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Lattice Boltzmann simulation of liquid flow in nanoporous media

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ABSTRACT

In this paper, a multi-relaxation-time lattice Boltzmann (LB) model for nanoscale liquid flow is established to investigate the liquid flow characteristics in nanoporous media. The slip length and effective viscosity obtained by molecular dynamics (MD) simulations are adopted to account for the nanoscale effect. First, the LB model for water flow in nanopores is built and water flow characteristics in nanoporous media are investigated. The fluid-solid interaction force shows significant influence on water flow in nanoporous media. The water flux through nanoporous media increases with the decrease of fluid-solid interaction force. In hydrophobic nanoporous media, the nanoscale effect can decrease the gap between water flow resistance in large pores and that in small pores, making the velocity distribution more uniform. In addition, the end effect caused by the bending of streamlines can induce significant additional flow resistance. Neglecting the end effect can greatly overestimate water flow ability. The pore structure also has significant influence on water flow in nanoporous media. With the increase of specific interfacial length, the nanoscale effect increases. Finally, the LB model for oil (octane) flow in quartz nanopores is also established by incorporating the MD simulation results. Oil flow simulation in quartz nanoporous media shows that the conclusions obtained for water flow are also applicable for oil flow.

1. Introduction

Unconventional oil and gas reservoirs are drawing more and more attention all over the world due to the development of advanced techniques such as horizontal drilling and multi-stage hydraulic fracturing, and also due to the depletion of conventional resources [1]. As an important type of unconventional resources, shale oil and gas reservoirs have been explored successfully in North America [2]. However, the hydrocarbon transport mechanisms in such reservoirs remain to be fully understood.

In recent years, with the help of advanced imaging techniques, such as atomic force microscopy (AFM), scanning electron microscope (SEM), focused ion beam scanning electron microscope (FIB-SEM), and micro- and nano-computed tomography (CT), the pore structures in shale rocks can be directly observed [3–5]. Compared with the conventional reservoir rocks, pores in shale rocks are quite small, usually at nanoscale. Oil and gas flow in such confined pore space is quite different from that in conventional pores. Gas flow in shale rocks have been widely investigated by different methods at different scales, including the MD method [6,7], lattice Boltzmann method (LBM) [8–13], pore-network model [14], physical experiments [15,16] and macroscale analytical models [17–24], etc. Knudsen number (Kn) which is defined as the ratio of molecular mean free path (λ) to the flow characteristic length is a key parameter characterizing gas flow in nanopores. Under high Kn, the rarefaction effect can greatly enhance gas flow in nanopores [9,10].

Because of the significant difference of physical properties between liquids and gas, the gas flow mechanisms in nanopores do not apply to liquid flow in nanopores. Liquid flow, especially water flow in nanopores has also been widely investigated. The nanoscale effect can either increase [25,26] or decrease [27,28] water flux in nanopores compared with that obtained by no-slip Hagen-Poiseuille equation, depending on the difference between fluid-solid interaction force and water intermolecular interaction force [29]. The continuum model with slip length and effective viscosity is widely used to quantitatively describe the nanoscale effect for water flow in nanopores [29–31], and the slip length and effective viscosity can be extracted by curve fitting the velocity profile obtained by MD simulations. Different fluid-solid interaction forces can induce different slip lengths and effective viscosity. If the fluid-solid interaction force is much larger than the water intermolecular interaction force, the water molecules will be stuck onto the solid surface, thus the water mobility near the solid surfaces will

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decrease. In this situation, the no-slip boundary condition is still valid on the solid surface and the viscosity of water near the solid surface will increase [28,29,32,33]. As a result, the nanoscale effect decreases the flow rate. If the fluid-solid interaction force is much smaller than the water intermolecular interaction force, water molecules will slip on the solid surface and the viscosity of water near the solid surface will decrease [29,34–36]. Then the nanoscale effect will increase the flow rate. The fluid-solid interaction force can be characterized by the wettability or contact angle (θ) that a water droplet can form on the walls [29,37]. The small θ means strong fluid-solid interaction force while the large θ means weak fluid-solid interaction force. Based on a comprehensive literature review on water flow in nanopores, Wu et al. [29] established a model describing water flow in nanopores based on Navier-Stokes (N-S) equation with effective viscosity and slip length. Both the fluid-solid interaction effect and the nanopore dimension are considered in this model and more details about the model will be introduced in the next section.

