High-resolution Simulation of Denitrification

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Experimental Study of Denitrification

Denitrification is a process where bacteria use nitrate as electron acceptor in the absence of oxygen. It is a potential source of nitrous oxide, an important greenhouse gas. It has been shown experimentally, that denitrification is also occurring in well aerated soils. The common assumption is, that anoxic zones are located within dense aggregates in a heterogeneous soil. To test this theory, laboratory experiments with an ensemble of artificial aggregates (Figure 1) from sintered glass have been conducted. The aggregates were inoculated with bacteria from two strains capable of denitrification up to different terminal products. The temporal evolution of the concentration of different intermediate products was measured over time (Figure 3).

Modelling and Numerical Solution

Mathematically, denitrification can be modelled as a reaction-diffusion process in a complex pore geometry. To evaluate the experiments, simulations of microbial growth and sustenance in the aggregates have been conducted using high-resolution pore space geometries obtained from X-ray micro-tomography (Figure 2). The model for denitrification consists of a system of coupled reaction-diffusion equations. It was solved numerically on a parallel computer cluster. The computational efficiency of the approach was evaluated and the influence of microbiological parameters (Michaelis-Menten constants) was tested, compared and adapted according to experimental data. The results will be the basis of an improved simulation of denitrification at the (heterogeneous) sample scale and the field scale.

Figure 1: Artificial aggregate (total size ≈ 8mm) used in the experiments.

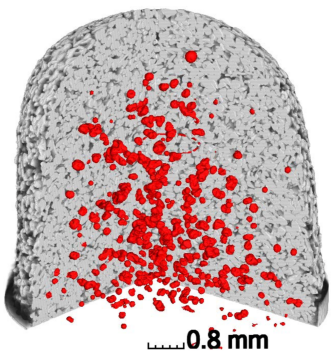

Figure 2: X-ray micro-tomography of one aggregate with some entrapped air in the generally water filled pore-space (dark grey) shown in red.

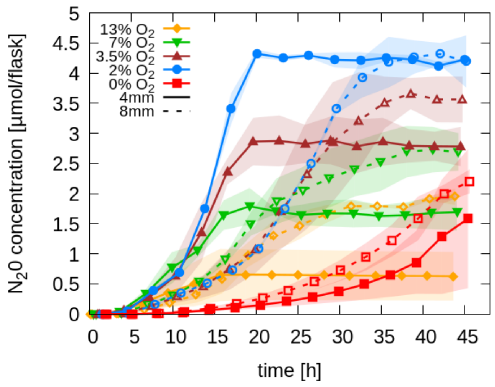

Figure 3: Temporal dynamic of the nitrous oxide concentration in the gas phase outside the aggregates during experiments with different oxygen concentrations.