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Prediction of capillary pressure-saturation relationship for primary drainage in a 3D fibrous porous medium using volume-of-fluid method

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ABSTRACT

The unsaturated flow through fibrous porous media at the macroscale is typically described using the Richards equation which requires constitutive relations for capillary pressure and relative permeability as a function of liquid saturation. In literature, these constitutive relations are typically estimated using reduced-order modeling approaches such as pore-network (PN) models, full-morphology (FM) method etc. In this paper, we determine quasi-static capillary pressure-saturation relationship (P_c-S) for primary drainage in a 3D isotropic fibrous medium by performing direct numerical simulations (at microscale) with the volume-of-fluid (VOF) method, which takes into account the detailed description of the pore structure and interface dynamics. As a first step, the accuracy of the VOF method was verified by simulating a test case of quasi-static drainage between two cylinders. Next, a grid-convergence study was performed to determine the optimal grid resolution required for the 3D simulations of quasi-static drainage. Using this grid, the P_c-S relationship for primary drainage in an isotropic fibrous structure was calculated from the direct simulations, and the results were compared with the P_c-S estimated using full-morphology method, which is a quasi-static reduced-order geometric approach. In the VOF method, no modeling assumptions are made on the geometry of the pore structure and the liquid propagation, and thus, the results from direct simulations can be used to gain insights into the limitations of the reduced-order models.

1. Introduction

Fibrous porous materials are utilized in a variety of applications such as sanitary products, performance apparel and drug delivery patches, etc., owing to their softness, high mechanical strength and unique properties in absorbing, storing, and releasing fluids [1,2]. As engineered fibrous materials become increasingly sophisticated, a fundamental understanding of the physical processes involved in unsaturated flow through fibrous materials is imperative for successful product design and development [3,4]. Traditionally, unsaturated flow through porous media at the macroscale is described using Richards equation [5].

Richards equation for unsaturated flow:

For two-phase flow through porous media, modified Darcy's law (Buckingham–Darcy law) in the absence of gravity is formulated as

$$q = -\left(\frac{kk_r(S)}{\mu}\right)\nabla P_c(S). \tag{1}$$

Here, q is the specific discharge or volumetric flow rate per unit area perpendicular to flow direction, k is the intrinsic permeability, k_r is the relative permeability (a dimensionless measure of the effective permeability of that phase), μ is the dynamic viscosity of the fluid, P_c is capillary pressure which is the pressure difference across the interface between two fluids, and S is the wetting-phase saturation. Combining the modified Darcy equation with the continuity equation (mass balance) results in the well-known Richards equation [5], which can be solved to obtain medium's saturation as a function of time and space,

$$\frac{\phi\partial S}{dt} = -\nabla.\left[\frac{kk_r(S)}{\mu}\nabla P_c\right] \tag{2}$$

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Here, ϕ is the porosity of the medium. It is important to note that both relative permeability and capillary pressure are dependent on liquid saturation (S) of a porous medium.

In order to predict liquid transport at the macroscale, Richards equation requires two constitutive relations: capillary pressure (P_c) and relative permeability (k_r) as a function of liquid saturation (S) [4]. These constitutive relations are usually determined from capillary desaturation experiments, which are cumbersome to perform. The desaturation experiment starts with a porous medium that is fully saturated with the wetting phase. The wetting phase is drained out of porous medium in a quasi-static manner by either injecting a non-wetting phase or by incrementally increasing the pressure of the non-wetting phase reservoir. This process is referred to as *primary drainage*. Following primary drainage, the direction of saturation change is reversed wherein the wetting-phase is imbibed into the system by displacing the non-wetting phase — this process is referred to as *primary imbibition*. Subsequently, above drainage-imbibition process is repeated to determine capillary pressure-saturation relationship during secondary drainage, secondary imbibition followed by the intermediate scanning curves.

