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Development of a new fully coupled biogeochemical reactive transport model to simulate microbial oxidation of organic carbon and pyrite under nitrate-reducing conditions

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Nitrate is one of the most abundant contaminants in groundwater due to wide agricultural application of nitrogen fertilizers. The EU WFD) suggests to limit the use of nitrate fertilizers and to monitor water quality with increased accuracy and frequency. However, several studies showed that applying the EU WFD regulations does not lead to improved results, as in many regions nitrate concentrations are still high or even showing increasing trends. Nitrate reduction by organic matter acting as electron donor (heterotrophic denitrification) is well proven and also pyrite is reported as important electron donor favouring nitrate reduction (autolithotrophic denitrification). Denitrification is controlled by the availability of reactive electron donors. However, the concentrations and spatial distribution of the electron donors and their specific reactivity are typically not known in detail and difficult to measure at the field scale.

Current numerical investigations of denitrification processes simulate nitrate reduction by organic carbon degradation based on the Monod approach. Pyrite oxidation is simulated at field scale with an empirical approach considering concentrations of pyrite, nitrate, and pH-values. However, current research does not account for i) effects of microbial growth and death cycles, ii) competitive oxidation of organic carbon and pyrite, or iii) transport of microorganisms. Addressing the gap in understanding the distribution and relevance of the different electron donors for long-term denitrification rates, the goal of our study was to design laboratory experiments that include all possible denitrification pathways and to develop a reactive transport model suitable to account for the complete suite of biogeochemical processes.

Laboratory experiments are analysed with a reactive transport model: i) to identify key processes driving denitrification, ii) to give sensitivities and uncertainties of the model parameters and observation data, iii) to derive key parameters that are needed to be monitored at field scale for a process-based observation of denitrification, and iv) to quantify limitations of the aquifer denitrification capacity.

Computed denitrification rates show that the key process for denitrification is oxidation of pyrite resulting in degradation rates up to 5 times higher than for heterotrophic denitrification. The reactive transport model allows to calculate relative concentration profiles of microbes along the column. During heterotrophic denitrification microbes increase up to 2.5 times after one month, then during autolithotrophic denitrification a new microbe concentration peak appears after 3 months that is 4 times above the initial microbial concentration. This microbial peak starts to move downward when the pyrite concentration starts to fall.

However, our numerical investigations demonstrate that the growth yield for heterotrophic denitrification is about two times larger than for autolithotrophic denitrification and thus the microbial energy yield is higher for heterotrophic denitrification. This might explain the observed preference of SOC compared to pyrite resulting in the temporal order of heterotrophic over autolithotrophic denitrification.

At the end of the experiment, after 5 months, about 85% of the SOC and 46% of the pyrite was depleted and in the outflow nitrate concentrations increase to 50% of the inflow concentration and thus the degradation capacity was highly limited.