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High-resolution Simulation of Denitrification

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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 different sized artificial aggregates from sintered glass and different oxygen levels were conducted. The aggregates were inoculated with Agrobacterium tumefaciens, a facultative anaerobic denitrifier with N2O as final denitrification product.

Mathematically, denitrification can be modelled as as a reaction-diffusion process in a complex pore geometry. To evaluate the experiments, simulations of microbial growth and sustenance in the aggregates were conducted using high-resolution pore space geometries obtained from X-ray micro-tomography. A new model for denitrification consisting of a system of nine coupled reaction-diffusion equations was developed, including a diffusion model with a transition between water and gas based on Henry's law.

In order to solve the occurring three dimensional, nonlinear and coupled system with a high spatial resolution numerically on a parallel computer cluster in reasonable time, an Operator Splitting approach is used for diffusion and reaction.

The computational efficiency of the approach is evaluated and the influence of microbiological parameters (Michaelis-Menten constants) is tested and the parameters are compared and adapted according to experimental data.