Quantification of aquifer DNAPLs degradation pathways using reactive transport simulation with isotopic fractionation

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Contamination of the environment by dense non-aqueous phase liquids (DNAPLs) is common in important aquifers of industrialized countries. Research in remediation of DNAPLs nourishes the importance of understanding and predicting their behavior and degradation pathways. Identifying reaction paths (microbially mediated or not) and quantifying them is an essential step to better define efficient rehabilitation methods.

Isotopic fractionation can be a powerful tool to investigate these reaction paths [1]. Moreover, soil and groundwater contamination remediation increasingly rely on reactive transport modeling and theoretical, algorithmic and numerical developments are in progress in HYTEC (a RT code developed at MINES ParisTech, [2]) to implement equilibrium and kinetic isotope fractionation.

In this study, an application is perfomed using HYTEC to model DNAPLs behavior in a fractured aquifer, based on data from [1]. Hydrodynamic simulation of the aquifer-aquitard system relies on a double porosity approach. Transport includes dissolution and diffusive control in the aquitard, and possible sorption of dissolved organic molecules on clay. Degradation is described by several (interlinked) chains of reactions. Carbon isotopes fractionation was taken into account during degradation reactions and sorption on organic matter.

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