Pore-scale lattice Boltzmann simulation of micro-gaseous flow considering surface diffusion effect

Junjian Wang^a, Qinjun Kang^b, Li Chen^{b,c}, Sheik S Rahman^{a,*}

^a*School of Petroleum Engineering, University of New South Wales, Sydney, NSW, Australia, 2033*

^b*Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, NM, USA, 87545*

^c*Key Laboratory of Thermo-Fluid Science and Engineering of MOE, School of Energy and Power Engineering, Xi'an Jiaotong University, Xi'an, Shanxi, China, 710049*

Abstract

Recent studies have shown that adsorbed gas and its surface diffusion have profound influence on micro-gaseous flow through organic pores in shale gas reservoirs. In this paper, a multiple-relaxation-time (MRT) LB model is adopted to estimate the apparent permeability of organic shale and a new boundary condition, which combines Langmuir adsorption theory with Maxwellian diffusive reflection boundary condition, is proposed to capture gas slip and surface diffusion of adsorbed gas. The simulation results match well with previous studies carried out using Molecular Dynamics (MD) and show that Maxwell slip boundary condition fails to characterize gas transport in the near wall region under the influence of the adsorbed gas. The total molar flux can be either enhanced or reduced depending on variations in adsorbed gas coverage and surface diffusion velocity. The effects of pore width, pressure as well as Langmuir properties on apparent permeability of methane transport in organic pores are further studied. It is found that the surface transport plays a significant role in determining the apparent permeability, and the variation of apparent permeability with pore size and pressure is affected by the adsorption and surface diffusion.

Keywords: lattice Boltzmann method, adsorbed gas, surface diffusion, micro-gaseous flow

1. Introduction

The emerging development of the unconventional gas reservoirs such as tight gas, coal seam gas and shale gas reservoir in last decades has raised the necessity for advancing our understanding of the physical laws governing the gas flow in nano-/micro- pores. In these reservoirs, the matrix pore space can be on the same order of magnitude as the mean free path of the gas molecules. According to the Knudsen number (Kn) and Mach number (M), the dynamics of nano-/micro- scale gas flow can be similar to that of rarefied gas flows[1]. Based on this assumption, a variety of slip models such as the extended slip N-S model[2] and empirical slip models[3, 4] were developed and widely applied to study gas transport in unconventional reservoirs. However, at reservoir conditions, the presence of a large amount of adsorbed gas is also

*Corresponding author at: School of Petroleum Engineering, UNSW, Sydney, NSW, Australia, 2033

Email address: sheik.rahman@unsw.edu.au (Sheik S Rahman)

Preprint submitted to Elsevier

August 7, 2016

very common in industrial applications especially in organic shale gas reservoir[5, 6], and the impact of surface diffusion of adsorbed gas may be significant on the gas transport process[7]. Consequently, some phenomenological models in a superposition form of surface diffusion, Knudsen diffusion, slip flow and viscous flow were proposed[8, 9, 10], and all of them conclude a fast mass transport of gas at nano- to micro-scale depending on Knudsen number and surface diffusivity. While this conclusion was adopted from methane flow in graphitic and the different potentials between gas and substrates[11] are ignored, an emerging number of molecular dynamics (MD) studies[1, 11, 12, 13] on different gas-surface interaction potentials have been carried out and they claimed the deficiency of previous slip and superposition models in characterizing the micro-gas flow in a confined system with an adsorbed gas field. Although MD provides the ultimate level of details of individual particles/molecules, its huge cost on account of the vast number of molecules required to simulate limits its further applications to a large simulation domain. In recent years, lattice Boltzmann method (LBM), a mesoscopic simulation approach, by combining aspects of particle-based (microscopic) and continuum-based (macroscopic) methods, renders it ideally suited to modelling microfluidics and micro-gaseous flow in unconventional reservoirs[14, 15].

Recently, LB algorithms were developed to characterize slip effect in shale at both representative elementary volume (REV)-scale and pore-scale. Chen et al.[16, 17] cite extended the generalised LBM for slip flow at REV-scale, in which Beskok and Karniadakis-Civan's correlation[4] was used to calculate the local apparent permeability. Chen and coauthors also developed a pore-scale LBM [18, 19] based on the Dusty gas model (DGM), which is a superposition of viscous flow and Knudsen diffusion, to estimate the apparent permeability and the Knudsen diffusivity of reconstructed organic shale, and their results match well with previous studies. Still the slip approach is a popular choice, and a variety of slip boundary conditions as a function of the tangential momentum accommodation coefficient (TMAC) such as the Maxwellian diffusive boundary condition[20], combined bounce back with specular reflection boundary condition (CBBSR)[21] or combined bounce back with diffusive reflection boundary condition (CBBDR)[22] were developed, and with these boundary conditions LBM can be recognized as an efficient alternative to solve Navier-Stocks (N-S) equation in tackling rarefied gas flow problems.

Most recently, a few attempts were made in literature to apply LBM to simulate micro-gaseous flow in kerogen/organic matter by considering the gas adsorption and/or surface diffusion effects. Wang et al.[23] estimated the apparent permeability of organic shale with the use of a generalised LBM, in which the surface diffusion is considered with the aid of DGM-generalised Maxwell Stefan (GMS) model. In order to account for the adsorbed gas effect, Allan and Mavko[24] as well as Li et al.[25] introduced the adsorbed gas as an immobile layer to organic pores which decreases the permeability by reducing pore space. Allan and Mavko[24] also claimed that the adsorption layer will change the TMAC, but this claim was not substantiated in their study. Fathi and Akkutlu [26] used Shan-Chen model to simulate gas flow in shale. The authors also used Langmuir slip boundary condition as proposed by Chen and Tian[27] to consider the interaction forces on the solid surfaces. The simulation results show that, when surface diffusion coefficient is larger than molecular diffusion coefficient at high pressure or when the gas flows in a capillary less than 20nm at low pressure, the fluid velocity at the wall can exceed the fluid velocity at the centre of the capillary. Later, both Ren et al.[10] and Li et al.[25] argued that the combination of Shan-Chen model and the Langmuir boundary condition might double count the gas-solid interactions, which could introduce some non-physical phenomena in simulations. In order to overcome the discrete effect, Ren et al.[10] treated the surface diffusion of adsorbed gas as a moving wall in a CBBSR boundary condition with the premise that the gas in bulk flow

is assumed to “slip” above the adsorption layer. However, the exchange of adsorbed gas and free gas resulting from the dynamic adsorption/desorption is not considered in their model.

