



Integrated modelling of enhanced *in situ* biodenitrification in a fractured aquifer: biogeochemistry and isotope geochemistry

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Enhanced *in-situ* biodenitrification is a feasible technology to recovery groundwater polluted by nitrates and achieves drinking water standards. Under optimum conditions, nitrate is reduced by autochthonous bacteria through different reactions until arrive to harmless dinitrogen gas. Isotopic fractionation monitoring in field applications allows knowing the exact degree and the real scope of this technology. Using the Rayleigh equation the change in the isotope ratio of the nitrate molecule ($\delta^{15}\text{N-NO}_3^-$, $\delta^{18}\text{O-NO}_3^-$) is related to the fraction of molecules remaining as a result of biodenitrification. However, Rayleigh application at field scale is sometimes limited due to other processes involved during groundwater flow such as dispersion or adsorption and geological media heterogeneities that interferes in concentration values. Then, include isotope fractionation processes in reactive transport models is a useful tool to interpret and predict data from *in-situ* biodenitrification.

We developed a reactive transport model of enhanced *in situ* application at field scale in a fractured aquifer that considers biogeochemical processes as well as isotope fractionation to enable better monitoring and management of this technology. Processes considered were: microbiological– exogenous and endogenous nitrate and sulfate respiration coupled with microbial growth and decay, geochemical reactions (precipitation of calcite) and isotopic fractionation ($\delta^{15}\text{N-NO}_3^-$; $\delta^{18}\text{O-NO}_3^-$ and carbon isotope network). The 2-D simulations at field scale were developed using PHAST code.

Modeling of nitrate isotope geochemistry has allowed determining the extent of biodenitrification in model domain. We have quantified which is the importance in decreasing of nitrate concentrations due to biodegradation (percentage of biodegradation, “B%”) and due to dilution process (percentage of dilution, “D%”). On the other hand, the stable carbon isotope geochemistry has been modeled. We have considered the isotopic carbon fractionation of different carbon species involved in enhanced biodenitrification: external organic carbon, biomass, inorganic carbon (in different forms) and calcite. The inclusion of carbon isotopes in the model, which are involved in both direct (oxidation of organic carbon) and indirect (carbonate mineral interaction) processes of enhanced biodenitrification, improves the evaluation of the overall model consistency due to the central role of carbon in the reaction network.