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Permeability of high-Kn real gas flow in shale and production prediction by pore-scale modeling

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ABSTRACT

Although shale gas has been commercially exploited, the gas transport mechanism in shale is still unclear. Because nanoscale pores are dominant in shale, the Knudsen number of the flow is relatively high so that the conventional Darcy's law fails. What is more, the shale gas in situ is under high pressure and high temperature so that the real gas (or non-ideal gas) effect is significant. Aiming at these two challenges, we did a pore-scale modeling by using lattice Boltzmann method in this work. We developed a pore-field-iteration (PFI) method to bridge up the pore-scale modeling results with the field-scale concerns, such as inflow performance relationship and decline curve analysis. Our results show that the high Knudsen effect leads to a higher gas flow rate, while the real gas effect causes lower gas flow rate. The gas production may be overestimated at early stage due to the real gas effect, while underestimated at late stage because of the high Knudsen number effect. These results may be very helpful for better understanding of gas transport mechanism in shale and for possible process optimization of shale gas developments in future.

1. Introduction

Shale gas is an unconventional gas resource with huge storage. With the gradual declination in conventional gas production, shale gas will play an important role in world energy supply. However, the mechanism of gas flow in shale is not clearly understood yet, as the conventional Darcy's law cannot describe the flow very well (Javadpour et al., 2007). Because of the lacking in fundamental theory and model, key problems such as how to interpret the history production data, how to predict the future production remain unsolved.

In physical view, there are two challenges in modeling the shale gas flow. The first one is the high Knudsen number (*Kn*) effect. As the nanoscale pores are dominant in shale (Loucks et al., 2009; Chalmers et al., 2012), the gas flow in shale has a relatively high *Kn* and the permeability in Darcy's law needs to be corrected. Many works have been done focusing on the high *Kn* effect. Klinkenberg (1941) first proposed a correction in which gas permeability increases with *Kn* linearly. After that, Beskok and Karniadakis (1999) presented a non-linear correction (termed as Beskok's correction here after for simplicity) for gas flow in straight channel and pipe, which is valid for a wide range of *Kn*. Latter, Civan (2010) extended Beskok's correction to flow in porous media, based on the use of hydrodynamic radius in defining the *Kn*. More recently, the pore-network modeling, in which the complex porous structure is simplified as pore nodes connected by pore bonds, has been used to capture the high *Kn* effect (Mehmani et al., 2013; Ma et al., 2014).

The second challenge is the real gas effect (or non-ideal gas effect). In most of the reservoirs, shale gas is a kind of supercritical fluid which cannot be treated as ideal gas. In 1966, Al-Hussainy et al. (1966) proposed the famous pseudo-pressure method to linearize the flow equations of real gas. No further works have been done regarding this problem until in recent years. Wang and Li (2003, 2007) and Wang et al. (2008) developed a Monte Carlo method based on the Enskog theory to simulate high *Kn* real gas flows, which is though very expensive in dealing with porous media and its application is merely limited to channel flow. Villazon et al. (2011) combined the Beskok's correction with the pseudo-pressure method, to consider both the *Kn* effect and real gas effect. Wang and Marongiu-Porcu (2015) recently used another correction to describe high *Kn* effect and coupled the real gas effect, formation compaction and gas desorption in their numerical simulations.

However, most of these models are in Darcy scale. They are accurate for regular porous media, but problematic for complex,

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heterogeneous and hierarchical structures like shale because of ignored effects of geometry details. With the developments of lattice Boltzmann method (LBM) which holds the advantage in tackling complex boundaries (Chen and Doolen, 1998), it becomes possible to directly simulate gas flows in complex structures, i.e. by pore-scale modeling (Chen et al., 2015). Pore-scale modeling is capable of capturing all the geometry details, therefore it is highly accurate for flow behavior in complex structure.

One challenge for pore-scale modeling of shale gas is the multiscale issue. The target is to understand and predict the production at field scale. However based on the computational cost, the pore-scale simulation is usually limited to very small volume (Chen et al., 2012). An efficient upscaling method is desperately desired to bridge the microscale simulation results and the macroscale prediction.

In this work, we firstly simulate the high *Kn* real gas flow at pore scale by using LBM. Several benchmarks are made to validate our numerical method. Then a multiple-scale integration method is proposed to upscale the pore-scale simulations to field-scale problems. To predict the production of shale gas, field-scale problems such as the inflow performance relationship (IPR) and decline curve analysis (DCA) are studied.

2. Numerical method

2.1. High Knudsen number effect

Knudsen number is defined as (Knudsen, 1933),

$$Kn = \frac{\lambda}{l}, \tag{1}$$

where λ and l are the mean free path of gas molecules and the characteristic length of the structure, respectively. The real gas mean free path model proposed by Bird (1983) is adopted here: $\lambda = \frac{\mu}{\rho}\sqrt{\frac{\pi M}{2RT}}$, where μ is the dynamic viscosity of gas; ρ is the gas density; M is the molar mass; T is the absolute temperature and R is the gas constant. For the characteristic length, the hydrodynamic tube radius of the well-known Kozeny–Carman model (Kozeny, 1927) is applied: $r = 2V_p/S_p$, where V_p is the total pore volume, S_p is the interface area between pore and solid matrix. For a straight channel, the channel height is taken as the characteristic length.

