The lattice Boltzmann method for isothermal micro-gaseous flow and its application in shale gas flow: a review

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Abstract

The lattice Boltzmann method (LBM) has experienced tremendous advances and been well accepted as a popular method for simulating various fluid flow problems in porous media. With the introduction of an effective relaxation time and slip boundary conditions, the LBM has been successfully extended to solve micro-gaseous transport phenomena. As a result, the LBM has the potential to become an effective numerical method for gas flow in shale matrix in slip flow and transition flow regimes. Additionally, it is very difficult to experimentally determine the permeability of extremely low permeable media like shale. In this paper an extensive review on a number of slip boundary conditions and Knudsen layer treatments used in LB models for micro-gaseous flow is carried out. Furthermore, potential applications of the LBM in flow simulation in shale gas reservoirs on pore scale and representative elementary volume (REV) scale are evaluated and summarised. Our review indicates that the LBM is capable of capturing gas flow in continuum to slip flow regimes which cover significant proportion of the pores in shale gas reservoirs and identifies opportunities for future research.

Keywords: shale, lattice Boltzmann method, micro-gaseous flow, slip flow

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1. Introduction

Shale gas reservoirs are thought to contain a significant proportion of hydrocarbon, and successful exploitation of such resource plays an increasingly important role in meeting world's demand for natural gas. Shale gas reservoirs are known to be fine grained sedimentary rocks which have complex porous structures with pores and fractures ranging from nano- to meso-scale[1][2], and in each level of pores and fractures different flow mechanisms are involved[3]. An in-depth understanding of flow processes involve in complex porous system in shale is essential for prediction of reservoir permeability and estimating production potential of shale gas reservoirs. This can be achieved by developing detailed descriptive transport simulators which are capable of predicting flow dynamics in shale.

Knudsen number (Kn), which is the ratio of the gas mean free path to the characteristic length of the media, is an important dimensionless parameter for gas transport in shale. Current studies conclude that gas transport through shale matrix can best be characterized by Kn in slip flow ($0.001 < Kn < 0.1$) and transition flow ($0.1 < Kn < 10$) regimes[4][5](see Fig.1). Under these conditions, continuum hypothesis is broken down and other rarefied gas transport mechanisms such as slip flow and Knudsen diffusion start to dominate the flow. Additionally, as a source rock, the presence of organic matter (kerogen) in shale matrix instigates other processes and adds complexities to gas flow simulation. Gas transport in nano-pores inside the kerogen involves adsorption/desorption as well as surface diffusion due to strong molecular interactions between gas and kerogen.

A variety of experimental and mathematical studies shows that rarefaction effects influence the shale permeability measurements by increasing the apparent permeability values[6][7][8][9][10][11][12][13]. The effect of adsorption gas and the following surface diffusion on the permeability of shale, however, is not well understood and less widely explored. On one hand, studies confirmed that the multilayer adsorption can take place in organic pores because of the capillary condensation phenomenon[14][15], which will lead to a lower permeability in shale reservoirs[16]. On the other, it is confirmed that surface diffusion can account for 25% of total flux at low pressure[17]. Wu et al.[18]stated that when the pore size is less than 2 nm, the contribution of surface diffusion to total mass transfer can be as much as 92.95%.

Figure 1: Knudsen number relationship to pore diameter and mean reservoir pressure at 400 K. Vertical dash line represent a typical reservoir pressure condition of 37 MPa. (Figure adapted from Javadpour et al.[3] and Sondergeld et al.[2])

