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Prediction of capillary hysteresis in a porous material using lattice-Boltzmann methods and comparison to experimental data and a morphological pore network model

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ABSTRACT

In this work we use two numerical methods which rely only on the geometry and material parameters to predict capillary hysteresis in a porous material. The first numerical method is a morphological pore network (MPN) model, where structural elements are inserted into the imaged pore space to quantify the local capillary forces. Then, based on an invasion–percolation mechanism, the fluid distribution is computed. The second numerical method is a lattice-Boltzmann (LB) approach which solves the coupled Navier–Stokes equations for both fluid phases and describes the dynamics of the fluid/fluid interface. We have developed an optimized version of the model proposed in [Tölke J, Freudiger S, Krafczyk M. An adaptive scheme for LBE multiphase flow simulations on hierarchical grids, Comput. Fluids 2006;35:820–30] for the type of flow problems encountered in this work. A detailed description of the model and an extensive validation of different multiphase test cases have been carried out. We investigated pendular rings in a sphere packing, static and dynamic capillary bundle models and the residual saturation in a sphere packing.

A sample of 15 mm in diameter filled with sand particles ranging from 100 to 500 μm was scanned using X-rays from a synchrotron source with a spatial resolution of 11 μm. Based on this geometry we computed the primary drainage, the first imbibition and the secondary drainage branch of the hysteresis loop using both approaches. For the LB approach, we investigated the dependence of the hysteresis loop on the speed of the drainage and the imbibition process. Furthermore we carried out a sensitivity analysis by simulating the hysteretic effect in several subcubes of the whole geometry with extremal characteristic properties. The predicted hysteretic water retention curves were compared to the results of laboratory experiments using inverse modeling based on the Richards equation.

A good agreement for the hysteresis loop between the LB and MPN model has been obtained. The primary and secondary drainage of the hysteresis loop of the LB and MPN model compare very well, and also the experimental results fit well with a slight offset of 10% in the amplitude. Differences for the first imbibition have been observed, but also large differences between two different experimental runs have been observed.

1. Introduction

In multiphase flow systems of two immiscible phases like air and water in a porous medium like a soil the flow and transport properties depend on the amount and the spatial distribution of the phases within the pore space. On the pore scale the phase distribution is controlled by the capillary forces depending on pore size, surface tension, and wettability. For that reason, the relationship between capillary pressure and liquid saturation (P_c–S_w relationship) is of high importance for the prediction of water flow and solute transport. Unfortunately, this relationship is ambiguous and depends on the preceding wetting and drainage processes. This phenomenon is denoted as hysteresis and was first documented by Haines in [2]. It is caused by different pore structures relevant for drainage and wetting processes. While the drainage of a large pore body may be prevented by surrounding small pore throats, the wetting of fine pores above a large pore is hampered by the weak capillary forces in the wide body. Additional hysteresis effects are caused by a difference in advancing and receding

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contact angle [3] and the inclusion of air in a first wetting process. Due to the inclusion of air in a wetting process, the water saturation after the primary drainage of a completely saturated porous medium remains smaller than the porosity for any following wetting processes. After a few drainage and wetting cycles, two bounding curves, denoted as main wetting and main drainage branch, can be determined. All processes within these bounding curves are denoted as scanning curves. To model water flow and solute transport correctly, the hysteretic relationship between capillary pressure and fluid saturation must be taken into account [4,5]. To quantify the hysteresis and the scanning curves, different approaches can be distinguished. On the macroscopic scale, the shape of the scanning curves can be deduced from the main wetting and drainage curves. With such a similarity or scaling approach, the shape of any scanning curve can be described [6–8]. While most approaches are based on the main drainage and wetting curve, it is possible to compute the whole hysteresis loop based on a single main curve [9]. In addition to these scaling approaches, two new descriptions on the macroscale based on the hysteron (the simplest hysteretic system described by an operator [10]) and the quantification of the continuous and non-continuous fluid phases [11] were recently introduced.

Secondly, the range of liquid saturation as a function of capillary pressure for wetting and drainage processes can be determined using pore network models. With a pore model consisting of a pore-body and a pore-throat distribution, the hysteresis of the hydraulic functions can be reproduced. The first pore network approaches were limited to cylindrical pore throats on a rectangular lattice [12]. To enhance the flexibility and to develop more realistic pore network models, different throat shapes [13] and other lattice types [14] were introduced. The drawback of these approaches is the uncertainty of the pore-throat and pore-body distribution function which are obtained from fitting, based on measured retention functions.

