



# Three-dimensional distribution of water and air in soil pores: Comparison of two-phase two-relaxation-times lattice-Boltzmann and morphological model outputs with synchrotron X-ray computed tomography data



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## ABSTRACT

Recent progress in the understanding of soil microbial processes at micrometric scales has created a need for models that accurately predict the microscale distribution of water, and the location of air–water interfaces in pores. Various models have been developed and used for these purposes, but how well they fare against real data has yet largely to be determined. In this context, for the first time, this article compares the prediction of two of these models to experimental data obtained on soil material. The distribution of water and air in soil samples constituted of repacked aggregates, equilibrated at three matric potentials (−0.5 kPa, −1 kPa and −2 kPa), was measured via synchrotron X-ray computed tomography at a resolution of 4.6 μm. Water distribution was simulated by a two-phase lattice Boltzmann model (LBM) and a morphological model (MOSAIC). Results indicate that, when one lifts the assumption, motivated by capillary theory, that a pore can drain only if a connecting pore is already full of air, MOSAIC gives an acceptable approximation of the observed air–water interfaces. However, discretization of pores as geometrical primitives causes interfaces predicted by MOSAIC to have nonphysical shapes. By contrast, LBM is able to predict remarkably well the location of air–water interfaces. Nevertheless, given the huge difference in computing time (minutes versus tens of hours) required to run these two models, it is recommended that further research be carried out on the development of both, in parallel.

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## 1. Introduction

Over the last decade, a significant body of work has been devoted to the response of soils, and especially of the vast stock of organic matter they contain, to changing climatic boundary conditions or to different agricultural practices. In that context, it has become increasingly clear that detailed knowledge is required of the different physical, (bio)chemical, and biological parameters that determine the activity of microorganisms at the microscopic scale. The demand for this information is not new. Several soil microbiologists have pointed

it out already for more than half a century [1]. However, not much could be done by way of a response until roughly 15 years ago, when significant technological breakthroughs allowed the geometry of the pore space in soils to be visualized, and the spatial heterogeneity of a number of chemical and mineralogical constituents of soils to be quantified at micrometric scales commensurate with fungal hyphae and even the most minute of bacteria or archaea [6–9,40,48].

The availability of such microscopic-scale data, combined with the anticipation of further advances in the very near future in terms of both laser and X-ray technologies opening up even brighter prospects, has prompted researchers to develop an array of sophisticated models at the pore scale. Among them, lattice-Boltzmann models (LBM) [20,29] are able to describe water, solute, and particulate transport in the interstitial space of soils, as well as the shape of

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air-water interfaces [13,53], without having to invoke the kind of simplifying assumptions about the geometry or topology of soil pores that were typical of earlier generations of models, based on traditional partial differential equations or capillary network idealizations. Similarly, agent- or individual-based models describe quantitatively the growth and metabolism of microorganisms much more realistically than traditional models, based on descriptions of population dynamics, and are able to account in great detail for the effects of the relative spatial distributions of fungi [13], bacteria [15,18,27,30], and the organic matter on which they feed. At the moment, the development of each of these different models is moving forward, in parallel with interdisciplinary efforts to combine them in order to describe various types of micro-scale scenarios and assess the nature of emergent properties of soil systems [13].

As with any type of modeling, part of the work of developing microscopic-scale models of soil processes consists of ensuring that model outputs are adequately approximating the reality they purport to represent. This is particularly important in the case of the spatial distribution of the aqueous phase in the pore space, because this distribution directly impacts the connectivity of liquid-filled pores as well as the rate and extent of air flow, all of which in turn influence directly the distribution and activity of microorganisms. A possible first step to assess the adequacy of a particular model to simulate water distribution in the soil pore space is to compare the results with other models, to make sure that there is general consistency among various alternative descriptions. Vogel et al. [51], for example, compare the outputs of pore network and morphology models with the predictions of a lattice-Boltzmann code, based on structural data relative to a homogeneous sintered borosilicate glass sample. Ideally, however, a further step in the evaluation of a given model should involve the comparison of model outputs to experimental data. Sukop et al. [46] measured the distribution of non-miscible phases in columns of quartz sand at a resolution of 20  $\mu\text{m}$ , and tried to simulate the results with a multicomponent, multiphase LBM. The outcome is generally satisfying, in terms of bulk concentrations of the different phases, even though detailed analysis of individual pores reveals numerous discrepancies between simulations and observations. A similar exercise has yet to be carried out with an actual soil sample, however.

