ba and ^{137m}Ba. The simulation results compared correctly with an analytical solution. A second reference is used to test the isotopic fractionation: carbon isotope partitioning as a function of pH and compared with results from the literature.

Work is continuing to improve the model. The resolution is based on the assumption of an overly predominant isotope, used as (user-defined) reference. The dominant isotope could change during the evolution of a system, or there could be two similar concentration isotopes. The first issue can be solved with a locally, automatically, adapted reference. The second requires an extension of the fractionation module. Finally, H and O are still a challenge due to the interference with the solvant.