Based on the above review, the application of LBM to gas flow at micro-scale is still in its infancy. Although many LB models have been proposed to capture adsorbed gas and/or surface diffusion, they are controversial to each other because the lack of complete knowledge of surface properties and surface interaction potentials. In this current study, we focus on the gas-surface interaction and we aim to present a new boundary condition for the LB model to couple the adsorbed gas and surface diffusion effects based on previous MD simulation observations. The paper is organized as follows: The physical representation and mathematical formulation of LBM with the new boundary condition are introduced in sections 2 and 3. The validation of numerical model is presented in section 4. Finally, in section 5, the role of adsorbed gas coverage and surface diffusion velocity on gas flow behaviour at micro-scale are discussed, and then a particular application to organic shale is studied to analyse the effects of pore width, pressure and Langmuir parameters on gas apparent permeability.

2. Inter-facial physics of gas-solid interaction

With the decrease of length scale, the ratio of surface to volume increases rapidly and surface forces become dominant. Surface-fluid interaction governs momentum and energy transport and the gas molecular kinetics are affected by the wall molecules. When a gas molecule comes into contact with the solid surface, it may experience various events such as elastic scattering, inelastic scattering, temporary or permanent adsorption, and mobile adsorption (surface diffusion)[28]. Within the kinetic theory framework of the Maxwell slip velocity model[29], the scattering of particles was classified as specular reflection and diffusive reflection. In the specular reflection model, the sticking time is virtually negligible and incident molecules undergo perfect elastic collision with the wall, such that there is no exchange of energy with the surface and the reflected molecules have the same velocity as that of the incident molecules. In the diffuse reflection model, incident molecules reside on the wall for a long time, during which it interacts with solid atoms and completely thermalized with the surface before scattering back, such that the net velocity of reflected molecules will be the same as that of the wall (see Fig. 1). While the Maxwell model and subsequent extensions of the model have shown moderate success in the prediction of flows on smooth surfaces or rarefied gas flow with extremely long adsorption time[30], some MD simulation studies[31, 32, 33, 34] argue their deficiency in capturing complete physics associated with complex problems such as short time adsorption/desorption-related effects and surface roughness effects.

Figure 1: Schematic of gas-solid interactions without considering moderate adsorption/desorption and surface diffusion based on Maxwell slip theory[29]. f_{in} represents incident molecules with a velocity $\mathbf{u}$; in sub-figure (a), f_{sr} represents specularly reflected molecules with the same velocity as that of incident molecules after undergoing perfect elastic collision with the wall; in sub-figure (b), f_{dr} represents diffusively reflected fluid molecules with the same velocity as that of the solid wall after the incident molecules adsorbed near the wall for a long time and totally forget the incident information.

91 When gas molecules are easy to be adsorbed near the wall under strong physical interactions,
 92 and in a situation where the potential energy barrier to diffusion is smaller than the energy of
 93 desorption for diffusion to occur, an adsorbed particle may remain mobile in a metastable phase
 94 while still being physically bound to the surface. This phenomenon is known as the surface
 95 diffusion[35] (see the movement of red gas molecules along the surface in Fig. 2). Besides, there
 96 is also a probability that adsorbed molecules may escape from the surface before reaching thermal
 97 equilibrium with the surface after a short time, and leave prematurely at a velocity $\mathbf{u}_{des}$ with
 98 a portion of its energy dissipated (see Fig. 2(c))[36]. Therefore, after the incident gas molecules
 99 collide with the solid wall, in addition to the reflected behaviours that could be expressed by
 100 Maxwell slip model, they would also be adsorbed on the surface and move in terms of surface
 101 diffusion or escape back into the bulk gas before reaching thermal equilibrium with the surface.
 102 (see Fig. 2(c)).

Figure 2: Schematic of gas-solid interactions considering surface diffusion and adsorption/desorption based on Maxwell slip theory[29] and inter-facial physics with adsorption field[35, 36]. Red molecules represent gas molecules being adsorbed physically on solid and moving forward with a total surface diffusion velocity $\mathbf{u}_{surface}$. (a) denotes the specular reflected gas molecules, (b) denotes the diffusive reflected gas molecules and (c) denotes the adsorption of incident gas molecules and the premature desorption of adsorbed gas molecules with a velocity $\mathbf{u}_{des}$.

103 A completely mathematical description of gas-surface interaction is under development.

104 However, as the adsorption phase contributes to transport of gas to a great extent in some cases,
 105 many studies have been carried out in regards to this aspect. The Langmuir model[37] and
 106 the Brunauer-Emmett-Teller (BET) model[38] are widely used to model adsorbing capacity of
 107 mono-layer adsorption and multilayer adsorption, respectively. Also, surface diffusion of ad-
 108 sorbed gas was introduced by hopping process[35] or random walk statistics[39] to explain the
 109 mass flow in excess to that predicted by Knudsen's model. Krishna and Wesselingh[9] proposed
 110 a Maxwell-Stefan approach combined with the Langmuir adsorption isotherm (which implicitly
 111 implies equilibrium), and yielded a reasonable expression for the description of surface diffusion
 112 which is confirmed by experimental work and simulation studies[40, 41]. In their approach the
 113 molar flux of surface diffusion in a single component system can be expressed as:

$$N_{surface} = q_{sat} \frac{D_s}{1 - \theta} \nabla \theta, \quad (1)$$

114 where D_s is the Maxwell-Stefan diffusivity that can be estimated from experimental studies or
 115 molecular dynamic (MD) simulations, q_{sat} is the Langmuir volume, and θ is the fractional cover-
 116 age of adsorbed gas which satisfies $\theta = q/q_{sat} = bP/(1 + bP)$ based on Langmuir model, where
 117 b is the Langmuir constant, P is the pressure, and q is the surface concentration. Therefore, the
 118 surface diffusion velocity $u_{surface}$ can be written as:

$$u_{surface} = \frac{N_{surface}M}{\rho_{ads}} = \frac{q_{sat}M}{\rho_{ads}} \frac{bD_s}{1 + bP} \nabla P, \quad (2)$$

119 where M and ρ_{ads} are molecular weight of adsorbed gas and the density of adsorbed gas, respec-
 120 tively.

121 3. Lattice Boltzmann model

122 3.1. LB equation

123 The multiple-relaxation-time (MRT)-LB equation derived from Boltzmann equation can be
 124 written as[42]:

$$f_i(\mathbf{x} + \mathbf{c}_i \delta_t, t + \delta_t) - f_i(\mathbf{x}, t) = \Omega_i(f), \quad (3)$$

125 where $f_i(\mathbf{x}, t)$ is the discrete distribution function for particles with velocities $\mathbf{c}_i$ at position $\mathbf{x}$ and
 126 time t , δ_t is the time step, and $\Omega_i(f)$ is the MRT discrete collision operator.