36 Generally, on the basis of pore size distribution, two possible mathemat-
 37 ical approaches are proposed to describe the gas transport mechanism and
 38 to calculate gas apparent permeability of organic shales. The first approach
 39 is to modify the non-slip boundaries in continuum model by accounting for
 40 slip boundary conditions. Beskok-Karniadaki[19] derived a unified Hagen-
 41 Poiseuille-type formula to take into account all flow regimes. Later, Civan
 42 and coworkers[20][21] and Florence et al.[22] proposed different forms of rar-
 43 efaction coefficient for Beskok-Karniadaki model. By simply adding the mass
 44 transfer of adsorbed gas into Beskok-Karniadaki model, the impact of the
 45 adsorption and surface diffusion on gas apparent permeability is studied by
 46 Xiong et al.[23]. The second approach is the superposition of various trans-
 47 port mechanisms. Javadpour[3] combined slip flow and Knudsen diffusion
 48 into gas flux equation and derived an equation for apparent permeability.
 49 Freeman et al.[5] used dusty gas model to account for Knudsen diffusion in
 50 shale gas reservoir. Singh et al.[24] combined viscous flow with Knudsen dif-
 51 fusion in their non-empirical apparent permeability model(NAP), and then
 52 validated with previous experimental data. Results have shown that the
 53 NAP can be used for Kn less than unity. Wu et al.[25] further proposed two

54 weighted factors for viscous flow and Knudsen diffusion, respectively. The
55 surface diffusion was also coupled in their apparent permeability model.

56 Most of the above mentioned analytical/semi-analytical studies are origi-
57 nally proposed based on simple geometries such as channels and tubes, and
58 are not suitable for more complex porous media, such as shales. Therefore,
59 the numerical methods of solving transport equations to obtain an estimate
60 for the permeability are attracting more attention. Especially after the cur-
61 rent well-established characterization techniques such as BIB-SEM, FESEM,
62 FIB-SEM and micro-CT enable us to identify a variety of pore structures in
63 shale matrix[1][26][27][28][29][30], the detailed rock images further promote
64 the use of image-based numerical simulation tools. Among them, the lattice
65 Boltzmann method (LBM), which is vastly different from traditional com-
66 putational fluid dynamics(CFD) methods, has proven to be an effective flow
67 simulation choice in porous media, as the geometry definition in LB model
68 is reduced to defining nodes as being either fluid or solid, which allows the
69 complex pore structure to be modelled with ease and allows for flexibility of
70 the parallelization.

71 Historically, the LBM was derived from lattice gas automata[31][32].
72 Later, it was shown that LB equation can also be directly derived by dis-
73 cretising the Boltzmann equation[33][34]. Shortly after its introduction, the
74 LBM became an attractive technique to study single/multi-phase flow[35][36]
75 [37][38][39] and reactive transport[40][41] in porous media, covering ground-
76 water flow[42], fabric materials[43] and fuel cells[44][45] etc. Detailed pore
77 structure obtained by FIB-SEM and micro-CT have made the LBM a pop-
78 ular alternative to direct numerical solution of the Navier-Stokes equation
79 for flows in tight rocks[46][47][48][49]. Because of its kinetic nature, the
80 LBM is, however, far more than just a N-S solver on pore scale[50]. Ad-
81 vances in micro electrical mechanical system (MEMS) and nanotechnology
82 have spurred interest in the use of the LBM for simulation of microfluidics
83 and tremendous efforts have been made to advance the LBM since 2002.
84 One noteworthy advance is its extension to simulation of gaseous flows in
85 slip flow regime [51][52][53][54][55][56][57][58]. Advances of the LBM have
86 also allowed us to simulate fluid flow in single capillary in transition flow
87 regime[59][60][61][62][63]. In previous studies, most of the micro-gaseous flow
88 was based on single relaxation time (SRT) model[52][55][56][57][59][64][65][66].
89 Luo[67] argued that slip velocity predicted by SRT is merely an artefact
90 at the solid boundaries. For this reason, other LB models, such as multi-
91 ple relaxation times (MRT)[60][62], two relaxation times (TRT)[68][69] and

92 Filter-matrix lattice Boltzmann (FMLB)[61] were proposed. Results of these
93 studies are in good agreement with that of the benchmark studies includ-
94 ing force-driven Poiseuille flow, pressure driven Poiseuille flow, and planar
95 Couette flow. For example, by incorporating the Bosanquet-type effective
96 viscosity and applying slip boundary conditions, Li et al.[62] successfully
97 used MRT models to simulate micro-channel gas flow at Kn of up to 3. This
98 also gives a similar result as that of MRT model with a Stops expression
99 of effective viscosity proposed by Guo et al[60]. Most Recently, Zhuo and
100 Zhong [61] developed a Filter-matrix Boltzmann model with Bosanquet-type
101 effective viscosity and produced reasonable results for micro-channel flow at
102 Kn of up to 10.