Pore-scale Modeling: In order to estimate the constitutive relations needed for the macroscale models, various microscale modeling approaches such as pore-network (PN) models, full-morphology (FM), lattice Boltzmann (LB), and smoothed particle hydrodynamics (SPH) methods have been used in the last two decades [6–13]. These numerical approaches differ in the amount of input data required, effort of data processing, and prediction potential [12]. Among these microscale modeling methods, PN modeling is the preferred method in literature as it is computationally less expensive, and thereby allows for modeling of larger domain sizes than possible with the other microscale approaches. However, in the PN method, the pore-space is idealized using primitive geometries and the fluid flow propagation is governed by simple set of rules [12]. Unlike the PN method, the FM method allows for a detailed representation of the porous geometry, and morphological openings are used to determine the flow (or open) paths inside the pore-space [14]. One disadvantage of the FM method is that it neglects the complex interplay between the various forces encountered during dynamic liquid propagation processes in the porous media [6,11,12,14]. In recent times, rapid increase in computing power and the development of robust numerical algorithms have enabled detailed numerical simulations of fluid flow through porous micro-structures using SPH and LB methods. The SPH and LB methods allow for sub-pore resolution and honor conservation equations in the appropriate limit [15–17]. However, the surface tension and contact angle are commonly implemented as special interaction forces acting between different particles and lattice nodes in SPH and LB methods, respectively and require calibration in some cases [18]. Also, porous structures like fibrous media pose an additional challenge to SPH and LBM methods, as capturing tortuous flow paths accurately would require using a large number of particles or a very fine grid.

An alternative to the PN, FM, SPH and LB microscale approaches is to perform direct numerical simulations using the finite-volume based Volume-of-Fluid (VOF) method. The VOF method relies only on conservation principles and solves a system of equations to model the flow field evolution of two or more immiscible fluids [18–22]. Unlike the other microscale modeling approaches, VOF method allows for explicit description of interface dynamics by directly including the effects of surface tension at the interface, and the wall adhesion between the wetting liquid and solid fibers (in the form of contact angle) [18,19]. Since no modeling assumptions are made on the geometry of the pore structure and flow propagation, direct numerical simulations with VOF method are computationally challenging but will provide valuable insight into the multi-phase flow dynamics at the porescale. The results from direct simulations can be used to understand the limitations of the reduced-order models (such as pore-network models, etc.), and for their calibration; verified reduced-order models can be used to study physical problems with larger length and time scales. To the best of authors' knowledge, no study has been reported using the VOF method to determine capillary pressure-saturation (P_c-S) relationship in a fibrous porous medium.

In this paper, we present the quasi-static P_c-S relationship for primary drainage in a 3D virtual isotropic fibrous structure determined using the finite-volume based VOF method. Two-phase flow simulations at the microscale were performed using the VOF method employed in OpenFOAM, an open-source CFD code (OpenCFD Ltd., v 2.0, www.openfoam.org). The accuracy of the two-phase calculations was established by simulating a test case of quasi-static drainage between two cylinders, and the numerical results were compared with the analytical solution published in the literature. The quasi-static P_c-S relationship for primary drainage in an isotropic fibrous structure was determined from the direct numerical simulation with VOF method. The results from VOF method were compared with the P_c-S relationship estimated using FM method (a reduced-order approach).

2. Methodology

The first part of this section presents the details of the construction of a 3D isotropic fibrous structure, following which we describe the conservation equations of the VOF method, and the boundary conditions used in the two-phase flow simulations. Finally, the computational grid generation is presented.

2.1. Generation of 3D virtual isotropic fibrous structure

A 3D virtual isotropic fibrous structure with a domain size of 2 mm ×2 mm × 1 mm was constructed using the commercial software GeoDict, a voxel-based code (Math2Market GmbH, GeoDict2012R1, www.geodict.com). The fiber diameter and porosity were kept constant at 50 μm and 0.8, respectively. In GeoDict, the fiber orientation distribution was controlled by a density function $p(\psi)$ defined in polar coordinates as,

$$p(\psi) = \frac{1}{4\pi}\left(\frac{\beta \sin\psi}{(1+(\beta^2-1)\cos^2\psi)^{3/2}}\right) \tag{3}$$

where, β is the anisotropy parameter which controls the fiber orientation of the micro-structure generation, and $\psi \in [0, \pi)$ is the through-plane angle [14]. Due to assumed isotropy in the xy-plane, the density function in Eq. (3) depends on through-plane angle only [14], and the fiber orientation is controlled by the value of β; for an isotropic structure, β is equal to unity. Fig. 1 shows the isotropic structure constructed in this study. The virtual isotropic structure constructed in GeoDict software was exported as a stereo-lithography (STL) file to create computational grids (described in Section 2.3) needed for the two-phase flow simulations.

2.2. Two-phase flow simulations: Volume-of-Fluid (VOF) method

Transient 3D simulation of quasi-static drainage of a wetting liquid through fibrous structure was conducted using the VOF method. The VOF method is a fluid fraction-based interface-capturing technique used for modeling the flow of a system of two or more incompressible, immiscible fluids [19,23,24]. The method is based on a whole-domain formulation that treats a two-fluid system as a single-fluid system with space-dependent physical properties. In the conventional VOF method, the continuity equation (Eq. (4)), momentum conservation equations (Eq. (5)), and a