Understanding denitrification at the pore scale

High-resolution Simulation of Denitrification

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In Short

- Denitrification is the microbial reduction of nitrate to dinitrogen, nitrous oxide or nitrogen.
- It occurs in soils, even if they are well aerated, presumably in so called "hot spots"
- In this project denitrification in hot spots is simulated by solving a diffusion reaction problem
- As images of the pore spaces from X-ray tomography will be used, a high spatial resolution is necessary, thus HPC is needed
- First simulations with lower resolution already gave first insights into the dynamic of hotspots and could reproduce experiments qualitatively

Facultative anaerobic bacteria can use nitrate as electron acceptor in the absence of oxygen, converting it from NO_3^- to NO_2^-, NO, N_2O and finally sometimes to N_2. This process is called denitrification. N_2O (laughing gas) is an important greenhouse gas. Although denitrification has been known for 200 years, the overall process is still not well understood. The DFG research unit DASIM (Denitrification in Agricultural Soils: Integrated Control and Modelling at Various Scales) tackles this issue by an interdisciplinary approach, combining researchers from soil science, microbiology and plant nutrition as well as different modelling approaches. The project of this research unit located at Clausthal University of Technology concentrates on the simulation of denitrification at the pore scale, assuming that microbial growth and sustenance is well understood in aqueous solution. The complex production and release pattern is assumed to be mainly a consequence of unresolved pore structure and heterogeneity.

At the pore scale, the problem can be described as a reaction-diffusion problem including the chemical components substrate, oxygen, NO_3^-, NO_2^-, NO, N_2O and N_2 as well as two groups of bacteria responsible for aerobic and anaerobic respiration.

Diffusion: While the bacteria are assumed to be immobile, all chemical components are transported by diffusion in a complex pore space. From high resolution X-ray tomography scans performed by cooperation partners at the Helmholtz-Institute for Environmental Research – UFZ, the distribution of air, water and solid in a sample can be determined (initially of artificial aggregates made from sintered glass). Thus the geometry of the pore space and the distribution of diffusion coefficients is well known. At the interface between liquid and gas phase Henry's law is assumed to be valid. Solving the diffusion problem with a sufficient spatial resolution (at least 500^3 voxel) is numerically challenging.

Reaction: Microbial activity within the water-filled pores is described as a reaction system. The model for the microbial behaviour is based on Michaelis-Menten kinetics and was created in close cooperation with the microbiologists of the research unit. It includes aerobic and anaerobic respiration as well as the switch of microorganisms from aerobic to anaerobic respiration. The parameters for the reaction are determined from batch experiments with bacteria grown in pure culture by our cooperations partners at Leibniz-University Hannover. Therefore, there is no need for parameter fitting.

The first goal of these simulations is to reproduce results from experiments conducted with a single strain of microorganisms in artificial hot spots from sintered glass. The experimental results were published in [1].

For efficiency reasons the diffusion reaction system is solved with an operator splitting approach. Diffusion of each component is solved separately. For the discretisation of the diffusion equation a Method of Lines approach is used with a cell-centered Finite-Volume scheme in space and an Implicit Euler or second-order Alexander scheme in time. This guarantees a discrete maximum principle and thus positivity of the solution. A Conjugate Gradient (if the matrix is symmetric, i.e. for liquids) or BiCGstab solver (if the matrix is not symmetric, i.e. for gases) is used for the linear systems with SSOR or an algebraic-multigrid scheme as preconditioner.

The reaction system is then solved with an explicit higher-order Runge-Kutta scheme for each grid cell.

The code is written in C++ based on the Distributed and Unified Numerics Environment (DUNE, see [2]). DUNE is a powerful and flexible C++ framework for the solution of partial differential equations. It provides different grids, base functions and a variety of sequential and parallel linear solvers. It is well suited for using it in High Performance Computing. In our case, an overlapping domain decomposition is used as parallelisation approach.

On the local compute cluster of the scientific computing group at TU Clausthal simulations were conducted up to a resolution of 152^3. In order to fully resolve the spatial structure of the hotspot, a resolu-

tion of 500^3 is needed. This requires a much larger compute cluster as provided by HLRN.

WWW

https://www.mathematik.tu-clausthal.de/personen/olaf-ippisch/

More Information

[1] S. Schlüter, S. Henjes, J. Zawallich, L. Bergaust, M. Horn, O. Ippisch, H.-J. Vogel, P. Dörsch *Front. Environ. Sci.* **6**, 17 (2018). doi:10.3389/fenvs.2018.00017

[2] https://www.dune-project.org

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