103 The rapid growth in unconventional gas, especially shale gas demands
104 a deeper understanding of the physics of fluid flow at the nanoscale to mi-
105 croscale. As a mesoscale method, the LB approach is an effective means
106 of dealing with flow problems whose scales are too small for the continuum
107 mechanics and too large for molecular methods. Although there have been
108 several excellent reports and reviews discussing the LBM for micro-gaseous
109 flow[70][71][72], the particular applications and strengths of LBM in simu-
110 lating gas flow in shale gas reservoir have not been well addressed. In this
111 review, we briefly introduce some ideas and equations fundamental to the
112 LBM. We also introduce the typical slip boundary conditions and Knudsen
113 layer treatments used in the LB algorithms for micro-gaseous flow, which
114 may be useful in shale gas flow simulation. Finally, we focus on recent de-
115 velopment in LB theory and applications for gas flow in shale, the feasibility
116 of these applications are also demonstrated.

117 2. Lattice Boltzmann method for isothermal micro-gaseous flow

118 In general, the lattice Boltzmann equation with a body force term can be
119 written as[73]:

$$f_i(\mathbf{x} + \mathbf{c}_i \delta t, t + \delta t) - f_i(\mathbf{x}, t) = \Omega_i(f_i) + \delta t \mathbf{F}_i, \quad (1)$$

120 where $\mathbf{c}_i$ indicates the finite number of discrete velocities of particles, f_i is the
121 distribution function of particles with speed $\mathbf{c}_i$, Ω_i is the collision term, $\mathbf{F}_i$
122 is the force term which is defined according to the collision operator, δx is the
123 uniform lattice spacing and δt is the time between two simulation iterations.

124 The microscopic variables (density and velocity) are defined as:

$$\rho(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t), \quad (2)$$

$$\rho(\mathbf{x}, t) \mathbf{u}^*(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t) \mathbf{c}_i + \frac{\delta t}{2} \mathbf{F}. \quad (3)$$

125 The most popular velocity sets for two dimensions and three dimensions
 126 are given in Fig.2(a) and Fig.2(b), respectively. When one considers appli-
 127 cations to micro-gaseous flow, some multi-speed or higher-order LB models
 128 such as D2Q21(Fig.2(c))[74] and D3Q39(Fig.2(d))[71][75] have also been de-
 129 veloped to increase the order of accuracy in the discretization of velocity
 130 phase space.

Figure 2: Discrete velocity models; (a) D2Q9 model, (b) D3Q19 model, (c) D2Q21 model, (d) D3Q39 model

131 2.1. Collision operators

132 The collision operators describe the collision behaviour of particles at
 133 every lattice location, which represents the variation of distribution functions
 134 caused by collision between particles. The requirements are that they should
 135 be physically correct and efficiently computable. In the following, collision
 136 operators commonly used in micro-gaseous flow are presented.

137 *2.1.1. Bhatnagar-Gross-Krook collision operator (BGK)*

138 Bhatnagar, Gross and Krook [76] proposed an efficient simplification op-
 139 erator to approximate the collision term as:

$$\Omega_i(f_i) = -\tau^{-1}(f_i - f_i^{eq}), \quad (4)$$

140 where, τ is the relaxation time and f_i^{eq} is the Maxwell Boltzmann distribution
 141 of $\mathbf{c}_i$ for a given macroscopic fluid velocity $\mathbf{u}$ and density ρ . The Maxwell-
 142 Boltzmann distribution describes the density distribution of a fluid in its
 143 equilibrium state to which every fluid strives. The equilibrium distribution
 144 f_i^{eq} in its discrete form can be expressed as:

$$f_i^{eq}(\mathbf{x}, t) = \rho(\mathbf{x}, t)\omega_i \left[1 + \frac{3(\mathbf{c}_i \cdot \mathbf{u})}{c^2} + \frac{9(\mathbf{c}_i \cdot \mathbf{u})^2}{2c^4} - \frac{3(\mathbf{u} \cdot \mathbf{u})}{2c^2} \right]. \quad (5)$$

