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A new boundary scheme for simulation of gas flow in kerogen pores with considering surface diffusion effect

Lingquan Wang [a,b], Zhong Zeng [a,b,c,*], Liangqi Zhang [a,b], Long Qiao [a,b], Yi Zhang [a,b], Yiyu Lu [a]

[a] State Key Laboratory of Coal Mine Disaster Dynamics and Control, Chongqing University, Chongqing 400044, China
[b] Department of Engineering Mechanics, Chongqing University, Chongqing 400044, China
[c] Chongqing Key Laboratory of Heterogeneous Material Mechanics (Chongqing University), China

HIGHLIGHTS

- A new slip boundary scheme for micro-scale LBM was proposed.
- The second order slip boundary was contained.
- The surface diffusion effect was considered.

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ABSTRACT

Navier–Stokes (NS) equations with no-slip boundary conditions fail to realistically describe micro-flows with considering nanoscale phenomena. Particularly, in kerogen pores, slip-flow and surface diffusion are important. In this study, we propose a new slip boundary scheme for the lattice Boltzmann (LB) method through the non-equilibrium extrapolation scheme to simulate the slip-flow considering surface diffusion effect. Meanwhile, the second-order slip velocity can be taken into account. The predicted characteristics in a two-dimensional micro-flow, including slip-velocity, velocity distribution along the flow direction with/without surface diffusion are present. The results in this study are compared with available analytical and reference results, and good agreements are achieved.

1. Introduction

Over the past decade, the fluid flow in microchannel has received a significant attention [1–3], particularly in shale gas reservoirs [4–6]. Shale gas is natural gas produced from shale, mainly including organic porous material (widely known as kerogen) and inorganic matrix [7]. Because the kerogen pores in shale should be regarded as nanoscale pores, some special nanoscale phenomena, including slip-flow and surface diffusion, should be considered in studying the mechanism of shale gas flow.

Gas transport in shale is usually characterized by the Knudsen number $Kn = \lambda/h$, where λ represents the mean free path of the gas and h is the characteristic length. Current studies distinguish the flow regimes according to the value of Kn: continuum flow ($Kn \leq 0.001$), slip flow ($0.001 < Kn \leq 0.1$), transition flow ($0.1 < Kn \leq 10$), and free molecular flow ($Kn > 10$) [7]. Gas flow in kerogen pores should be slip flow or transition flow [7,8] and then continuum hypothesis is broken

* Corresponding author at: State Key Laboratory of Coal Mine Disaster Dynamics and Control, Chongqing University, Chongqing 400044, China.
E-mail address: zzeng@cqu.edu.cn (Z. Zeng).

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down. In addition, shale gas reservoirs are located in deep underground with high pressure, a large amount of shale gas adsorbs on the shale surface and the adsorbed gas will diffuse along the shale surface. Though a variety of experiments and analytical solutions study shale gas flow [9–13], simulations on containing the effects of both the slip-flow and surface diffusion are still rare. The main strategies for simulating shale gas flow have molecular dynamics (MD) approach, and mesoscopic approach. Nevertheless, the MD approach has expensive computational costs and high statistical noises limit for its applications in simulating shale gas flow [7]. Therefore, the mesoscopic approach, such as lattice Boltzmann method (LBM), has been used to simulate shale gas flow [14–18].

LBM has shown its superiority to delineate the shale gas flow, due to its kinetic origin and computational efficiency. So far, the LBM has been successful in modeling slip gas flow and transition flow. To our knowledge, the first order velocity slip model can be used to capture slip gas flow and the transition flow can be displayed with second order velocity slip model. A detailed review for the application of LBM in micro-gaseous flows has been introduced by Amit Agrawal [19]. To simulate the velocity slippage in the slip/transition regime, LBM can be applied with coupling various slip boundary implementation schemes. The boundary implementation schemes in the above literatures can be divided into two kinds: a kind based on the non-equilibrium extrapolation approach, such as Langmuir slip model [20,21] and a kind related to the bounce-back approach, such as Discrete Maxwellian (DM) boundary [22] and Bounceback-Specular-Reflection (BSR) boundary [23]. As pointed out by Guo [24], the bounce-back approach is difficult to extend to arbitrary boundary conditions. Meanwhile, the Langmuir slip model cannot display the second order velocity slip. Thus, no matter which kind of approach has its limitations. However, this puzzle can be solved in this paper.