127 In D2Q9 model, the discrete velocity $\mathbf{c}_i$ is defined as $\mathbf{c}_1 = (0, 0)$, $\mathbf{c}_2 = -\mathbf{c}_4 = (1, 0)c$, $\mathbf{c}_3 =$
 128 $-\mathbf{c}_5 = (0, 1)c$, $\mathbf{c}_6 = -\mathbf{c}_8 = (1, 1)c$, $\mathbf{c}_7 = -\mathbf{c}_9 = (-1, 1)c$. where $c = \delta_x/\delta_t$ is the lattice speed with
 129 δ_x being the lattice spacing. The MRT collision operator is given by:

$$\Omega_i(f) = -(\mathbf{M}^{-1}\mathbf{S}\mathbf{M})_{ij}(f_j - f_j^{eq}), \quad (4)$$

130 where $\mathbf{M}$ is a orthogonal transformation matrix and $\mathbf{S} = \text{diag}(\tau_\rho, \tau_e, \tau_\varepsilon, \tau_j, \tau_q, \tau_j, \tau_q, \tau_s, \tau_s)^{-1}$ is a
 131 diagonal matrix.

132 The distribution function f_i and its equilibrium distribution function f_i^{eq} can be projected onto
 133 the moment space, and the following results can be obtained:

$$\mathbf{m} = \mathbf{M}\mathbf{f} = (\rho, e, \varepsilon, j_x, q_x, j_y, q_y, p_{xx}, p_{xy})^T, \quad (5)$$

$$\begin{aligned} \mathbf{m}^{eq} &= \mathbf{M}\mathbf{f}^{eq} = (\rho, e^{eq}, \varepsilon^{eq}, j_x, q_x^{eq}, j_y, q_y^{eq}, p_{xx}^{eq}, p_{xy}^{eq})^T \\ &= \rho(1, -2 + 3|\mathbf{u}|^2, 1 - 3|\mathbf{u}|^2, u, -v, u, -v, u^2 - v^2, uv)^T, \end{aligned} \quad (6)$$

where $\mathbf{f} = (f_1, f_2, \dots, f_9)^T$ and $\mathbf{f}^{eq} = (f_1^{eq}, f_2^{eq}, \dots, f_9^{eq})^T$; ρ is the density, e is the energy mode, ε is related to energy square, (j_x, j_y) are the momentum components, (q_x, q_y) correspond to energy flux, (p_{xx}, p_{xy}) are related to the diagonal and off-diagonal components of the stress tensors; u and v are the components of the velocity $\mathbf{u}$, respectively.

For isothermal gas flow, the macroscopic density, momentum, and the shear viscosity are recovered by:

$$\rho = \sum_i f_i, \quad \rho \mathbf{u} = \sum_i \mathbf{c}_i f_i, \quad \mu = \rho c_s^2 (\tau_s - \frac{1}{2}) \delta_t, \quad (7)$$

where $c_s = \sqrt{RT} = c / \sqrt{3}$ is the sound speed, in which R is the gas constant and T is the temperature.

To account for the effect of gas molecule/wall interactions, generally two kinds of corrections on mean free path and/or viscosity are proposed in the literature. Zhang et al.[43] and Guo et al.[44] introduced different effective Knudsen number expressions considering the distances of the gas from the solid walls. Besides, Guo et al.[42] and Li et al.[45] averaged the effect of the Knudsen layer to the whole flowing area and proposed the simplified effective Knudsen number expressions. More discussions on Knudsen layer effect can be found from our previous review paper[15]. In this study, the average effective Knudsen number proposed by Guo et al.[42] is used, and the relaxation time τ_s is chosen as:

$$\tau_s = \frac{1}{2} + \sqrt{\frac{6}{\pi}} N Kn \frac{2}{\pi} \arctan(\sqrt{2} Kn^{-3/4}), \quad (8)$$

where N is the grid number in the direction of the characteristic length. Note that the fact that $c = \sqrt{3} c_s = \sqrt{3RT} = \delta_x / \delta_t = 1$ has been used in the above deduction.

3.2. Boundary conditions

3.2.1. Wall boundaries

The wall boundary conditions are required to appropriately describe the momentum exchanges between gas molecules and solid walls, so as to capture the slip motion and adsorption/desorption of gas molecular in organic shale. In order to take account of the adsorption/desorption as well as the surface diffusion effects that are illustrated in Fig.2, inspired by the work of Levesque et al.[36, 46] and their co-workers[47], we firstly proposed a similar propagation scheme in the slip boundary condition for micro-gas flow. In the new boundary condition, the solid wall is assumed to be covered by a certain amount of adsorbed gas and the adsorption/desorption is in equilibrium, therefore the density of both free gas and adsorbed gas remains constant. The transport of the adsorbed gas is following the surface diffusion rule and it is assumed to be independent to the transport of the free gas. The influence of premature desorption of adsorbed gas on free gas transport is introduced to the new boundary condition by the definition of a “post-desorption distribution functions” $f_i^{des}(\mathbf{x})$, and $\mathbf{u}_{des}$ is assumed to be the same as $\mathbf{u}_{surface}$. The distribution function of fluid boundary nodes $f_i^{BC}(\mathbf{x})$ is defined as:

$$f_i^{BC}(\mathbf{x}, \rho, \mathbf{u}) = \theta f_i^{des}(\mathbf{x}, \rho, \mathbf{u}_{surface}) + (1 - \theta) f_i^{fr}(\mathbf{x}, \rho, \mathbf{u}_w), \quad (9)$$

$f_i^{fr}(\mathbf{x})$ is the reflected distribution function contributed from the free gas. $f_i^{des}(\mathbf{x})$ holds the free gas density and with the surface velocity $\mathbf{u}_{surface}$ according to its definition.

170 In order to calculate the distribution function associated with free gas particles $f_i^{fr}(\mathbf{x})$, the
 171 kinetic boundary condition proposed by Tang et al.[20] is introduced, where $f_i^{fr}(\mathbf{x})$ is a combina-
 172 tion of the specular reflection distribution function, f_i^{sr} with the completely diffusive distribution
 173 function, f_i^{dr} , and it can be expressed as:

$$f_i^{fr}(\mathbf{x}) = r f_i^{dr}(\mathbf{x}) + (1 - r) f_i^{sr}(\mathbf{x}), (\mathbf{c}_i - \mathbf{u}_w) \cdot \mathbf{n} > 0, \quad (10)$$

174 where the specular reflected distribution function, f_i^{sr} satisfies:

$$f_i^{sr}(\mathbf{x}) = f_{i'}(\mathbf{x}), \quad (11)$$

175 with $\mathbf{c}_{i'} = \mathbf{c}_i - 2[(\mathbf{c}_i - \mathbf{u}_w) \cdot \mathbf{n}]\mathbf{n}$ being the specular velocity of $\mathbf{c}_i$, and $\mathbf{n}$ is the unit normal vector.
 176 The diffusive distribution part is derived by Ansumali and Karlin[48] and can be calculated as:

$$f_i^{dr}(\mathbf{x}) = \frac{\sum_{(\mathbf{c}_j - \mathbf{u}_w) \cdot \mathbf{n} < 0} |(\mathbf{c}_j - \mathbf{u}_w) \cdot \mathbf{n}| f_j(\mathbf{x})}{\sum_{(\mathbf{c}_i - \mathbf{u}_w) \cdot \mathbf{n} > 0} |(\mathbf{c}_i - \mathbf{u}_w) \cdot \mathbf{n}| f_i^{eq}(\mathbf{x})} f_i^{eq}(\mathbf{x}). \quad (12)$$

