



Reactive transport models for denitrification in a fractured limestone aquifer

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The simulation of reactive transport of nitrate and other solutes becomes very complicated when fractured and karstified media are concerned due to the large heterogeneity and complexity of water-rock interactions. We consider a carbonate aquifer (Upper Muschelkalk) in the catchment of river Ammer close to Tübingen (Germany), which was exposed to nitrate contamination for at least half a century. The fate of nitrate and its distribution in the aquifer is controlled by physical and chemical processes including redox-reactions and diffusion processes in the rock matrix. Since the contribution of individual processes to denitrification is not known, we tested several modeling scenarios for their appropriateness to describe measured nitrate concentrations.

A reactive transport model based on residence time as a scaling factor was developed to simulate long-term redox evolution in the micritic limestone aquifer. The role of biotic and abiotic iron oxidation and type and content of iron-bearing minerals as electron-donors were studied in a series of modeling scenarios. Different mineral combinations and redox-reactions inside the rock matrix and within the fracture were considered.

The scenario analysis shows that observed nitrate concentrations can be described even without any biotic nitrate reduction in the rock matrix. Iron-bearing minerals (siderite and pyrite) serve as major electron donors. Therefore the model is sensitive to all processes controlling iron concentrations, e.g. oxygen input into the aquifer since the last glacial maximum (approx. 12000 years ago), which led to pyrite oxidation in the rock matrix. The location of the denitrification front depends non-linearly on iron mineral contents in the rock matrix. Results show that a mix of pyrite and siderite is essential, if only one of them is present, denitrification almost ceases. Given a certain initial mineral content of less than 2%, denitrification showed to be at maximum if fractions of pyrite and siderite are equal.