

Quantification of aquifer DNAPLs degradation pathways using reactive transport simulation coupled 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. The use of chlorinated solvents became widespread during World War II in manufacturing industries although the ensuing contamination was recognized far later (1970s). Observed levels of contamination usually range from $\mu\text{g/L}$ to mg/L (dissolved). DNAPLs pollution induces great challenges on groundwater remediation as the DNAPLs behavior is complex: these solvents are denser than water, can penetrate soils and host rocks below the water table, have low liquid viscosities and interfacial tensions with water, are volatile, have low absolute solubility but high solubility relative to drinking water limits, they are not delayed by aquifer materials and have low degradability. All these characteristics make chlorinated solvents widespread pollutants with high persistency (Pankow and Cherry, 1996).

Research in remediation solution 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 (Wanner et al., 2018).

Soil and groundwater contamination remediation increasingly rely on reactive transport modeling to understand processes behind present pollution states and their possible evolutions. Theoretical, algorithmic and numerical developments are in progress in HYTEC (a reactive transport code developed at MINES ParisTech, Van der Lee et al., 2003) to implement equilibrium and kinetic isotope fractionation. Reactive transport modeling also takes into account biogeochemical reactions and processes and new perspectives are emerging to investigate biogeochemical cycles of various elements (e.g. C,N) as well as transport, weathering or contamination processes.

The use of reactive transport code hand in hand with field data allow to confirm processes identified on field as well as bringing to light processes that are not clearly noticeable when observing contaminated soils and aquifers. The combination of both also provides significant elements to quantify the highlighted degradation processes and possible competitions. The analysis and modeling of isotope fractionation is perfectly in line with this approach: as an example, carbon fractionation occurs in DNAPLs degradation reactions such as dichloroelimination or dehydrohalogenation, which can be the result of in situ microbial activity, but also during reaction with the medium (sorption for example).

In this study we propose to use some of HYTEC isotope fractionation new functionality for an unusual RT code application : to model DNAPLs behavior and quantify their degradation in a fractured aquifer presenting double porosity characteristics.