177 To match the second order slip boundary condition with a half-way reflection mode, the
 178 contribution of the diffusive reflection part, r in Eq. 10 and the relaxation time, τ_q must be
 179 chosen as[49]:

$$r = 2(1 + \sqrt{\frac{\pi}{6}} A_1)^{-1}, \quad (13)$$

$$\tau_q = \frac{1}{2} + \frac{\pi A_2 (2\tau_s - 1)^2 + 3}{8(2\tau_s - 1)}, \quad (14)$$

180 where A_1 and A_2 are functions of tangential momentum accommodation function, σ [44]:

$$A_1 = \frac{2 - \sigma}{\sigma} (1 - 0.1817\sigma), \quad (15)$$

$$A_2 = \frac{2}{\pi} + \frac{1}{2} A_1^2. \quad (16)$$

182 For the calculation of “post-desorption distribution functions” $f_i^{des}(\mathbf{x})$, we introduced the
 183 boundary condition proposed by Inamuro et al.[50]. $f_i^{des}(\mathbf{x})$ is assumed to be the equilibrium
 184 distribution function with a counter slip velocity to ensure the gas at the fluid boundary has the
 185 velocity, $\mathbf{u}_{surface}$ and the density, ρ :

$$f_i^{des}(\mathbf{x}) = f_i^{eq}(\mathbf{x}, \rho', u'), \quad (17)$$

186 and for lower fluid boundary nodes, we have:

$$\rho = \frac{1}{1 - v_{surface}} [f_1 + f_2 + f_4 + 2(f_5 + f_8 + f_9)], \quad (18)$$

$$\rho' = 6[(\rho v_{surface} + f_5 + f_8 + f_9)/(1 + 3v_{surface} + 3v_{surface}^2)], \quad (19)$$

$$u' = \frac{1}{1 + 3v_{surface}} \{6[(\rho u_{surface} - (f_2 + f_9 - f_4 - f_8))/\rho'] - u_{surface} - 3u_{surface} v_{surface}\}, \quad (20)$$

where $u_{surface}$ and $v_{surface}$ are the x and y components of the velocity $\mathbf{u}_{surface}$, respectively. With an assumption that the surface diffusion is along the channel ($v_{surface} = 0$), and in consistent with the half-way boundary condition used to calculate $f^{fr}(\mathbf{x})$, $u_{surface}$ needs to be replaced with $u'_{surface}$, and $u'_{surface}$ is given as:

$$u'_{surface} = u_{surface} + 4u_{max}(\frac{1}{2}\delta x/H)(1 - (\frac{1}{2}\delta x/H)), \quad (21)$$

where u_{max} is the maximum streamwise velocity, H is the channel height, and $u_{surface}$ can be calculated based on Eq. 2.

3.2.2. Inlet/outlet

In order to specify the pressure on flow boundaries, the extrapolated boundary conditions[22] are employed at inlet/outlet ends of the channel. The inlet and outlet are located at $x = (1, y)$ and $x = (N_x, y)$ with $y \in [1, N_y]$, the ghost nodes are defined at the positions $x = (0, y)$ and $x = (N_x + 1, y)$. The following equations are used to determine the unknown distribution based on a linear extrapolation scheme:

$$f_i(0, y) = 2f_i(1, y) - f_i(2, y), i = \{2, 6, 9\}, \quad (22)$$

$$f_i(N_x + 1, y) = 2f_i(N_x, y) - f_i(N_x - 1, y), i = \{4, 7, 8\}, \quad (23)$$

after this, in order to realize the pressure boundary condition, the extrapolated density needs to be renormalized to the prescribed density:

$$\rho_{new}(1, y) = \frac{N_y \rho_{in}}{\sum_{y=1}^{N_y} \rho(1, y)} \rho(1, y), \quad (24)$$

$$\rho_{new}(N_x, y) = \frac{N_y \rho_{out}}{\sum_{y=1}^{N_y} \rho(1, y)} \rho(N_x, y). \quad (25)$$

The renormalized values are used in the equilibria to carry out the ensuring collision step. This procedure ensures the pressure profile is consistent with flow field inside the channel[22].

4. Numerical validation

The simulation runs are carried out by assuming $\theta = 0$ and the results are compared with that of DSMC and IP-DSMC results as reported by Shen et al. [51], which are suitable for modelling micro-gaseous flow and have been extensively used for such validation purposes. In this case, the ratio of the length to the height, L/H is 100, and a uniform lattice $N_x \times N_y = 2100 \times 21$ is adopted. The outlet gas density ρ_{out} is 1, and pressure ratio of inlet and outlet p_{in}/p_{out} is taken as 1.4 for $Kn_{out} = 0.0194$ and 2 for $Kn_{out}=0.194$, respectively. The convergence criterion towards the steady state is set as follows:

$$\sqrt{\frac{\sum_i |\mathbf{u}(\mathbf{x}_i, t_n) - \mathbf{u}(\mathbf{x}_i, t_n - 1000\delta t)|^2}{\sum_i |\mathbf{u}(\mathbf{x}_i, t_n)|^2}} < 10^{-12} \quad (26)$$

211 The normalized streamwise velocity $U = u/u_{max}$ predicted by this study for $Kn_{out} = 0.0194$
 212 and $Kn_{out} = 0.194$ are shown in Fig. 3. It can be seen from the figure that the overall velocity
 213 profile are in good agreement with those of the DSMC/IP-DSMC and the LBM is applicable for
 214 slip flow and the early part of transition regime which covers a large portion of flow in shale.

Figure 3: Normalized streamwise velocity at different Knudsen number

215 The molar fluxes through a channel with $H = 5nm$ and $L = 50nm$ at $T = 338.7k$ predicted
 216 by DGM under different pressures are also presented for validation. By the superposition of
 217 convective transport and Knudsen diffusion, Veltzke and Thöming[52] proposed the DGM for
 218 channel and tube flow and concluded that the mass flux estimated by DGM fits the experimental
 219 data well in the slip regime and the beginning of transition regime. The molar flux estimated
 220 based on DGM for a single channel can be written as:

$$N_{DGM} = -\frac{1}{RT}(D_k + \frac{K_0}{\eta}P)\nabla P, \quad (27)$$

221 where D_k is Knudsen diffusivity, K_0 is the absolute permeability, and η is viscosity. The compar-
 222 isons are shown in Fig.4, and the simulation results estimated based on LB model are comparable
 223 to those of the DGM.

