

Modeling of enhanced *in situ* biodenitrification in fractured aquifer: Biogeochemical interactions and isotope fractionation

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Enhanced *in situ* biodenitrification (EIB) is a feasible technology to clean up nitrate-polluted groundwater and achieve drinking water standards. We developed a reactive transport model that considers biogeochemical processes as well as isotope fractionation to enable better monitoring and management of this technology. In this work, we applied this model to interpret data from batch experiments on EIB. Furthermore, 2-D simulations at field scale are in progress to model an EIB pilot conducted in a fractured aquifer system. The used codes were PHREEQC for batch scale and PHAST for field scale. The fractured media were modeled as equivalent continuum media with two hydraulic conductivity zones. The flow model was validated with experimental data from a tracer test with bromide. The reactive transport model at batch and field scale was validated with experimental values of Vidal-Gavilan *et al.* (2013) [1]. The preliminary results show that parameters determined in batch experiments can be used as first estimates to reproduce field observations provided groundwater flow is well known. Moreover, the inclusion of isotope fractionation processes allowed to determinate the real scope and exact degree of EIB at field scale.

[1] Vidal-Gavilan, G., Folch A., Otero N., Solanas, A.M., Soler A., 2013. App.Geochem (in press).

Uptake of $\text{Pb}^{2+}_{(\text{aq})}$ by baryte-celestine solid-solution crystals

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The interaction of dissolved toxic metals with minerals frequently leads to dissolution-coprecipitation processes in which the metal ion incorporates into the solid phase substituting for the major ion in lattice positions. The fact that the solubility of a minor constituent in a solid solution is smaller than the solubility of its equivalent pure solid explains the environmental relevance of these coprecipitation reactions. Interaction studies are typically carried out by using stoichiometric minerals as host phases. However, in most cases the effectiveness of this removal mechanism could be significantly increased using suitable solid-solutions instead of pure minerals. In this work we study the interaction of Pb-bearing aqueous solutions with baryte (BaSO_4) and intermediate (5-15 % molar Sr) members of the $(\text{Sr},\text{Ba})\text{SO}_4$ solid solution.

Compositionally homogeneous crystals of the solid solution were obtained by precipitation & aging in a closed reactor at 90°C. The obtained precipitates were checked for compositional homogeneity by considering the full width at half maximum intensity values (FWHM) of some selected reflections of the XRD patterns. The precipitate compositions were determined by analyzing the remaining solutions by ICP-AES. Moreover, samples of each precipitate were analyzed by SEM-EDS.

The interaction experiments were carried out in closed reactors at 25°C. The aqueous composition was analyzed repeated times during the experiments, which lasted one month. In the case of the interaction with strontian baryte, lead incorporates into the solid phase while some barium and a large proportion of strontium incorporate to the aqueous solution. As result the aqueous solution becomes depleted in lead at a significantly greater extent than during the interaction with pure baryte.

Future work will deal with the implementation of an equilibrium model for the $(\text{Pb},\text{Sr},\text{Ba})\text{SO}_4\text{-H}_2\text{O}$ system. An added implication is related to the effectiveness of Sr-bearing baryte as a sequestering phase for radium. The interaction with baryte leads to a significant removal of dissolved Ra^{2+} , but the depletion could be considerably greater using strontian baryte.

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