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Pore-scale simulation of shale gas production considering the adsorption effect

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ABSTRACT

A microscale lattice Boltzmann (LB) model considering the adsorption effect was established and adopted to simulate shale gas production in microscale porous media. The adsorption effect was incorporated into the LB model by introducing the interaction forces between solids and gas particles, and the adsorption parameters were determined by the molecular simulation method through a novel process proposed in this paper. First, the grand canonical Monte Carlo (GCMC) method was adopted to simulate gas adsorption in a slit pore. Then the LB model was also adopted to do the same simulation under the same conditions. By matching the results of LB model with those of molecular simulation, the adsorption parameters in LB model under different conditions were obtained. Then the proposed LB model was adopted to simulate gas production processes in an organic porous medium and an inorganic porous medium with the same geometry. The effects of adsorption on pore-scale gas storage, recovery and production were all analyzed. The simulation results show that adsorption can greatly increase the gas storage in organic porous media, while the gas recovery of organic porous medium is always lower than that of inorganic porous medium since the adsorbed gas is difficult to produce. In addition, the organic porous media will not always produce more gas than the inorganic porous media. Whether the adsorption effect will increase the gas production or not depends on the excess adsorption curve.

1. Introduction

In the past decades, the exploitation of unconventional oil and gas reservoirs has been drawing more and more attention all over the world due to the advanced techniques such as horizontal drilling and multi-stage hydraulic fracturing [1]. As an important type of unconventional resource, shale gas reservoirs have been explored successfully in North America. Shale gas reservoir is different from the conventional reservoirs mainly in two aspects. One is that most pores in shale rocks are quite small, usually in nanoscale [2–4]. The other is that there exists organic matter in shale rocks which has strong interaction force with gas and will adsorb gas onto its surface [5,6].

Gas flow in microscale porous media can be characterized by Knudsen number (Kn) which is defined as the ratio of molecular mean free path to the characteristic length of the porous medium. Based on Knudsen number gas flow can be divided into four regions [3]: continuum flow region ($Kn < 0.001$), slip flow region ($0.001 < Kn < 0.1$), transient flow region ($0.1 < Kn < 10$) and free molecular flow region ($Kn > 10$). For gas flow in porous media, the molecular mean free path near the solid walls will be cut off because of the existence of the walls, so gas flow near the solid walls is different from that in the bulk area of the flowing channel. This flowing area affected by the solid walls is called the Knudsen layer [7]. In the continuum flow region and slip flow region, the Knudsen layer only occupies a small part of the flowing channel, so the effect of Knudsen layer can be ignored and the continuum hypothesis is still valid. While in the transient flow region and free molecular flow region, the Knudsen layer occupies a very large part of the flowing channel, even the whole flowing channel. As a result, the effect of Knudsen layer must be considered and the continuum hypothesis is no longer applicable. The particle based method should be adopted to investigate the gas flow characteristics, such as the molecular simulation, direct simulation Monte Carlo (DSMC) method, lattice Boltzmann method (LBM) etc.

Molecular simulation has been successfully adopted to investigate gas flow and gas adsorption in nanopores. Both non-equilibrium molecular dynamics (NEMD) [8,9] and equilibrium molecular dynamics (EMD) [10] have been adopted to simulate the molecular movement of gas in nanopores. The GCMC method provides a convenient route to simulate isotherms, and describes the methane adsorption behavior on carbonaceous materials [11]. As the molecular simulation can describe the exact

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interaction forces between molecules, it is thought to be an accurate method. However, as it needs to describe the information of each molecule, it demands a lot of computation resources. As a result, it is only suitable to simulate gas behavior in pores with just a few nanometers.

LBM has also been adopted to simulate gas flow in microscale pores since 2002 [12]. In the first few years, the researchers mainly focused on gas flow simulation in the slip flow region and different relaxation time expressions and slip boundary conditions were proposed [13–16]. With the increase of Knudsen number, the effect of Knudsen layer becomes increasingly critical. For gas flow beyond the slip flow region, the effect of Knudsen layer must be considered. Many efforts have been done to extend LBM beyond the slip flow regime, including the physically based strategies and phenomenologically motivated based strategies [17]. The former one deals with the Knudsen layer by establishing high-order LB models. They are typically derived by projecting the Boltzmann equation onto a Hermite basis. By truncating at various levels in the Hermite expansions, one can obtain differing orders of accuracy for the LB method [17,18]. In addition, in highly rarefied gas flows, both rarefaction and nonlinear effect by compressibility interplay. The higher terms in the equilibrium distribution function are mainly related to the compressibility and the discrete velocity set is related to the rarefaction [19]. Many researchers have theoretically analyzed and numerically evaluated the accuracy of high-order LB models for capturing non-equilibrium effects in rarefied gas flow [20–23]. Although the high-order LB model is more reasonable for microscale gas flow, because it requires higher order velocity models and very complicated numerical treatments for complex surface geometry, it is not practical for gas flow simulation in microscale porous media. On the other hand, the latter one deals with the Knudsen layer by adopting the effective relaxation time modified by Knudsen number. Since this strategy is simpler without losing of accuracy, it is more popular and has been successfully used to simulate gas flow in micro-channels under both small and large Knudsen numbers [24–26]. However, this kind of LB model [24–26] cannot be used to simulate gas flow in microscale porous media under large Knudsen numbers because of the inadequate symmetry of the discrete model [27]. To overcome this defect, the regularization procedure must be considered [27,28].

