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# Numerical modeling of slippage and adsorption effects on gas transport in shale formations using the lattice Boltzmann method

Yang Ning [a], Yang Jiang [a, b], Honglin Liu [c], Guan Qin [a, *]

[a] Petroleum Engineering Program, Department of Chemical & Biomolecular Engineering, University of Houston, Houston, TX 77204, USA
[b] SinoFTS Petroleum Services Ltd., Beijing 100101, China
[c] Institute of Petroleum Exploration & Development – Langfang Branch, PetroChina Company Limited, Langfang 102801, China

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ABSTRACT

Shale formations consist of numerous nanoscale pores within a range of 2 nm–50 nm; the shale gas flow within this size range under typical shale reservoir pressure and temperature will fall into the slip flow or the transitional flow regime $0.001 < K_n < 10$. Besides nano-pores in shale, there exist a number of mesoscopic and macroscopic pores with size larger than 50 nm, and many micrometer fractures. Natural gas, mainly methane, flows through nanoscale pores, mesoscale, and macroscopic pores or fractures during the production period. Gas slippage described by the Klinkenberg effect reduces viscous drag near the pore walls and influences permeability. In shale, the majority of gas molecules are adsorbed in kerogen that is considered to be organic source rocks. Within nano-pores and meso-pores, Darcy's law cannot effectively describe this type of transport phenomena due to its continuum assumption. Alternatively, the kinetic-based lattice Boltzmann method (LBM) becomes a strong candidate for simulating an organic-rich shale reservoir that contains a large number of nano-pores. In this paper, we present a multiple-relaxation-time (generalized) LBM, which is considered to be one of the most efficient LBM models. For gas flow in a confined system, its molecular mean free path is corrected depending on the size of the confined system and the distance of the gas molecules from the pore walls. Gas slippage on pore walls is captured with a combined bounce-back specular reflection boundary condition. In addition, adsorbed gas in shale has a significant influence on gas transport in shale gas production. Here, we propose to incorporate inter-molecular and adsorptive forces into the generalized LBM algorithm to capture gas adsorptions in organic nano-pores. Therefore, this approach is able to simulate gas flow with adsorption effect. Many factors are believed to control the flow mechanisms in these types of pores, including the pore size distribution, the specific surface area, and the adsorptive feature of the pore walls. The simulation results agree well with the existing data for high Knudsen flows between 2D parallel plates. Accounting for the adsorption and slippage effects, flow phenomena are investigated by varying different controlling factors in both simple and complex structures. The permeability of methane is also determined for complex porous geometries.



## 1. Introduction

Shale gas is becoming a significant source of unconventional natural gas. The production of shale gas mainly depends on its characteristics, including its pore size distribution, organic richness, natural/factitious fractures, *etc.* A significant portion of shale gas is stored in nano-pores within kerogen pockets that are 200 nm to 500 nm in size, and nano-pores have sizes in the range of 2 nm–50 nm (Ambrose et al., 2010; Adesida et al., 2011; Wei et al., 2013; Kang et al., 2011). Consequently, it is essential to understand the natural gas flow mechanisms in nano-pores in order to predict long-term shale gas production and shale gas reserves. In nano-pores, a dimensionless number, the Knudsen number ($K_n$), is important for describing the flow mechanisms. The Knudsen number is defined as the ratio of the molecular mean free path $\lambda$ to a representative physical length of the interest, which is the representative diameter of nano-pores. The molecular mean free path is the average distance that a molecule travels between two successive collisions. It is a function of pressure, temperature, and the type of gas molecules. With different Knudsen numbers, the flow regime falls into the following four categories: continuum flow

* Corresponding author.
*E-mail address:* gqin@uh.edu (G. Qin).

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($K_n < 0.001$), slip flow ($0.001 < K_n < 0.1$), transitional flow ($0.1 < K_n < 10$), and free molecular flow ($K_n > 10$). Natural gas flow in nano-pores is considered to be either a slip flow or a transitional flow regime, depending on pore condition, size of nano-pore and type of gas molecules. In both of these flow regimes, the continuum assumption of fluid flow breaks down and Navier–Stokes (N–S) equations, with a regular no-slip boundary condition, cannot be applied because the gas slippage effect becomes significant. A large portion of natural gas in shale formations is claimed to be adsorbed in kerogen pockets because of the organic nature of kerogen (Kang et al., 2011), so we must take the adsorption/desorption effect into account to effectively describe the mechanism and storage of gas flow in shale formations. Permeability is a key parameter for describing the flow characteristics of hydrocarbons in oil and gas reservoirs. In shale formations, Darcy's law cannot be used to characterize permeability as it has been derived from N–S equations via homogenization (Whitaker, 1986). Accurately determining permeability can significantly improve the prediction of production in either numerical reservoir simulations or empirical methods. In gas reservoirs, the slippage of gas molecules at the pore wall gives apparently higher permeability than would be obtained by liquid measurements, which is known as the Klinkenberg effect (Klinkenberg, 1941). This effect may have a significant impact on gas flow behavior, especially in low permeability media. Klinkenberg stated that effective gas permeability is a pressure-dependent property and it is a linear function of the reciprocal mean pressure. Shale reservoirs have different characteristics from conventional gas reservoirs, and the permeability of shale is dependent of multiple conditions, such as pore pressure, temperature and organic content, and so on. Therefore, different modified Klinkenberg slippage theories have been proposed based on higher-order dependency between gas permeability and pore pressure (Moghadam and Chalaturnyk, 2014; Fathi et al., 2012; Ziarami and Aguilera, 2012).