145 Suga [71] summarized $\mathbf{c}_i$, the sound speed c_s and the weight parameter
 146 ω_i in accordance with each subfigure of Fig.2 (see Table 1).

Table 1: Parameters of the discrete velocity models for 2D/3D

Models	c_s^2/c^2	$\mathbf{c}_i/c$	w_i
D2Q9	1/3	(0,0)	4/9($i = 0$)
		($\pm 1, 0$), ($0, \pm 1$)	1/9($i = 1 - 4$)
		($\pm 1, \pm 1$)	1/36($i = 5 - 8$)
D2Q21	2/3	(0,0)	91/324($i = 0$)
		($\pm 1, 0$), ($0, \pm 1$)	1/12($i = 1 - 4$)
		($\pm 1, \pm 1$)	2/27($i = 5 - 8$)
		($\pm 2, 0$), ($0, \pm 2$)	7/360($i = 9 - 12$)
		($\pm 2, \pm 2$)	1/432($i = 13 - 16$)
		($\pm 3, 0$), ($0, \pm 3$)	1/1620($i = 17 - 20$)
D3Q19	1/3	(0,0,0)	12/36($i = 0$)
		($\pm 1, 0, 0$), ($0, \pm 1, 0$), ($0, 0, \pm 1$)	2/36($i = 1 - 6$)
		($\pm 1, \pm 1, 0$), ($\pm 1, 0, \pm 1$), ($0, \pm 1, \pm 1$)	1/36($i = 7 - 18$)
D3Q39	2/3	(0,0,0)	1/12($i = 0$)
		($\pm 1, 0, 0$), ($0, \pm 1, 0$), ($0, 0, \pm 1$)	1/12($i = 1 - 6$)
		($\pm 1, \pm 1, \pm 1$)	1/27($i = 7 - 14$)
		($\pm 2, 0, 0$), ($0, \pm 2, 0$), ($0, 0, \pm 2$)	2/135($i = 15 - 20$)
		($\pm 2, \pm 2, 0$), ($\pm 2, 0, \pm 2$), ($0, \pm 2, \pm 2$)	1/432($i = 21 - 32$)
		($\pm 3, 0, 0$), ($0, \pm 3, 0$), ($0, 0, \pm 3$)	1/1620($i = 33 - 38$)

147 The forcing term, $\mathbf{F}_i$ can be specified with respect to the relaxation pa-
 148 rameter τ and the body force $\mathbf{F}$ as[73]:

$$F_i = (1 - \frac{1}{2\tau})\omega_i[\frac{\mathbf{c}_i - \mathbf{u}}{c_s^2} + \frac{\mathbf{c}_i \cdot \mathbf{u}}{c_s^4}\mathbf{c}_i] \cdot \mathbf{F}. \quad (6)$$

149 Also in order to be valid, the LB equation requires the parameter to fulfil
 150 the following relation:

$$\mu = \rho c_s^2 (\tau - \frac{1}{2}) \delta t, \quad (7)$$

151 where, μ is the dynamic viscosity of the fluid.

