LATTICE BOLTZMANN METHOD FOR AIR-WATER DISTRIBUTION MODELING AT THE PORE SCALE

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In unsaturated porous media, processes such as diffusion or reactive transport of pollutants including biodegradation mechanisms are strongly dependent on the air-water distribution in the pores. Thus, air phase can act as a barrier to those processes and modify the pathways for pollutants, nutrients or micro-organisms leading to unexpected non linear impact of the saturation level on these processes as well as threshold effects. The modeling of the air-water distribution in pores is thus the first step needed to access the impact of saturation on the biological functioning of soils.
In order to model the air-water distribution at the pore scale, lattice Boltzmann methods appear as an interesting alternative because of their ability to capture the complex geometry of real soil structures in a simple way and their simple programming rules that allow to add or modify physical processes through the introduction of corresponding forces. We started from an existing Two Relaxation Time (TRT) lattice Boltzmann model and added a classical cohesive force to build a one component two-phase flow model. The model was found to well match static one component two-phase flow theory and presents a close-to-theory equation of state, phase diagram and Laplace law. We introduced water-solid affinity (contact angle) by adding an additional cohesive force between fluid sites and solid sites.
In order to test our LB model ability to simulate real air-water distribution in soil pores, we compared the results to selected 3D computed tomographic (CT) images of air-water distribution measured in a small soil cube (6x6x6 mm3). The soil cube was equilibrated at a fixed water potential close to saturation (- 5 hPa) and the monochromatic beam of Synchrotron-based-radiation (SR) achieved such a precise density level that soil, water and air were clearly distinguishable. The measurements were performed at the SR-µCT facility operated by the GKSS research centre at HASYLAB (Hamburger Synchrotron Strahlungslabor) belonging to the DESY (Deutsches Elektronen Synchrotron) in Hamburg (Germany). On the basis of the 3D pore description, we filled the pore with a fluid of mean density according to the observed mean saturation and let the system evolve subject to cohesion forces and full wetting of the walls. At this saturation, spontaneous phase separation occurred in the pore. When equilibrium was reached, the calculated air bubble was compared to the tomographic one with an unexpected high level of accuracy.