In recent years, more and more researchers adopted LBM to simulate gas flow in shale rocks and some new phenomena have been found [24–26,29–33]. To consider the adsorption effect in organic matter, different strategies have been proposed. Fathi et al. [24] considered the adsorption effect by using the Langmuir boundary condition. Ning et al. [31] introduced the interaction forces between solids and gas. Ren et al. [25] calculated the adsorbed gas velocity based on Langmuir isotherm and modified the pore size with the thickness of the adsorbed layer. And Li et al. [34] introduced the thickness of adsorption layer into LBM according to MD simulation. The method of Ning et al. [31] is more reasonable since it is based on the nature of physical adsorption. However, as LBM is a mesoscopic method, it cannot describe the exact interaction forces between the solids and gas molecules. So the accuracy of these LB models considering the adsorption effect is questionable.

As introduced above, the molecular simulation method is a microscopic simulation method. It can directly describe the molecular movement and the interaction forces between molecules. However, it is very difficult to be extended to simulate gas flow and adsorption in relatively large porous media because of its high computational costs. LBM is a mesoscopic simulation method. It describes the movement of gas particles composed of a mass of molecules. Although LBM can be used to simulate gas flow in relatively large porous media, the exact adsorption parameters in the LB model is unknown. To combine the advantages of these two simulation methods, a novel process was proposed in this paper. In this process, the adsorption effect is considered by introducing the interaction forces between solids and gas particles in LBM, and the adsorption parameters were determined by the molecular simulation. Then the proposed LB model was adopted to simulate gas production processes in an organic porous medium and an inorganic porous medium with the same geometry. The effects of adsorption on pore-scale shale gas storage, recovery and production were all analyzed based on the simulation results.

2. Numerical methods

2.1. Microscale lattice Boltzmann model considering the adsorption effect

2.1.1. Shan-Chen-type lattice Boltzmann model

Because of the high pressure in shale gas reservoir, the ideal equation of state (EOS) is no longer applicable. The single-component Shan-Chen model [35,36] was firstly proposed for multi-phase flow. By introducing the interaction forces between fluid particles, the non-ideal EOS can be simulated. In addition, different potential functions results in different EOS [37]. In this paper, although there is no phase separation, the Shan-Chen model is applied to introduce the Peng–Robinson (P–R) EOS into our model to consider the high pressure effect. As this paper mainly focuses on 2D simulation, the D2Q9 discrete velocity model is used. The basic evolution equation with the Bhatnagar–Gross–Kr ook (BGK) collision approximation is shown as follows. Unless otherwise stated, all units in this paper are lattice units.

$$f_\alpha(\mathbf{r}+\mathbf{e}_\alpha\delta_t, t+\delta_t) - f_\alpha(\mathbf{r},t) = -\frac{1}{\tau}(f_\alpha - f_\alpha^{eq}) + \delta_t F_\alpha \tag{1}$$

where f_α is the density distribution function of α direction; $\alpha = 0, 1, 2, \ldots, 8$, which means that there are 9 velocity directions; $\mathbf{r}$ is the spatial location of the particles; $\mathbf{e}_\alpha$ is the velocity of α direction; t is time; δ_t is time step; τ is the relaxation time; F_α is the force term; f_α^{eq} is the local equilibrium distribution function of α direction expressed as follows:

$$f_\alpha^{eq} = w_\alpha \rho \left[1 + \frac{\mathbf{e}_a \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_a \cdot \mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}^2}{2c_s^2}\right] \tag{2}$$

where ρ and $\mathbf{u}$ are the macroscopic density and velocity, respectively; c_s is the lattice sound speed; w_α is the weight factor of α direction.

To introduce the non-ideal EOS into the model, Shan and Chen [35] introduced the interaction force between fluid particles:

$$\mathbf{F}(\mathbf{r},t) = -G\psi(\mathbf{r},t)\sum_{\alpha=1}^{8}\omega_\alpha\psi(\mathbf{r}+\mathbf{e}_\alpha\delta_t,t)\mathbf{e}_\alpha \tag{3}$$

where $\mathbf{F}$ is the interaction force between fluid particles; G is a parameter that controls the interaction strength between the fluid particles; ψ is the potential function that depends on the fluid density. The P-R EOS is introduced into the model by the following format of ψ [37].

$$\psi = \sqrt{\frac{2\left(\frac{\rho RT}{1-c\rho} - \frac{a\alpha(T)\rho^2}{1+2c\rho-c^2\rho^2} - c_s^2\rho\right)}{c_s^2 G}} \tag{4}$$

where $a = 0.45724R^2T_c^2/P_c$; R is the universal gas constant; T_c and P_c are the critical temperature and critical pressure of the gas; $\alpha(T) = \left[1 + (0.37464 + 1.54226\omega - 0.26992\omega^2) \times (1 - \sqrt{T/T_c})\right]^2$; ω is the acentric factor, and $\omega = 0.011$ for methane; T is temperature. We set $a = 2/49$, $c = 2/21$, and $R = 1$ in the simulation [37].