Figure 4: Molar flux at different pressure ($T=338.7\text{K}$, $H=5\text{nm}$, $L=50\text{ nm.}$)

5. Simulation examples

5.1. Influence of adsorbed gas and surface diffusion on micro-gaseous flow

In order to qualify the influence of adsorbed gas and its surface diffusion on micro-gaseous flow, in this section, the normalized streamwise velocity distribution of the free gas and the total molar flux at different θ and D_s are analysed. Methane flow through channels with $P_{in} = 22\text{MPa}$ and $P_{out} = 20\text{MPa}$ at $T = 338.7\text{K}$ are considered. $N_x \times N_y = 41 \times 803$ lattice and $N_x \times N_y = 41 \times 403$ lattice are adopted to discretize $5 \times 100\text{nm}$ and $10 \times 100\text{nm}$ micro-channels, respectively. Extrapolated boundary conditions are applied to the inlet and outlet boundaries, and the proposed boundary condition is applied to the solid wall. Before starting the simulation, f^{eq} with $\mathbf{u} = 0$ and ρ satisfying linear distribution from ρ_{in} and ρ_{out} are adopted as the initial value of distribution function f_i at each lattice. Based on the fact that the adsorbed gas molecules need to overcome additional resistance of the wall, the surface diffusion velocity is assumed to be no larger than the slip velocity without the consideration of adsorption and surface diffusion[10, 25], and the normalized slip velocity satisfies $U_s = 4A_1K_n + 8A_2K_n$ [49]. When the gas adsorption reaches a maximum, the density of the adsorbed gas $\rho_{ads,sat}$ is assumed to be 340kg/m^3 according to Ambrose et al.'s work[53], and therefore the density of the adsorbed gas at different θ satisfies $\rho_{ads} = \theta\rho_{ads,sat}$.

5.1.1. Influence of θ and D_s on normalised streamwise velocity

The normalised stream-wise velocities of the free gas at different adsorbed gas coverages and different surface diffusion velocities are shown in Fig.5. When $\theta = 0$, the variation of $u_{surface}$ does not influence the free gas flow because there is no adsorbed gas in the system (Fig.5 (a)). The gas slip at the solid surface is controlled by the interaction of free gas molecules with solid molecules and the rarefaction dominate the flow which leads to a large slip velocity at the boundary. When $\theta = 1$, the slip velocity of the free gas at the solid surface is completely determined by the desorbed gas, and it vanishes to zero at $u_{surface} = 0$ (Fig.5 (d)). This results is consistent with a very recent MD study performed by Wang et al.[11], who claimed that the gas flow in confined micro-channel manifests a parabolic velocity profile with zero slip velocity at the solid surface when an immobile adsorption layer is formed, and the slip model based on kinetic theory[54]

fails to capture the flow behavior. When the solid surface is partially covered by an amount of
 adsorbed gas, the slippage of the free gas is determined by the interactions with both solid wall
 and the adsorbed gas, and the “dynamic similarity” of rarefied gas flow and micro-scale confined
 flow breaks down. At a certain coverage, the gas slip at the wall decreases with the decreased
 $u_{surface}$ as a result of the premature short-time desorption of adsorbed gas (Fig.5 (b) and (c)).
 Compared different sub-figures in Fig.5, when $u_{surface} = u_s$, the increase with coverage does not
 influence the slip velocity as according to the assumption of $u_{des} = u_{surface}$, otherwise, the slip
 of the free gas is decreased with the increase of adsorbed gas coverage θ at a certain $u_{surface}$.
 Previous MD studies have concluded that the near wall velocity profile shows reduced gas slip
 with the increased surface-gas potential strength/ more explicit adsorption[1, 11, 13, 55, 56], and
 this phenomenon is confirmed by current LB simulation results in this study.

Figure 5: Normalized velocity U at different surface coverage θ and surface diffusion velocity $u_{surface}$. Width=5nm, length=100nm, $T = 338.7K$, $P_{in} = 22MPa$ and $P_{out} = 20MPa$.

5.1.2. Influence of θ and D_s on molar flux

The molar flux of the free gas N_{free} , the molar flux of the adsorbed gas $N_{surface}$ and the total molar flux $N_{free} + N_{surface}$ at different θ and $u_{surface}$ of 5nm and 10nm wide channels are shown

in Figs. 6 and 7, respectively. In Fig. 6 (a) and Fig. 7 (a), the variations of N_{free} with θ are consistent with the velocity profiles shown in Fig.5. It remains as a constant at different θ when $u_{surface} = u_s$, and it decreases with the increase of θ because the $u_{surface}$ is assumed to be smaller than u_s . $N_{surface} = 0$ at $u_{surface} = 0$ as the adsorbed gas is immobile, otherwise, $N_{surface}$ shows a linearly increase with the increase of θ because the adsorbed gas density close to the solid surface is much larger at a larger θ . Also, $N_{surface}$ increases with the increase of $u_{surface}$ as a larger $u_{surface}$ indicates a stronger mobility of the adsorbed gas. Compared N_{free} with $N_{surface}$, it can be concluded that the molar flux produced by surface diffusion is more significant than that of free gas at a large adsorption coverage if the adsorbed gas is mobile in the system. In a 5nm wide channel, the $N_{surface}$ can exceed N_{free} at $u_{surface} = u_s$ and $u_{surface} = 0.8u_s$ if the solid surface is covered by enough adsorbed gas (Fig.6(a)). In Fig. 6 (b) and Fig. 7 (b), the variation of N_{total} shows a changeable trend with θ at different $u_{surface}$. At low $u_{surface}$, N_{total} decreases with θ because the adsorbed gas contributes very little to the total mass flow. However, at high $u_{surface}$, since the adsorbed gas density is much larger than that of free gas, the adsorbed gas contributes substantial mass flux, and N_{total} starts to increase with θ . These results are consistent with a recent non-equilibrium molecular dynamics (NEMD) study on gas transport in nanopores. Wu and Zhang[12] performed several NEMD simulations on gas flow through illite and graphene channels, and they concluded that the total mass flux is significantly influenced by the gas mobility in adsorption region, and the mass flux can either be enhanced or reduced by adsorbed gas.

Figure 6: Variation of molar flux with adsorption gas coverage at different surface diffusion velocity. The molar flux of free gas is indicated by solid line and the molar flux of adsorbed gas is indicated by dash line. Width=5nm, length=100nm, $T = 338.7K$, $P_{in} = 22MPa$ and $P_{out} = 20MPa$.

Figure 7: Variation of molar flux with adsorption gas coverage at different surface diffusion velocity. The molar flux of free gas is indicated by solid line and the molar flux of adsorbed gas is indicated by dash line. Width=10nm, length=100nm, $T = 338.7K$, $P_{in} = 22MPa$ and $P_{out} = 20MPa$.