Alternatively, the pore size distribution can be deduced from images of the pore space. In Øren et al. [15] the reconstructed pore space is transformed into a pore network that is used as input to a two-phase network model. Based on this work Valvatne et al. [16] constructed a network with the same topology as a scanned sandstone sample and modified the size distribution to obtain the same permeability. To apply this network to other media, the main drainage branch must be fitted to describe the wetting branch.

Finally, to predict the hysteresis loops without any fitting based on the measured pore space geometry, a direct numerical simulation of the two-phase Stokes problem can be performed. A suitable method for this task is the lattice-Boltzmann method. Pan et al. [17] applied successfully a lattice-Boltzmann approach based on the Shan–Chen [18] multiphase extension for a packing of glass beads and compared the results to experiments. Nevertheless this approach needs numerical experiments to determine the material parameters. In a later study [19] the focus moved to the determination of relative permeabilities. By using a multiple-relaxation-time (MRT) lattice-Boltzmann approach, more realistic capillary numbers could be reproduced. In [20] the primary drainage curve (without hysteretic effects) for a porous medium was simulated by a lattice-Boltzmann approach. The medium consisted of sintered glass and the geometry was obtained by tomography. The LB results were compared to the results of a full-morphological and a pore network model and a good agreement for the three models was observed. However, these results have not been compared to experimental data.

In this study we use a MPN model and an LB approach to predict hysteresis in the capillary pressure–saturation relationship for the measured pore structure of a sand sample. The LB approach is based on the multiple-relaxation-time (MRT) model with an optimized multiphase extension given in [1] and further optimized for Stokes flow in porous media. This approach permits higher viscosity ratios and lower capillary numbers than previous LB multiphase extensions. To obtain a geometric representation suitable for the LB solver, the surface of the sand particles was reconstructed from the voxel matrix by a marching-cube algorithm and the description of the fluid behavior at the solid walls was improved by the accurate determination of the distance of the fluid nodes to the particle boundaries [21]. Also the numerical resolution of the setups was higher as in previous studies. An extensive validation for the model developed has been carried out. Complex test cases like pendular rings, a (dynamic) capillary tube bundle and the residual water saturation in a periodic array of spheres are set up and analyzed in detail.

We compare our predictions for the capillary hysteresis using the MPN and LB model to laboratory measurements, where inverse modeling based on the Richards equation was applied to compute the drainage and imbibition curves. In addition, a few equilibrium states between water saturation and capillary pressure were analyzed to validate the results of the inverse modeling.

Furthermore we carried out a sensitivity analysis by simulating the hysteresis in several subcubes of the whole geometry with extremal characteristic properties.

The paper is organized as follows: In Section 2 the laboratory experiments and the methods to determine the hysteresis curves by an inverse fitting procedure are described. Section 3 introduces the morphological pore network model and the results for the capillary hysteresis. Section 4 discusses the lattice-Boltzmann approach and the results for the saturated permeability and the capillary hysteresis. In Section 5 the results for the different models are compared and conclusions are given. In Appendix A a detailed description of the lattice-Boltzmann model is given and in Appendix B various test cases for multiphase flows are carried out to validate the lattice-Boltzmann method.

2. Material, experimental setup and inverse parameter fit

2.1. Materials and samples

To predict the fluid distribution within the pore structure we scanned a sand sample of 1.5 cm in diameter and 1 cm in height using X-rays from a synchrotron source. The tomography was carried out at the Hamburger Synchrotron Laboratories (HASYLAB) in Germany. The particle size of the sand material ranged from 0.1 to 0.5 mm. Based on the imaged X-ray attenuation the density distribution of the solid material can be reconstructed. The reconstructed density map was segmented into a black and white image of pore space and solid phase with a voxel resolution of $r_v = 11\ \mu m$. A voxel (*vo*lumetric pi*xel*) is a volume element, representing a value on a Cartesian grid in three-dimensional space and is commonly used as the basic unit of a three-dimensional image. The tomography of this sand material is described in more detail in [22]. To avoid effects at the boundary between the sand and the container, a cube from the center of the cylinder with 800^3 voxels was analyzed with respect to geometrical properties and fluid distribution. In case of the lattice-Boltzmann approach the computation of the hysteresis in the relationship between capillary pressure and liquid saturation is very time consuming and was determined for a subcube with 200^3 voxels. The results may depend on the chosen section within the whole sample with 800^3 voxels. To estimate the sensitivity of the results on the chosen section, we focused on two subcubes with extremal properties. For that purpose, we computed characteristic geometrical properties for various subcubes. We shifted the origin of the analyzed subcube in intervals of 20 voxels in *x*-, *y*- and *z*-direction from position 0,0,0 to 600,600,600 within the large image. Totally, $31^3 = 29{,}791$