152 2.1.2. Multiple Relaxation Times collision operator (MRT)

153 The MRT-LB model is the most general form within the theoretical frame-
 154 work of the LB equation and kinetic theory. The MRT collision operator
 155 relaxes the kinetic moments separately, which can be retrieved from the dis-
 156 tribution functions. The MRT collision operator is defined as follows[77]:

$$\Omega(f) = -(\mathbf{M}^{-1}\mathbf{S}\mathbf{M})(\mathbf{f} - \mathbf{f}^e). \quad (8)$$

157 In D2Q9 model, $\mathbf{f} = (f_0, f_1, \dots, f_7, f_8)^T$ denotes the column vector of the
 158 distribution functions, $\mathbf{S}$ is the non-negative relaxation matrix:

$$\mathbf{S} = \text{diag}(\tau_\rho, \tau_e, \tau_\epsilon, \tau_j, \tau_q, \tau_j, \tau_q, \tau_s, \tau_s)^{-1}, \quad (9)$$

159 and $\mathbf{M}$ is an orthogonal transform matrix, which maps the distribution func-
 160 tions onto the moment space, and defined as:

$$\mathbf{M} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & 1 \end{bmatrix}. \quad (10)$$

161 The distribution function and equilibrium function can be projected onto
 162 the moment space by using the transform matrix:

$$\mathbf{m} = \mathbf{M}\mathbf{f} = (\rho, e, \epsilon, j_x, q_x, j_y, q_y, p_{xx}, p_{xy})^T, \quad (11)$$

163

$$\begin{aligned}\mathbf{m}^{eq} &= \mathbf{M}\mathbf{f}^{eq} = (\rho, e^{eq}, \epsilon^{eq}, j_x, q - x^{eq}, j_y, q_y^{eq}, p_{xx}^{eq}, p_{xy}^{eq})^T \\ &= \rho(1, -2 + 3|u|^2, 1 - 3|u|^2, u, -v, u, -v, u^2 - v^2, uv)^T,\end{aligned}\quad (12)$$

164 all of these moments have a physically meaningful interpretation: ρ is the
 165 density; e is the energy mode; ϵ is related to the energy square; j_x and j_y
 166 are the x and y components of the momentum; q_x and q_y correspond to the
 167 x and y components of the energy flux, p_{xx} and p_{xy} and are related to the
 168 diagonal and off-diagonal component of the stress tensor. u and v are x and
 169 y components of velocity $\mathbf{u}$.

170 The forcing terms, $\mathbf{F}_i$ can also be mapped onto the moment space which
 171 gives the vector $\bar{\mathbf{F}}$ as:

$$\bar{\mathbf{F}} = (0, 6\mathbf{u} \cdot \mathbf{F}, -6\mathbf{u} \cdot \mathbf{F}, \mathbf{F}_x, -\mathbf{F}_x, \mathbf{F}_y, -\mathbf{F}_y, 2(u\mathbf{F} - v\mathbf{F}_y), (u\mathbf{F} + v\mathbf{F}_y))^T. \quad (13)$$

172 MRT is able to overcome the deficiencies of the BGK collision operator
 173 because it has more degrees of freedom, which can also be used to increase
 174 the numerical stability of the method significantly[78].

175 2.1.3. Two relaxation time collision operator (TRT)

176 The scheme for two relaxation time was developed by Ginzburg [79], for
 177 which the collision operator is split into symmetric and anti-symmetric parts
 178 as:

$$\Omega_i(f_i) = -\tau_s^{-1}(f_i^s - f_i^{seq}) - \tau_a^{-1}(f_i^a - f_i^{aeq}), \quad (14)$$

179 where relaxation time, τ_s related to shear viscosity, and relaxation time, τ_a
 180 related to energy fluxes. The symmetric and anti-symmetric components of
 181 distribution function and equilibrium distribution function can be computed
 182 as:

$$f_i^s = \frac{f_i + \bar{f}_i}{2}, f_i^{seq} = \frac{f_i^{eq} + \bar{f}_i^{eq}}{2}, \quad (15)$$

183

$$f_i^a = \frac{f_i - \bar{f}_i}{2}, f_i^{aeq} = \frac{f_i^{eq} - \bar{f}_i^{eq}}{2}. \quad (16)$$

184 The TRT model is comparable with SRT model in the simplicity of imple-
 185 mentation and computational efficiency, but retains the advantages of MRT
 186 model in terms of accuracy and stability[68][78].