5.2. Application of the LBM to study gas flow in organic shale

In this section, the LB model with the proposed boundary condition is used to study gas flow in organic shale considering the surface diffusion of adsorbed gas. It is noted that the gas flow in porous shale is conventionally modelled as capillaries. Here, pressure driven methane flow through 100nm long micro-channels with width ranges from 5nm to 40nm are considered, and extrapolated boundary conditions are applied to the inlet and outlet boundaries. The outlet pressure ranges from 10MPa to 50MPa, and the inlet pressure is 2MPa higher than outlet pressure. Langmuir adsorption isotherm model is used to describe the adsorption of methane into shale matrix, and the Maxwell-Stefan approach is applied to describe the transport of adsorbed gas. Therefore, $\theta = bP/(1 + bP)$ and $u_{surface}$ can be expressed as a function of Langmuir properties and surface diffusivity with Eq. 2. Because the apparent permeability of gas is one of the most important petro-physical parameters to porous shale, and its variation with rock properties and production conditions usually attracts many discussions, the influences of pore width, pressure and Langmuir properties on gas apparent permeability are discussed. Based on a sensitivity analysis, parameters affecting apparent permeability of organic shale are quantified. The apparent permeability is calculated with $k_{app} = N_{total}M\mu/(\rho_{free}\nabla P)$. Since the specific values of surface diffusivity and Langmuir property of shale samples are still not clear and more experiments will likely be done in the future, in this study a wide range of parameter analysis is considered. D_s from 0 to $1 \times 10^{-5}m^2/s$, b from 0.125 to $1 MPa^{-1}$ and q_{sat} from 1000 to 8000 mol/m^3 [23] are used for the following discussions.

5.2.1. Influence of the pore width

In order to study the influence of pore width on gas apparent permeability, the variations of K_{app} and the ratio of K_{app} to intrinsic permeability K_0 with pore width at different surface diffusivities are simulated using the LB model developed in this study and the results are shown in Figs.8 and 9. The permeability without adsorbed gas is also presented for the purpose of comparison. Temperature, the Langmuir volume (q_{sat}), and the Langmuir constant (b) are set to be 338.7K, 8000 mol/m^3 and $1 \times 10^{-6}Pa^{-1}$, respectively. From Figs.8 and 9 it can be seen that, at low surface diffusivity, pore width has a negligible effect on K_{app} . When surface diffusion is noticeable, the pore width has a significant influence on both K_{app} and K_0 . With the increase

in pore width, both K_{app} and K_0 increase, and the K_{app}/K_0 reaches a Plateau at pore diameter of about $40nm$. This behaviour can be explained by the fact that in larger pores, the flux from viscous flow is predominant and the surface effects which include the gas slip and the surface diffusion are almost negligible. As a consequent of this, K_{app} becomes approximately equal to K_0 . Moreover, the effect of pore diameter on K_{app} is more pronounced at high surface diffusivity especially at low pressures, and difference in K_{app} and K_0 is increased with the increase of D_s in a certain pore space. Comparing cases with and without adsorbed gas, K_{app} considering adsorbed gas is smaller than that without considering adsorbed gas at low D_s . When D_s reaches an order of $10^{-6}m^2/s$, with the increase of D_s , a significant underestimation of K_{app} can be observed at high surface diffusivity in small pores, which is in good agreement with previous pore-scale numerical studies[8, 57].

Figure 8: K_{app}/K_0 and K_{app} at $P_{in} = 22MPa$ and $P_{out} = 20MPa$

Figure 9: K_{app}/K_0 and K_{app} at $P_{in} = 12MPa$ and $P_{out} = 10MPa$

5.2.2. Influence of pressure

The variations of K_{app} and K_{app}/K_0 with average pressure are shown in Figs. 10 and 11. Temperature, Langmuir properties and surface diffusivity are the same as those in Sec.5.2.1. Figs.10 and 11 illustrate that, at extremely low surface diffusivity, as the immobile adsorbed gas restricts the surface flow, the effect of pressure on the K_{app} is diminished and K_{app} approximately equals K_0 . Otherwise, since the increased pressure reduces the mobility of adsorbed gas and the rarefaction, the K_{app} and K_{app}/K_0 decrease with the increase in average pressure especially in smaller pores, which is consistent with the macroscopic behavior of shale gas production[58]. At low pressure, both gas slip and the surface diffusion of adsorbed gas contribute to the increased K_{app} , and when D_s reaches to an order of $10^{-6} \text{ m}^2/\text{s}$, the K_{app} is larger than cases without adsorbed gas. The results also indicate that, at high pressure conditions such as reservoir condition, although the rarefaction and slip effects are negligible, the surface diffusion of adsorbed gas can have significant contribution of total mass flux and finally leads to a large K_{app} compared to K_0 at high surface diffusivity.

Figure 10: K_{app}/K_0 and K_{app} at Width = 5nm and Length = 100nm

Figure 11: K_{app}/K_0 and K_{app} at Width = 10nm and Length = 100nm

5.2.3. Influence of Langmuir properties

In an effort to better understand the role of adsorbed gas on apparent permeability of shale, the effects of Langmuir volume (q_{sat}) and Langmuir constant (b) on K_{app} are evaluated and the results are shown in Figs.12 and 13. The inlet pressure, outlet pressure, the pore width, and length are set as 22MPa, 20MPa, 10nm and 100nm, respectively. From Fig.12 it can be seen that for constant value of b , an increase in q_{sat} leads to an increase in $u_{surface}$ which results in a larger K_{app} , especially at high surface diffusivities. This is also evident in Eq.2 that q_{sat} is the controlling parameter for velocity of adsorbed gas. The influence of b , however, is of two folds: b controls both θ and $u_{surface}$ at a certain pressure condition. Fig.13 shows that, with low surface diffusivity, the influence of b on $u_{surface}$ is negligible, and that the K_{app} decreases with b as more gas tends to be adsorbed on the solid surface. As D_s increases, the effect of b on $u_{surface}$ becomes noticeable, and the K_{app} starts to increase with b .

Figure 12: Variation of K_{app} with q_{sat}

Figure 13: Variation of K_{app} with b

6. Conclusion

In this study, a MRT lattice Boltzmann model with a new boundary condition to account for adsorbed gas and surface diffusion effects is employed to study gas flow in organic shale and to estimate apparent permeability. The effects of pore width, pressure, and Langmuir properties on apparent permeability have been carried out.