However, the research work of oil flow in nanopores is quite limited. In recent years, Wang et al. [38,39] adopted MD method to investigate the oil adsorption and transport phenomenon in organic nanopores represented by graphite slits. The multiple adsorption layers were observed and the effects of different factors influencing oil adsorption were analyzed [38]. In addition, significant slip velocity and fast mass transport of oil were observed in organic nanopores [39]. However, the graphite slits are adopted in this research which have quite smooth surface and can generate extremely large slip lengths. Using the simple graphite slits to represent the complex kerogen pores in shale rocks may be questionable. Given quartz is the major inorganic component in the pore networks of shale matrix, Wang et al. [40] also simulated oil flow in quartz nanopores by MD method. They concluded that by incorporating the slip length and effective viscosity, the N-S equation can reasonably describe oil flow in quartz nanopores. Besides the MD method, other methods were also adopted to investigate oil transport in nanopores. Using the computational fluid dynamic (CFD) method, Afsharpoor et al. [41] found that the effects of pore geometry and slip velocity must be considered when using the pore network model to simulate liquid flow in shale. However, in their investigation, the wall effect on viscosity was ignored and the slip length was given artificially. Based on MD simulation results, experimental and theoretical studies, a mathematical model was derived by Cui et al. [42] to calculate the liquid permeability in shale organic nanopores. Zhang et al. [43] also established new apparent liquid permeability models to consider the effects of velocity slip, physical adsorption and wettability on nanoscale liquid flow. Although the mathematical models can incorporate different mechanisms, the reliability of these models needs further validation.

Although MD method is the most accurate method to model liquid flow in nanopores, the high computational cost restricts it from simulating a large domain. To investigate liquid flow in nanoporous media, other methods with higher computational efficiency should be adopted, among which LBM is a good choice. As a mesoscale simulation method, LBM has been successfully applied to many areas, including multiphase and multi-component flow [44–49], thermal flow [50], reactive flow [51,52], etc. In recent years, the LBM has also been adopted to simulate gas flow in nanoporous media [8–10,53]. There are two kinds of LB models to simulate nanoscale gas flow. One is the high-order LB model [54,55] which needs more discrete velocities to capture the non-equilibrium effects in rarefied gas flow. The other is the LB model with effective viscosity considering the effect of Knudsen layer. In this case, the LBM is essentially used to solve the N-S equation supplemented with the slip velocity and effective viscosity to account for the nanoscale effect. As introduced above, the slip length and effective viscosity are also introduced into the continuum model (N-S equation) to account for the nanoscale effect for nanoscale liquid flow [29,40]. Therefore, the LB model developed for nanoscale gas flow should also be applicable for nanoscale liquid flow. In this study, the nanoscale effect for liquid flow in nanopores is firstly incorporated into the pore scale lattice Boltzmann model and the liquid flow characteristics in nanoporous media are studied in detail. We find the end effect has significant influence on liquid flow in nanoporous media. This paper is arranged as follows. First, a LB model proposed by Guo et al. [53], which is originally used to model microscale gas flow, is modified to simulate liquid flow in nanoporous media. The slip length and effective viscosity for water flow in nanopores obtained by MD simulation is incorporated into this model to simulate water flow in nanoporous media. Both water flow characteristics and its influencing factors are investigated. Then, the LB model for oil flow in quartz nanopores is proposed based on the MD simulation results of Wang et al. [40] and oil flow characteristics in quartz nanoporous media are also studied.

2. Theory and model description

2.1. Theory of water flow in nanoporous media

As stated in the introduction, water flow in nanopores is strongly dependent on the fluid-solid interaction force. Wu et al. [29] established a model describing water flow in nanopores considering the fluid-solid interaction effect and nanopore dimension. In Wu's model, the N-S equation is supplemented with the slip length and effective viscosity. The relationship between slip length and wettability, as well as the link between effective viscosity, wettability and confinement are established. The slip length can be calculated by [29,56]:

$$l_s = C/(\cos\theta + 1)^2, \tag{1}$$

where l_s is the slip length, which is defined as the ratio of slip velocity to the shear rate at the solid walls; C is a constant for a certain fluid which should be fitted with experimental or MD simulation data, for water, $C = 0.41$ [29]; θ is the contact angle of water. This relationship matches well with the MD simulation results for θ up to 150° [29,56].

Affected by the fluid-solid interaction force, the viscosity of water near the solid walls will be changed. Considering the interface region affected by the solid walls, the area-weighted-average effective viscosity μ_{eff} can be calculated by [29,57]:

$$\mu_{eff} = \mu_i \frac{A_i}{A_t} + \mu_\infty \left(1 - \frac{A_i}{A_t}\right), \tag{2}$$

where μ_i and A_i are the viscosity and area of water in the interface region, respectively; μ_∞ is the bulk viscosity of water in the middle of the channel; A_t is the total cross-sectional area. The area of interface region is dependent on the thickness of the interface region, which is 0.7 nm for water according to experiments and MD simulations [29].

The viscosity of water in the interface region is also dependent on the wettability [29]:

$$\frac{\mu_i}{\mu_\infty} = -0.018\theta + 3.25 \tag{3}$$

Incorporating the slip length and effective viscosity, the modified N-S equation can be adopted to describe water flow in nanopores. However, for water flow in short channels or tubes, because of the bending of streamlines at the entrance or exit of the channels or tubes, additional hydrodynamic resistance can be