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Water and air distribution in 3D computed tomography images to use in silico studies of fungal resilience and biodiversity in soils

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Little is known about the behaviour and spread of fungi in soils despite the relevant role they play in the ecosystems. In silico studies with appropriate pore scale models can help untangle the effect of the soil structure in the resilience and biodiversity of the fungal communities and, by extension, of the soil system itself. Furthermore, the water content of the soil affects the connectivity of the water and gas phases, which may impact unevenly the different microbial communities found in soils, e.g., fungi prefers air filled pores while bacteria requires water for growing. The change in the microbial communities ultimately may affect the ecosystem services that the soil is delivering. To date, despite the enormous development of the X-ray computed tomography technology, the microscale distribution of water is still very difficult to obtain. Nonetheless, modelling approaches at pore scale has been developed to this end. Among them, the lattice-Boltzmann approach has demonstrated to produce physically accurate water distributions in natural and reconstructed soils. The aim of the present contribution is to obtain a new set of 3D images of air-water interfaces at two water saturation levels (80 and 20%) in a material constituted of soil aggregates repacked at different densities. The water levels chosen allow alternative images having either a well-connected gas or water phase. The soil was repacked in triplicate at 5 bulk densities: 1.2, 1.3, 1.4, 1.5, and 1.6 g cm^{-3} and packed into cylinders, 50 mm in diameter and 40 mm high. For each resulting soil column angular-projection images were collected using a Metris X-Tek HMX micro-tomography system. Three-dimensional volumetric data sets were reconstructed with the VGStudio MAX using a filtered back-projection algorithm and a voxel (volumetric picture element) size of 24 μm. From the centre of each soil-sample image we selected a cube of 512x512x512 voxels. The water-air distributions in the images were computed using a two-phase Two Relaxation Times Lattice-Boltzmann Model described in Genty and Pot (2013, *Transp Porous Media* 96:271-94). The interface water-air was obtained by thresholding the water particles distribution at the end of the computations using the theoretical density value of 1.225 as assumed in the literature. An iterative procedure changing the initial amount of water particles in the image's pore space was developed to obtain thresholded images with a water content in the range of $SW_T \pm 0.5$, where SW_T is the water saturation level (%) targeted in the simulation. The development of the procedure described was motivated by the existence of unconnected pores naturally generated during the compaction of the soil. The water saturation levels of 80 and 20 % allow a good connectivity of the water and air phases, respectively. With the saturation level of 80 %, the connectivity of the water phase relative to the connectivity of the pore space remains approximately constant. However, with the saturation level of 20%, the connectivity of the air phase relative to the connectivity of the whole pore space decreases with the compaction increase.