187 2.2. Capture gas-solid interfacial slip

188 In traditional fluid mechanics, the assumption of non-slip at a solid bound-
 189 ary is used as the boundary condition. The non-slip assumption, however,
 190 breaks down at micro- and nanoscales[80][81]. Generally, the interfacial slip
 191 is generated by hydrophobicity in liquid flow and by Knudsen effect for gas
 192 flow[82]. To capture the liquid-solid interfacial slip, the Shan-Chen inter-
 193 particle potential model is usually used, where the solid-liquid interaction is
 194 modelled via an explicit solid-liquid intermolecular potential to predict be-
 195 haviours at the interface[82][83][84]. This approach appears to have a sound
 196 physical basis. However, it may face with more restrictive constraints in ac-
 197 tual practice[53] and no definitive results have been provided to demonstrate
 198 its ability to capture gas slip in transition flow regime[85].

199 To capture the gas slip at the solid boundary, single phase LB model is
 200 widely used, and the slip boundary condition is adopted to implicitly consider
 201 the solid-fluid interaction. Tremendous efforts have been devoted to develop
 202 accurate and efficient boundary schemes for the LBM. In the following section
 203 we summarize typical boundary conditions that could be useful for micro-gas
 204 simulations.

205 2.2.1. Bounce-back boundary condition(BB)

206 The half way bounce-back scheme [86] is typically utilized for its simplic-
 207 ity and its second-order accuracy. This boundary condition assumes that a
 208 particle which collides with the wall is reflected in opposite direction, which
 209 means that its momentum is reversed. In the implementation, particles leav-
 210 ing a boundary fluid node x bounce back from the boundary to the original
 211 site in the reversed lattice velocity, this behaviour can be described by Eq.
 212 17 as:

$$f_i^{bb}(\mathbf{x}, t + \delta t) = f_i^*(\mathbf{x}, t), \quad (17)$$

213 where f_i^* denotes the opposing distribution function to f_i leaving x after
 214 collision at time t such that $c_i = -c_{\bar{i}}$. The bounce-back boundary condition
 215 was used by Nie et al.[87] to mimic the microscopic flow, however, lately it
 216 has been shown that the boundary slip observed from Nie et al.[87] with a
 217 pure bounce-back scheme is just a numerical artefact[33] and cannot reflect
 218 the physical slip over the surface.

219 2.2.2. Specular reflection boundary condition(SR)

220 The specular reflection boundary condition is motivated by the obser-
 221 vation of elastic collisions between a relatively light particle and a heavy

222 boundary, the physical effect of such a collision is that the velocity compo-
 223 nent, which is orthogonal to the boundary, is reversed. This is described by
 224 the following equation for the D2Q9 model:

$$f_i^{sr}(\mathbf{x}) = f_{i'}^*(\mathbf{x}), \quad (18)$$

225 where, $f_{i'}^*$ and f_i^{sr} are approaching and specular reflecting distribution func-
 226 tions as shown in Fig.3. This boundary condition is applied by Lim et al.[88]
 227 to investigate pressure driven and shear driven micro-channel flows, however,
 228 it was found that the mesh size has a significant effect on the numerical re-
 229 sults in their work[88][89] and pure specular reflection may overestimates the
 230 slip velocity[90].

