Measurement and prediction of pore scale air and water phase distribution in soil using SR-µCT and LBM

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Diffusion processes in soils depend strongly on the distribution of the air and water phase at the pore scale. Water menisci may block gas transport and thus limit oxygen supply to roots and microorganisms while the air phase may act as a barrier for diffusion of nutrients and contaminants within the liquid phase by increasing diffusion path lengths. Hence, both liquid and gaseous diffusion control numerous biogeochemical reactions in soils, e.g. turnover and biodegradation of nutrients and pollutants by microorganisms.

Modelling of the air-water distribution in pores is a promising approach to assess the impact of saturation on biological functioning of soils. Lattice Boltzmann Models (LBM) have the potential to predict air-water phase distribution based on physical forces while explicitly capturing the complex pore geometries in structured soils. The LBM requires as input data knowledge of the architecture of the pore space which is easily obtained by X-ray microtomography. However, to validate modelling results also the air-water interface in unsaturated soil has to be detected. This is challenging because of the relatively low attenuation contrast between air and water compared to the attenuation contrast between mineral phase and pore space. The high photon fluxes and very good signal to noise ratios obtained with Synchrotron-based X-ray microtomography (SR-µCT) allowed us to determine the 3D configuration of water menisci at the relevant spatial scale without using contrast enhancing dopants such as potassium iodine. This provided a reference dataset for the LBM which is not obscured by modified fluid properties resulting from a dopant.

To model the air-water distribution at the pore scale an existing Two Relaxation Time Lattice Boltzmann Model (TRT-LBM) was modified by adding a classical cohesive force to build a one component two-phase flow model (Shan and Chen, 1994). The model was found to well match static one component liquid-gas theory and presents a close-to-theory equation of state, phase diagram and Laplace law (Genty and Pot, 2012). We further introduced water-solid affinity (contact angle) by adding an additional cohesive force between fluid sites and solid sites (Raiskinmaki et al., 2000). Simulated air-water phase distribution was compared with the real water configuration in a structured soil. For this purpose small soil cubes (6x6x6 mm³) were equilibrated with water at a fixed matric potential close to saturation (-5 hPa) with the aid of a hanging water column and scanned at beamline W2 (HARWI II) at a voxel resolution of 4.43 µm. Air, water and mineral phases could clearly be distinguished in the tomograms. The water in larger macropores showed the expected characteristic configuration as water menisci which is due to wetting properties of the solid surface and capillary forces of the pore space (Fig. 1).

On the basis of the 3D pore geometry, we filled the pore with a fluid of initial homogeneous density calculated from the observed mean saturation and let the system evolve subject to cohesion forces and full wetting of the pore walls. Spontaneous phase separation initiated from interactions with the solid walls occurred in the pore. When equilibrium was reached, the calculated air bubble was compared to the tomographic one with a surprisingly high level of accuracy (Fig. 2). The results obtained from this study proof the ability of LBM simulations to predict air-water phase distributions in complex porous media such as soil. This is very promising as LBM in combination with other modelling approaches allows us to study the influence of water configuration as a function of matric potential on carbon turnover processes which is part of on-going research.
Figure 1: Tomograms showing the mineral matrix (medium to light grey), liquid water phase within larger pores (light grey) and air (dark grey). Due to the wetting properties of the solid phase and capillary forces the liquid water configures as characteristic water menisci within the larger air filled pores.

Figure 2: 3D view of the gas bubble inside a single pore of 250µm diameter obtained from the SR-μCT measurement (left top figure) and simulated by the LBM (right top figure). Below are 2D sections of the pore in the plane (x,y) at two different z coordinates The solid phase is not drawn. The gas phase is shown in blue and the liquid phase in orange.

References