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Kinetics and reactive transport of N2O in a nitrate-contaminated shallow aquifer: How to transfer static Batch Experiments to highly-transient Field Conditions?

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N2O-production and reduction within the exchange zone are highly variable in space and time and depend on complex reaction rates. The ongoing controversial discussion about the relevance of indirect N2O-emission from shallow groundwater has a high degree of uncertainty, because data interpretation is mainly based on regression and on over-simplified steady-state and homogeneous flow models. Moreover prediction models often use non-site specific data sets from literature. For realistic reactive transport modeling of N2O we derived a comprehensive site-specific data set of kinetic constants for the depth-dependent heterotrophic and autotrophic denitrification process at the Fuhrberger Feld aquifer. Parameter identification was conducted for incubation experiments using both first-order kinetics and Michaelis-Menten kinetics.
The main question is: How to transfer these kinetic rates obtained from static laboratory experiments to field conditions? For the deeper autotrophic zone we found that the incubation experiments are in good qualitative agreement with field observations, since steady-state flow conditions with nearly constant reducing redox conditions can be assumed. In contrast, N2O-production of the heterotrophic exchange zone of shallow groundwater is highly transient related to fluctuating groundwater level (GWL). Therefore, laboratory incubations of aquifer material yielded substantially lower N2O concentrations than measured in the field. Thus, the laboratory results are hardly transferable to field conditions. For the first time we develop a reactive transport model that accounts for day-scale changes of the observed GWL and for the short-term fluctuations between anaerobic and aerobic conditions in the exchange zone. We show that the two process time scales (time scale for a typical GWL-fluctuation and time for N2O-production) are responsible for N2O-production and that under certain conditions N2O- accumulation can be observed.

References

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