To simulate high *Kn* flow, lattice Boltzmann method (LBM) is used because of two aspects: (1) it has solid physical foundation since the lattice Boltzmann equation is derived directly from Boltzmann equation (He and Luo, 1997; Chen and Doolen, 1998), which is the fundamental transport law available for high *Kn* flow; (2) LBM has a high efficiency in dealing with complex boundaries of porous structure (Wang and Chen, 2007; Wang et al., 2007a). LBM describes the evolution of the discrete distribution function, which can be written as

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = \Omega_i(f), \quad i = 0, 1, \cdots, n-1 \tag{2}$$

where f_i ($\mathbf{x}$, t) is the discrete distribution function; Ω_i (f) is the discrete collision operator and n is the number of the discrete velocities. For numerical accuracy, the 3-dimension 19-speed model (D3Q19) is used in this work (Wang and Kang, 2009). There are usually two models for the collision operator: single relaxation time model (SRT) (Qian et al., 1992; Wang et al., 2007b) and multiple relaxation time model (MRT) (Higuera et al., 1989; Lallemand and Luo, 2000). For the numerical stability concerns of SRT model for variable-viscosity flows in porous media, the MRT model is applied in the present work (d'Humieres et al., 2002; Pan et al., 2006):

$$\Omega_i = -\sum_j \left(\mathbf{M}^{-1}\mathbf{S}\mathbf{M}\right)_{ij}\left(f_j - f_j^{eq}\right). \tag{3}$$

The features of high *Kn* flow mainly include two aspects: (1) a gas slip adjacent to the wall; (2) a lower effective viscosity of gas. In LBM, the wall gas slip can be captured by the discrete diffuse boundary condition (or the discrete Maxwellian boundary condition) (Ansumali and Karlin, 2002), and the gas viscosity is described by the Bosanquet-type effective viscosity model,

$$\mu_e = \frac{\mu}{1 + aKn}, \tag{4}$$

with the empirical parameter $a = 2.2$, suggested by Beskok and Karniadakis (1999).

To validate our numerical method, the channel flow is simulated as a benchmark. The grid is 200 × 10 and the fluid density ρ is doubled from 1 kg/m^3 to 256 kg/m^3 successively. Other parameters are listed in Table 1. The fluid is treated as ideal gas. Fig. 1(a) compares the cross-section velocity profile obtained by present LBM simulation with Beskok's model (Beskok and Karniadakis, 1999) and Fig. 1(b) compares the normalized mass flow rate $Q = \frac{\rho u_{avg}}{(-dp/dx)H}\sqrt{\frac{2RT}{M}}$ in the present work with Cercignani's theoretical solution (Cercignani et al., 2004). The agreement between our numerical simulations and the theoretical models is very good. Thus the present numerical framework for high *Kn* flow is reliable for further exploration.

2.2. Real gas effect

In the present work, the shale gas is considered as pure methane for simplicity, since the mole fraction of methane is usually more than 90% in shale gas. Real gas effect also involves two aspects: (1) the equation of state (EOS) of real gas, (2) variable properties of real gas. For the first aspect, Redlich–Kwong (RK) EOS is able to give a simple but accurate description for gas at high pressure and temperature (Shah and Thodos, 1965), which is written as

$$p = \frac{RT}{V_m - b} - \frac{a}{\sqrt{T}V_m(V_m + b)}, \tag{5}$$

where p is the gas pressure; V_m is the molar volume; a and b are constants. The RK equation works well as is shown in Fig. 2 (a) through a comparison with NIST standard data (Setzmann and Wagner, 1991). For the second aspect, the pressure-dependent dynamic viscosity is considered, which is usually a constant at a certain temperature for ideal gas. The NIST dynamic viscosity data for methane (Younglove and Ely, 1987) is adopted in the present work as is shown in Fig. 2 (b).

To accurately capture the real gas effect, our simulation should be reliable for variable properties of gas, which means the numerical results must be independent with relaxation time in LBM. Therefore, the non-slip flow in body centered cube (BCC) array of spheres is simulated as a validation. The parameters are given in Table 2 and the results are presented in Fig. 3 (similar results reported in Ref. (Pan et al., 2006)). The MRT model for collision

Table 1
Parameters for high *Kn* flow simulation.

Temperature T (K)	373
Molar mass M (kg/mol)	0.016
Pressure gradient ∇p (MPa/m)	−1
Channel height H (nm)	10
Dynamic viscosity μ (kg m^{-1} s^{-1})	1×10^{-5}