The fact that attenuation of X-rays by water is quantitatively not very different from that by organic matter makes it very difficult experimentally to distinguish water from soil constituents under many circumstances. To palliate this difficulty, some authors have used other liquids, like decane, instead of water [43], or doped Soltrol, a NAPL, with a marked contrast with water [3], or they have added various contrast agents to the water, to modify its X-ray attenuation [46,49]. Another option is to work with porous media that do not contain any organic matter. For example, Brusseau et al. [10] and Culligan et al. [12] show air-water interfaces in 3D computed tomography (CT) images of repacked sand and glass beads, respectively, at a resolution of about 12  $\mu\text{m}$  using synchrotron X-ray CT. More recently, Andrew et al. [4] show detailed air-water interfaces and are able to successfully measure contact angle of  $\text{CO}_2$ -brine interfaces onto the solid surface of limestone at a small resolution of 2  $\mu\text{m}$ .

Working with a real soil material, Carminati et al. [11] adopt yet another approach, in that they focus on the water that occupies part of the volume in larger pores, located between aggregates. They are able under these conditions to clearly observe pendular rings of water between two clay-loam soil aggregates at a resolution close to 6  $\mu\text{m}$ . Tippkötter et al. [47] adopt a similar focus, in undisturbed soil samples, and are able with a table-top X-ray CT scanner to visualize the presence of water films coating the inner surfaces of meso- and macropores. These data obtained by Carminati et al. [11] and Tippkötter et al. [47], or equivalent CT data obtained in other soils, could in principle be used to assess whether existing pore-scale models of water distribution in soils are adequate.

In this general context, a first objective of the research reported in the present article was to obtain a new set of 3D images of air-water interfaces at a few  $\mu\text{m}$  resolution at defined matric potentials in a material constituted of repacked soil aggregates. A second objective was to simulate air-water distribution in this material using two mathematical models to find out which approach is the most promising in order to describe quantitatively the retention of water in soils. The two models, namely a two-relaxation-times (TRT) lattice-Boltzmann model, and the pore morphology model of Monga et al. [35], were chosen because of their contrasting features. The former model is capable of describing very realistically the physics of phase separations, as well as the hydrophobic or hydrophilic properties of the soil solid phase [20] but it presents the relative disadvantage of being very demanding in terms of computational resources. By contrast, the far simpler morphology-based model provides a compact description of pore space and has lower computational costs, but it presents the possible drawback of relying on a simplified description of soil physical laws.

## 2. Material and method

### 2.1. Soil preparation

Soil samples were obtained in the La Cage field site (Versailles, France) from the surface horizon of a silt loamy Albeluvisol [14] with 17% clay, 56% silt and 27% sand. The soil was passed through a 2 mm sieve, and soil aggregates between 2 and 3.15 mm in size were collected from the coarse fraction. The gravimetric moisture content of the aggregates was adjusted at 0.205  $\text{kg kg}^{-1}$ , which was hypothesized to amount to 80% of 'field capacity' (defined by a matric potential of  $-32\text{ kPa}$  or  $\text{pF}=2.5$ ). The aggregates were then packed uniformly at a bulk density of 1200  $\text{kg m}^{-3}$  into cylinders, 50 mm in diameter and 40 mm high. The resulting soil columns were subsequently sawed to about 8 mm thick slices. Nine  $6 \times 6 \times 8\text{ mm}^3$  soil cubes were sampled out of each slice with the help of a razor blade in order to minimize disturbance during cutting. The samples were stored in a cold chamber at 4°C before further processing.

### 2.2. Miniaturized suction device

We developed a miniaturized experimental suction device to equilibrate the small soil cubes at fixed matric potentials close to water saturation. The design was specifically conceived to enable measurements at the Synchrotron radiation microtomography (SR- $\mu\text{CT}$ ) facility. Nine syringes, 1 cm in diameter, were half-filled with 90–125  $\mu\text{m}$ -diameter glass beads, and subsequently connected at the bottom end to a hanging water column. Each soil cube was placed on top of the glass beads in a syringe and after matric potential was equilibrated, the sample was secured in place with a parafilm pellet to prevent any movement during scanning. After that, the syringes were sealed at the top with parafilm. The volume of the air phase above the soil cubes was thus kept as small as possible to prevent evaporation during the tomography scans.

The soil cubes were first equilibrated at a matric potential of  $-2\text{ kPa}$  for two days using de-aired water. Then, all soil cubes were slowly saturated and were kept equilibrated at 0 kPa for 1 h in order to remove residual entrapped air. The time duration of this process was initially longer but several cubes collapsed and the whole procedure was repeated with new cubes for a shorter time. Then the syringes, in series of three, were directly equilibrated at specific matric potentials of  $-0.5\text{ kPa}$ ,  $-1\text{ kPa}$ , and  $-2\text{ kPa}$ , respectively, for 24 h. For scanning, the syringe was detached from the hanging water column after closing a valve at its bottom tip. Thus, each soil cube was imaged at only one matric potential, with three replicates for each matric potential.

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