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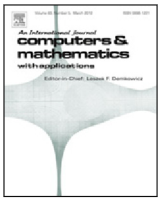

Three-dimensional lattice Boltzmann simulations of high density ratio two-phase flows in porous media

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ABSTRACT

A three-dimensional multiphase lattice Boltzmann model is implemented to study the spontaneous phase transport in complex porous media. The model is validated against the analytical solution of Young's and Laplace's laws. Afterward, three-dimensional porous layers are randomly generated to investigate droplet penetration into a substrate, liquid transport in a porous channel as well as extraction of a droplet from a porous medium. Effects of several geometrical and flow parameters such as porosity, density ratio, Reynolds number, Weber number, Froude number and contact angle are considered. A parametric study of the influence of main non-dimensional parameters upon the impact of liquid drops on permeable surface is performed. Results show that while increasing Froude number causes spreading of the droplet on the surface, increasing Reynolds number, Weber number, porosity and liquid-air density ratio will enhance the penetration rate into the surface. Furthermore, increasing the contact angle decreases both the spreading and the penetration rate at the same time. In the same way, for the liquid transport in a porous channel, it is found that increasing the porosity and Reynolds number will result in increasing penetration rate in the channel. For the extraction of a droplet from a porous medium, it is shown that by increasing the gravitational force and/or porosity the droplet extracts faster from the substrate.

1. Introduction

Multiphase flow in porous media is of both industrial and fundamental interests. Typical applications can be found in oil and gas transport in rock shells, groundwater flows, composite manufactories, ink-jet printing and coating among others [1–3]. Although most of physical phenomena engaged in such applications are micro/meso-scale, they are classically treated as macro-scale phenomena [4,5] where mass, momentum and species balances are solved along with a constitutive equation such as Darcy's law and its extension for multiphase flows [6,7]. This methodology, however, has difficulties in considering the complex porous media morphologies with different heterogeneities and requires some inputs for semi-empirical equations, e.g. permeability or wetting. In addition to the above-mentioned problem, in conventional Computational Fluid Dynamics (CFD) techniques, in order to accurately capture the dynamic phase interfaces (i.e. fluid–fluid and/or fluid-solid), a proper use of an interface tracking method such as Level Set (LS) and/or Volume of Fluid (VoF) is indisputable [8,9] which bring further complications at pore-scale. Even the macroscopic meshless methods that inherently can capture the dynamic

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interfaces [10–12] may not always realize the effects that are associated with the micro-scale structure [13,14]. Therefore, the use of micro/meso-scale numerical tools became inevitable part of pore-scale modelling in the last two decades [15].

Lattice-Boltzmann Method (LBM) is one of the promising and efficient numerical tools for the simulation of fluid mechanics problems at pore-scale level. LBM consists of finite number of fictitious particles, represents an ensemble of molecules, with a given distribution on a discrete lattice mesh. The fluid system evolution is governed by microscopic interactions between these particles based on mesoscopic kinetic equations which results in particle weight redistributions on the same lattice. The macroscopic variables are then calculated through the moment integration of these distribution functions. Due to its particular nature and its local dynamics, LBM shows some advantages such as facility in implementation and parallelization, handling complex geometry, incorporating microscopic interactions, and inherently tracking the dynamic interface contact line, over conventional CFD techniques. Therefore, LBM attracts many attentions for simulations of the pore-scale phenomena in the last decade [15].

For multiphase flow in porous channels many works have been conducted in the last two decades. Among others one can mention the followings; Shan and Chen (SC) [16] proposed a multi-phase and multi-component LBM to simulate fluid flow in simple, e.g. micro-channel, and complex geometry, such as a porous medium. Their model was adopted for a gas–liquid phase change where each component was treated to be immiscible with the others. Angelopoulos et al. [17] proposed a Swift free-energy-based single component multiphase (SCMP) LBM model to simulate vapour-fluid flow in porous media. They studied the critical flooding phenomena under strong wettability conditions in a pore structure, such as formation of thin films and snap-off in narrow throats. Pan et al. [18] simulated dynamic distributions of the non-wetting phase during primary drainage by using multi component multiphase (MCMP) SC model. To relieve the numerical stability and accuracy issues of Pen et al.'s simulation, Li et al. [19] extend the multiple-relaxation-time Lattice Boltzmann model of MCMP SC.

Hao et al. [20] conducted free-energy LBM simulation of a gas diffusion layer (GDL) in a packed-sphere bed. They studied the effects of phase wettability, relative permeability of a porous material and its anisotropy on the non-wetting phase saturation. Mukherjee et al. [21] simulated the two-phase flows phenomena in the porous media of a proton exchange membrane fuel cells (PEMFC). They rigorously studied the influence of structure—wettability on the underlying two-phase behaviour and flooding dynamics in porous channels. In their work, the mobile fluid phase relative permeability is solved by using Brinkman equation. Han et al. [22] simulate the liquid water transport dynamics in the porous layer of a PEMFC. Their studies focus on the effects of the porous layer porosity and boundary liquid saturation on two-phase transport behaviours. It is noted that most of the above-mentioned studies are two-dimensional and limited to low density ratios and/or limited range of porosities.

On the other hand, results on droplet penetration/extraction into/from porous regions are scarcer. Taghilou and Rahimian [23] used the multiphase model of Lee [24] to simulate the penetration of droplet into a randomly generated porous medium. This work was recently extended by Latifiyan et al. [25] for the droplet evaporation during penetration in the porous media. It is noted that both of the above-mentioned works are two-dimensional and do not involve the wide range of medium porosity and fluid density ratios. More recently, Ge et al. [26] studied the two-dimensional droplet spreading and permeating on the porous substrates with hybrid-wettability. However, the work by Frank et al. [27] is of few three-dimensional investigations that studied the spreading of a liquid droplet on different porous surfaces. Still the porous surface in the latter work was a simple pore-space made of parallel holes of infinite length. Once more the densities of the fluid and the vapour phases in both works are of the same order of magnitude and the surface porosity is either two-dimensional or is an extension of it.

Interested readers are invited to read the three recent literature reviews on LBM for more information about its methodology and its diverse application in pore-scale [15,28,29].

As it can be seen from most of these works, the available literatures in simulation of multiphase flow and droplet penetration in porous media by LBM are limited to two-dimensional methods/problems. In this paper, the Lee's method, is extended to three-dimensional discretization and is used to simulate high density ratio droplet penetration in randomly reconstructed porous media. Therefore, although the primary goal of this work is the extension of previous works [23–26] to 3D; it is also extending the range of physical parameters investigated in available literature, i.e. mainly to higher density ratios as well as wider range of porosities.

The code is validated by Laplace's law, relaxation of square droplet and also different equilibrium contact angles where simulation results are compared with Cahn's wetting theory. The process of the droplet penetration in the porous substrate is then shown in detail. The effects of different parameters including, Froude number (Fr), Reynolds number (Re), Weber number (We), porosity (ε), contact angle (θ), and density ratio (ρ_l/ρ_v) are investigated. Finally, the current 3D LBM methodology is extended for the multi-phase transport in a porous channel and the extraction of a droplet from a porous substrate to show the effectiveness of the utilized method for diverse pore-scale applications. To the authors best knowledge, the only available LBM results of the latter problem, i.e. droplet extraction from a porous medium, are in two-dimensional and presented by Taghilou and Rahimian [23]. Therefore, this manuscript also opens new horizon for treating such a problem using LBM.

2. Numerical model

Several LBM models have been developed to treat the multiphase problems. Some widely used models are for instances free-energy models [30], Shan–Chen model [16], and finite difference LBM [31]. One of the main drawbacks of these

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