The numerical modeling of gas flow in organic nano-pores requires proper numerical techniques. The Boltzmann equation is well-accepted for modeling gas flows across all types of flow regimes. The lattice Boltzmann equation is a discretized form of the continuous Boltzmann equation and it models the distribution function of fluid particles. Two types of lattice Boltzmann method (LBM) models include the single-relaxation-time model, based on the Bhatnagar-Gross-Krook (BGK) approximation (Bhatnagar et al., 1954), and the multiple-relaxation-time (generalized) model (d'Humieres, 1992). Generalized LBM relaxes various moments (*i.e.,* density, energy, momentum, heat flux, stress tensor, *etc.*) to their equilibrium states at different relaxation times during collisions, which provides great advantages regarding its theories, parameter selections, and numerical stability over the BGK LBM (Lallemand and Luo, 2000). Standard LBM is a second order approximation of the continuous Boltzmann equation and it has the same accuracy with N–S equations as the continuous Boltzmann equation. LBM and N–S equations have been successfully applied to modern computational fluid dynamics for thermodynamic quasi-equilibrium flows. However, their standard formulations are inadequate to simulate extremely low speed flows with high Knudsen numbers (*i.e.*, $K_n \gg 0.001$) in which the fluids are in a thermodynamic non-equilibrium state (Meng et al., 2012). For high Knudsen flows, the failure of the standard LBM can be attributed to its insufficient ability to describe the Knudsen layer (a kinetic boundary layer over a solid surface), and its thickness is comparable to gas molecular mean free path (Guo et al., 2006; Shan et al., 2006). Within the Knudsen layer, the thermodynamic quasi-equilibrium state cannot be achieved due to insufficient collisions between the gas molecules, and gas slippage cannot be ignored. Therefore, a more effective LBM model to capture gas slippage within the Knudsen layers is needed.

In the past decade, LBM has been widely used in modeling high Knudsen flow due to its theoretical advantages over N–S equations. In a high Knudsen flow, the kinetic Knudsen layer is a dominant portion of the whole flow region and the slippage effect becomes important. The failure to characterize the Knudsen layer can significantly influence the ability to model the flow mechanisms. Modifying the gas mean free path in the Knudsen flow region has been proven to be able to improve the flow prediction (Guo et al., 2006; Shan et al., 2006; Zhang et al., 2006; Niu et al., 2007; Sbragaglia and Succi, 2005; Guo et al., 2007, 2008). One of the relaxation times in generalized LBM is related to the gas molecule's mean free path or the fluid viscosity, so this relaxation time needs to be adjusted to capture flow behavior within the Knudsen layers. Moreover, a proper boundary condition that can accurately describe the gas slippage on solid boundaries is required. The most widely used non-slip bounce-back boundary condition in LBM, which strictly guarantees the conservation of mass and momentum, cannot be applied for high Knudsen flows. Therefore, Zhang et al. (2006) proposed an effective mean free path with a diffuse scattering boundary condition for high Knudsen flows. Niu et al. (2007) and Suga et al. (2010) applied higher order moments and an effective relaxation time to model the Knudsen layer. Guo et al. (2007, 2008) proposed an extended Navier–Stokes formulation based on an effective mean free path and applied it into the generalized LBM with a combination of bounce-back and specular reflection (CBBSR) boundary conditions (Sbragaglia and Succi, 2005). The combination of bounce-back and specular reflection is used to describe the slippage on the solid boundary, while the portion of the specular reflection is found related to the effective relaxation time (Guo et al., 2008). Chen and Tian (2009) proposed another boundary condition based on the Langmuir slip model.

Another important issue in shale gas transport is the adsorption effect, as a significant amount of natural gas stored in shale formations is absorbed gas that can be quantified using Langmuir isotherms (Kang et al., 2011). Shale gas transport can be dominated by the release of absorbed gas from the nano-pores. The hopping of gas molecules between the adsorbed gas and the free gas requires an intermolecular force. Shan and Chen (1993) have introduced an intermolecular potential among different phases, which adds an attraction or repulsion to the elastic collisions. Sukop and Or (2004) have introduced an intermolecular potential between solid walls and fluid particles to capture the adsorption effect based on Shan and Chen's work (Shan and Chen, 1993). Fathi et al. (2012) first applied the adsorptive force onto LBM to capture adsorbed gas in kerogen capillary tubes. Since intermolecular potentials are incorporated into LBM, the equation of state (EOS) needs to be modified accordingly (He and Doolen, 2002; Sukop and Thorne Jr., 2006) in order to include the non-ideality effect. By accounting for the adsorptive/cohesive forces among particles, we can capture the adsorption and interphase phenomenon. Recently, Ren et al. (2015) calculated the transports of the adsorbed gas and the free gas separately. The transport of the adsorbed gas was solved by the surface diffusion theory, where the amount of the adsorbed gas was quantified by the Langmuir isotherm. In the meantime, transport of the free gas was solved by the non-ideal LBM method.

In this paper, we first discuss the generalized LBM with an effective relaxation time associated with the effective mean free path of the gas. This effective mean free path is defined as a function of the Knudsen number and the location in the confined system, and it is always smaller than what would be obtained from a bounded system. For high Knudsen flows, gas molecules no longer have zero velocity near solid walls due to the strong slippage effect. In this regard, a proper boundary condition, combined bounce-back specular reflection (CBBSR), is discussed to capture the slippage