By introducing an extra “post-desorption term” in kinetic boundary condition to reflect adsorbed gas with the aid of Langmuir adsorption model, the results of current LB model match reasonably well with previous studies and capture critical phenomena observed by MD simulations. Neglecting the adsorbed gas results in slip of the free gas, and it is consistent with the kinetic theory predictions. Presence of adsorbed gas breaks down the dynamic similarity between rarefied and nano-/micro-scale gas flows based on the Knudsen numbers. Current LB model shows reduced gas slip with the decrease of surface diffusion velocity and stick when an immobile adsorbed gas layer is formed near the solid surface. The new boundary condition overcomes the shortage of previous slip boundary conditions in LB model that indicates substantial velocity slip on the solid walls.

The sensitivity studies confirm that, unlike the intrinsic permeability, the apparent permeability of organic shale is a dynamic parameter and should be adjusted during the production. The apparent permeability increases with the increase of pore radius and the decrease of pressure, and it is controlled by the Langmuir properties. The adsorbed gas and its surface diffusion have a profound effect in determining the apparent permeability, and the gas apparent permeability can be either enhanced or reduced depending on variations in surface diffusion of adsorbed gas under different conditions.

Results of this study can help improve our understanding on solid-gas interactions near the wall and gas adsorption as well as surface diffusion in organic shale. The proposed LB model will be extended in porous shale in future studies.

7. Acknowledgements

The authors thank the support from SCOPE, UNSW and the LDRD program of LANL. J.W. thanks the financial support from the China Scholarship Council (CSC). L.C. thanks the support from National Nature Science Foundation of China (No. 51406145, 51136004), and Q.K. thanks the support from a DOE oil & gas project.

8. References

- [1] M. Barisik, A. Beskok, Surface–gas interaction effects on nanoscale gas flows, *Microfluidics and nanofluidics* 13 (5) (2012) 789–798.
- [2] F. Javadpour, D. Fisher, M. Unsworth, Nanoscale gas flow in shale gas sediments, *Journal of Canadian Petroleum Technology* 46 (10) (2007) 55–61.
- [3] A. Beskok, G. E. Karniadakis, Report: a model for flows in channels, pipes, and ducts at micro and nano scales, *Microscale Thermophysical Engineering* 3 (1) (1999) 43–77.
- [4] F. Civan, C. S. Rai, C. H. Sondergeld, Shale gas permeability and diffusivity inferred by improved formulation of relevant retention and transport mechanisms, *Transport in Porous Media* 86 (3) (2011) 925–944.
- [5] P. Charoensuppanimit, S. A. Mohammad, K. A. Gasem, Measurements and modeling of gas adsorption on shales, *Energy & Fuels* 30 (3) (2016) 2309–2319.
- [6] Y. Wu, J. Li, D. Ding, C. Wang, Y. Di, A generalised framework model for the simulation of gas production in unconventional gas reservoirs, *SPE Journal* 19 (05) (2014) 845–857.
- [7] Z. Zhai, X. Wang, X. Jin, L. Sun, J. Li, D. Cao, Adsorption and diffusion of shale gas reservoirs in modeled clay minerals at different geological depths, *Energy & Fuels* 28 (12) (2014) 7467–7473.

- [8] K. Wu, X. Li, C. Wang, W. Yu, Z. Chen, Model for surface diffusion of adsorbed gas in nanopores of shale gas reservoirs, *Industrial & Engineering Chemistry Research* 54 (12) (2015) 3225–3236.
- [9] R. Krishna, J. Wesselingh, The maxwell-stefan approach to mass transfer, *Chemical Engineering Science* 52 (6) (1997) 861–911.
- [10] J. Ren, P. Guo, Z. Guo, Z. Wang, A lattice boltzmann model for simulating gas flow in kerogen pores, *Transport in Porous Media* (2014) 1–17.
- [11] S. Wang, Q. Feng, F. Javadpour, Y.-B. Yang, Breakdown of fast mass transport of methane through calcite nanopores, *The Journal of Physical Chemistry C* 120 (26) (2016) 14260–14269.
- [12] T. Wu, D. Zhang, Impact of adsorption on gas transport in nanopores, *Scientific Reports* 6.
- [13] M. Barisik, A. Beskok, law of the nano-wall in nano-channel gas flows, *Microfluidics and Nanofluidics* 20 (3) (2016) 1–9.
- [14] J. Zhang, Lattice boltzmann method for microfluidics: models and applications, *Microfluidics and Nanofluidics* 10 (1) (2011) 1–28.
- [15] J. Wang, L. Chen, Q. Kang, S. S. Rahman, The lattice boltzmann method for isothermal micro-gaseous flow and its application in shale gas flow: a review, *International Journal of Heat and Mass Transfer* 95 (2016) 94–108.
- [16] L. Chen, W. Fang, Q. Kang, J. D. Hyman, H. S. Viswanathan, W.-Q. Tao, Generalized lattice boltzmann model for flow through tight porous media with klinkenberg’s effect, *Physical Review E* 91 (3) (2015) 033004.
- [17] L. Chen, Q. Kang, Z. Dai, H. S. Viswanathan, W. Tao, Permeability prediction of shale matrix reconstructed using the elementary building block model, *Fuel* 160 (2015) 346–356.
- [18] L. Chen, Q. Kang, R. Pawar, Y.-L. He, W.-Q. Tao, Pore-scale prediction of transport properties in reconstructed nanostructures of organic matter in shales, *Fuel* 158 (2015) 650–658.
- [19] L. Chen, L. Zhang, Q. Kang, H. S. Viswanathan, J. Yao, W. Tao, Nanoscale simulation of shale transport properties using the lattice boltzmann method: permeability and diffusivity, *Scientific reports* 5.
- [20] G. Tang, W. Tao, Y. He, Lattice boltzmann method for gaseous microflows using kinetic theory boundary conditions, *Physics of Fluids (1994-present)* 17 (5) (2005) 058101.
- [21] S. Succi, Mesoscopic modeling of slip motion at fluid-solid interfaces with heterogeneous catalysis, *Physical review letters* 89 (6) (2002) 064502.
- [22] F. Verhaeghe, L.-S. Luo, B. Blanpain, Lattice boltzmann modeling of microchannel flow in slip flow regime, *Journal of Computational Physics* 228 (1) (2009) 147–157.
- [23] J. Wang, L. Chen, Q. Kang, S. S. Rahman, Apparent permeability prediction of organic shale with generalized lattice boltzmann model considering surface diffusion effect, *Fuel* 181 (2016) 478–490.
- [24] A. M. Allan, G. Mavko, The effect of adsorption and knudsen diffusion on the steady-state permeability of microporous rocks, *Geophysics* 78 (2) (2013) D75–D83.
- [25] Z.-Z. Li, T. Min, Q. Kang, Y.-L. He, W.-Q. Tao, Investigation of methane adsorption and its effect on gas transport in shale matrix through microscale and mesoscale simulations, *International Journal of Heat and Mass Transfer* 98 (2016) 675–686.
- [26] E. Fathi, Lattice boltzmann method for simulation of shale gas transport in kerogen, *SPE Journal* 18 (1) (2013) 27–37.
- [27] S. Chen, Z. Tian, Simulation of microchannel flow using the lattice boltzmann method, *Physica A: Statistical Mechanics and its Applications* 388 (23) (2009) 4803–4810.
- [28] S. Brull, P. Charrier, L. Mieussens, Gas-surface interaction and boundary conditions for the boltzmann equation, *Kinetic and related models* 7 (2) (2014) 422–450.
- [29] J. C. Maxwell, On stresses in rarified gases arising from inequalities of temperature, *Philosophical Transactions of the royal society of London* 170 (1879) 231–256.
- [30] W.-M. Zhang, G. Meng, X. Wei, A review on slip models for gas microflows, *Microfluidics and nanofluidics* 13 (6) (2012) 845–882.
- [31] S. K. Bhatia, M. R. Bonilla, D. Nicholson, Molecular transport in nanopores: a theoretical perspective, *Physical Chemistry Chemical Physics* 13 (34) (2011) 15350–15383.
- [32] B.-Y. Cao, Non-maxwell slippage induced by surface roughness for microscale gas flow: a molecular dynamics simulation, *Molecular Physics* 105 (10) (2007) 1403–1410.
- [33] B.-Y. Cao, J. Sun, M. Chen, Z.-Y. Guo, Molecular momentum transport at fluid-solid interfaces in mems/nems: a review, *International journal of molecular sciences* 10 (11) (2009) 4638–4706.
- [34] V. Sokhan, D. Nicholson, N. Quirke, Fluid flow in nanopores: an examination of hydrodynamic boundary conditions, *The Journal of Chemical Physics* 115 (8) (2001) 3878–3887.
- [35] K. Higashi, H. Ito, J. Oishi, Surface diffusion phenomena in gaseous diffusion. i. surface diffusion of pure gas, *Nippon Genshiryoku Gakkaishi (Japan)* 5.
- [36] M. Levesque, M. Duvail, I. Pagonabarraga, D. Frenkel, B. Rotenberg, Accounting for adsorption and desorption in lattice boltzmann simulations, *Physical Review E* 88 (1) (2013) 013308.
- [37] I. Langmuir, The adsorption of gases on plane surfaces of glass, mica and platinum., *Journal of the American*