In addition, currently the attempts on lattice Boltzmann simulations of shale gas flow with considering the effects of surface diffusion are still few. To our best knowledge, Junjie Ren et al. [7] present a novel LB model with taking account of the effects of surface diffusion, gas slippage, and adsorbed layer. Junjian Wang et al. [25] proposed a propagation LB scheme in the slip boundary condition considering the effect of surface diffusion. Then, Yuan et al. [14] and Junjian Wang et al. [15] studied the influence of surface diffusivity depending on the adsorption coverage. However, all these literatures have adopted the BSR boundary scheme or its modification. Thus, we tried to propose a new boundary implementation scheme, based on the non-equilibrium extrapolation approach, to capture both the slip and surface diffusion effects in kerogen pores.

In this paper, a new boundary implementation scheme was developed. We proposed a new slip boundary condition, which is based on the finite difference scheme and then it was incorporated into the LB method by amending the non-equilibrium extrapolation scheme. The scheme is not only suitable to capture the second order velocity slip with a parameter θ_b referring to accommodation coefficient related to slip coefficient A_1, but also convenient to contain surface diffusion effect with a parameter θ referring to the fraction of the surface covered by adsorbed atoms at thermal equilibrium. To validate the present scheme, we performed an isothermal micro-Poiseuille flow and then we applied the scheme to the shale gas flow with considering the surface diffusion effect.

2. Lattice Boltzmann model for micro-flow

The evolving equation of the LB model for micro-flow has been developed in [26,27]

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot f_\alpha = -\frac{1}{\tau_f}\left(f_\alpha - f_\alpha^{eq}\right) + F_\alpha \tag{1}$$

where $\mathbf{e}_\alpha$ denotes the discrete velocity in direction α and f_α^{eq} denotes the discrete equilibrium distribution function. τ_f is the relaxation time. F_α denotes the discrete body force term. For two-dimensional nine-directional (D2Q9) square lattice with $c = \sqrt{3RT}$ (where T is the average temperature and R is the universal gas constant), the equilibrium density distribution f_α^{eq} and the discrete forcing term F_α are, respectively, chosen as:

$$f_\alpha^{eq} = \omega_\alpha \rho (1 + \frac{3\,(\mathbf{e}_\alpha \cdot \mathbf{u})}{c^2} + \frac{9(\mathbf{e}_\alpha \cdot \mathbf{u})^2}{2c^4} - \frac{3(\mathbf{u}\cdot\mathbf{u})}{2c^2}) \tag{2}$$

$$F_\alpha = \omega_\alpha (1 - \frac{1}{2\tau_f})(\frac{3\,(\mathbf{e}_\alpha \cdot \mathbf{F})}{c^2} + \frac{9\,(\mathbf{e}_\alpha \cdot \mathbf{u})\,(\mathbf{e}_\alpha \cdot \mathbf{F})}{c^4} - \frac{3(\mathbf{u}\cdot\mathbf{F})}{c^2}) \tag{3}$$

where $\mathbf{F}$ is the external force with the weight factors: ω_0=4/9; ω_{1-4} =1/9, and ω_{5-8} =1/36. The discrete velocities $\mathbf{e}_\alpha$ are given as:

$$\mathbf{e}_\alpha = \begin{cases} (0,0), & \alpha = 0 \\ \left(\cos\left[\dfrac{(\alpha-1)\,\pi}{2}\right], \sin\left[\dfrac{(\alpha-1)\,\pi}{2}\right]\right), & \alpha = 1\text{–}4 \\ \sqrt{2}\left(\cos\left[\dfrac{(2\alpha-9)\,\pi}{4}\right], \sin\left[\dfrac{(2\alpha-9)\,\pi}{4}\right]\right) c & \alpha = 5\text{–}8 \end{cases} \tag{4}$$

where $c = \delta_x/\delta_t$ denotes the lattice velocity, δ_x and δ_t are the lattice spacing and time step, respectively. The effective kinematic viscosity ν is determined by

$$\nu = \frac{1}{3}(\tau_f - 0.5)c^2\delta_t \tag{5}$$