- Chemical society 40 (9) (1918) 1361–1403.
- [38] S. Brunauer, P. H. Emmett, E. Teller, Adsorption of gases in multimolecular layers, *Journal of the American chemical society* 60 (2) (1938) 309–319.
- [39] D. Theodorou, J. Wei, Diffusion and reaction in blocked and high occupancy zeolite catalysts, *Journal of Catalysis* 83 (1) (1983) 205–224.
- [40] J.-H. Moon, Y.-J. Park, M.-B. Kim, S.-H. Hyun, C.-H. Lee, Permeation and separation of a carbon dioxide/nitrogen mixture in a methyltriethoxysilane templating silica/ α -alumina composite membrane, *Journal of membrane science* 250 (1) (2005) 195–205.
- [41] A. Marković, D. Stoltenberg, D. Enke, E.-U. Schlünder, A. Seidel-Morgenstern, Gas permeation through porous glass membranes, *Journal of Membrane Science* 1 (336) (2009) 32–41.
- [42] Z. Guo, T. Zhao, Y. Shi, Physical symmetry, spatial accuracy, and relaxation time of the lattice boltzmann equation for microgas flows, *Journal of Applied physics* 99 (7) (2006) 074903.
- [43] Y.-H. Zhang, X.-J. Gu, R. W. Barber, D. R. Emerson, Capturing knudsen layer phenomena using a lattice boltzmann model, *Physical Review E* 74 (4) (2006) 046704.
- [44] Z. Guo, C. Zheng, B. Shi, Lattice boltzmann equation with multiple effective relaxation times for gaseous microscale flow, *Physical Review E* 77 (3) (2008) 036707.
- [45] Q. Li, Y. He, G. Tang, W. Tao, Lattice boltzmann modeling of microchannel flows in the transition flow regime, *Microfluidics and nanofluidics* 10 (3) (2011) 607–618.
- [46] M. Levesque, O. Bénichou, B. Rotenberg, Molecular diffusion between walls with adsorption and desorption, *The Journal of chemical physics* 138 (3) (2013) 034107.
- [47] J.-M. Vanson, F.-X. Coudert, B. Rotenberg, M. Levesque, C. Tardivat, M. Klotz, A. Boutin, Unexpected coupling between flow and adsorption in porous media, *Soft matter* 11 (30) (2015) 6125–6133.
- [48] S. Ansumali, I. V. Karlin, Kinetic boundary conditions in the lattice boltzmann method, *Physical Review E* 66 (2) (2002) 026311.
- [49] Z. Guo, B. Shi, T.-S. Zhao, C. Zheng, Discrete effects on boundary conditions for the lattice boltzmann equation in simulating microscale gas flows, *Physical Review E* 76 (5) (2007) 056704.
- [50] T. Inamuro, M. Yoshino, F. Ogino, A non-slip boundary condition for lattice boltzmann simulations, *Physics of Fluids* (1994-present) 7 (12) (1995) 2928–2930.
- [51] C. Shen, D.-B. Tian, C. Xie, J. Fan, Examination of the lbm in simulation of microchannel flow in transitional regime, *Microscale Thermophysical Engineering* 8 (4) (2004) 423–432.
- [52] T. Veltzke, J. Thöming, An analytically predictive model for moderately rarefied gas flow, *Journal of Fluid Mechanics* 698 (2012) 406–422.
- [53] R. J. Ambrose, R. C. Hartman, M. Diaz-Campos, I. Y. Akkutlu, C. H. Sondergeld, Shale gas-in-place calculations part i: New pore-scale considerations, *SPE Journal* 17 (01) (2012) 219–229.
- [54] G. Karniadakis, A. Beskok, N. Aluru, *Microflows and nanoflows: fundamentals and simulation*, Vol. 29, Springer, 2006.
- [55] J. Sun, Z.-X. Li, Effect of gas adsorption on momentum accommodation coefficients in microgas flows using molecular dynamic simulations, *Molecular Physics* 106 (19) (2008) 2325–2332.
- [56] M. Barisik, A. Beskok, Molecular free paths in nanoscale gas flows, *Microfluidics and Nanofluidics* 18 (5-6) (2015) 1365–1371.
- [57] K. Wu, Z. Chen, X. Li, Real gas transport through nanopores of varying cross-section type and shape in shale gas reservoirs, *Chemical Engineering Journal* 281 (2015) 813–825.
- [58] T. Yang, X. Li, D. Zhang, Quantitative dynamic analysis of gas desorption contribution to production in shale gas reservoirs, *Journal of Unconventional Oil and Gas Resources* 9 (2015) 18–30.