Figure 3: Illustration of the reflection process (in the left image, the distributions before the collision are highlighted. In the right image, the specular reflected distributions after collision with the wall are shown)[91]

231 2.2.3. Maxwellian diffuse reflection boundary condition(MD)

232 The Maxwellian diffusive reflection boundary condition is derived from
 233 the continuum kinetic theory for non-absorbing walls. The underlying idea of
 234 this boundary condition is that impinging particles lose the memory of their
 235 movement direction and are scattered back following a Maxwellian distribu-
 236 tion in which the wall density, ρ_w and the wall velocity, u_w are known. The
 237 fully diffusive boundary condition can be described by the following equation
 238 [92]:

$$f_i^{dr}(\mathbf{x}) = \frac{\sum_{(c_k - u_w) \cdot n < 0} |(c_k - u_w) \cdot n| f_k^*(\mathbf{x})}{\sum_{(c_k - u_w) \cdot n > 0} |(c_k - u_w) \cdot n| f_k^{eq}(\rho_w, u_w)} \cdot f_i^{eq}(\rho_w, u_w) \quad (19)$$

239 with $(c_k - u_w) \cdot n > 0$. The condition $(c_k - u_w) \cdot n < 0$ enforces that
 240 all incidental distributions are summed up and then redistributed over the

241 outgoing distributions such that they obey the equilibrium distribution with
 242 mass conservation. The process of the boundary treatment is illustrated in
 243 Fig. 4.

Figure 4: Illustration of the diffuse process(in the left image, the distributions before the collision and in the right image, the diffusive distributions collided with the wall are shown. The thickness of the arrows indicates the value of the distributions)[91]

244 This boundary condition has been implemented in LB model and the
 245 the results show good agreement with the analytical solution of Boltzmann
 246 equation for Kramer’s problem as the Kn tends to be zero[92], the similar
 247 concepts are used to simulate micro-gaseous flow at higher Kn using D2Q9
 248 LBM [52] and high-order LBM[93]. Later Chai et al.[94] argued that the slip
 249 velocity is overpredicted when MD scheme is applied to Poiseuille flow in a
 250 micro channel.

251 2.2.4. Combined form

252 The above mentioned three boundary conditions normally are not directly
 253 applied in the LB method, some improved version of the boundary conditions
 254 are proposed recently to mimic the macroscopic slip boundary condition by
 255 introducing a combination coefficient to control the boundary slip, which
 256 includes:

257 The combined specular with diffusive reflection boundary condition(MR)
 258 [66][57][95][96]:

$$f_i(\mathbf{x}) = (1 - \sigma)f_i^{sr}(\mathbf{x}) + \sigma f_i^{dr}(\mathbf{x}). \quad (20)$$

259 The combined bounce-back with specular reflection boundary condition
 260 (BR)[54]:

$$f_i(\mathbf{x}) = (1 - r)f_i^{sr}(\mathbf{x}) + r f_i^{bb}(\mathbf{x}). \quad (21)$$

261 The combined bounce-back with diffusive reflection boundary condition
 262 (MB)[58]:

$$f_i(\mathbf{x}) = (1 - \chi)f_i^{bb}(\mathbf{x}) + \chi f_i^{dr}(\mathbf{x}). \quad (22)$$

Historically, there is no consensus on how to choose combination coefficients [55][58][61][62][66][97]. Recent studies[58][60][98] indicate that the analytic solution of LBM with bounce-back or combined boundary conditions in Poiseuille flow is just a parabolic profile of N-S equation shifted by a numerical slip, u_s , and when combined boundary conditions are applied, by setting this numerical slip u_s to Maxwellian slip boundary condition, the combination coefficients can be obtained[58][60]. A detailed analysis of three kinds of combined form of boundary conditions are given by Zheng et al.[99] in which they pointed out that if one chooses combination coefficient equal to tangential momentum accommodation coefficient (TMAC)(TMAC=0.8 is used in their case studies), the discrete effects of the boundary conditions will induce large numerical errors. Specifically, MR overestimates the slip velocity, while BR and MB underestimate the slip velocity (see Fig.5), and the three boundary conditions cause large errors in the slip velocity (> 60% for the BR scheme, > 20% for the MB scheme, and > 40% for the MR scheme) within the slip regime (see Fig. 6). For micro-tube flow, the Maxwell-type second order slip boundary can be expressed as:

$$u_s = A_1 K n \left. \frac{\partial u}{\partial y} \right|_{wall} - A_2 K n^2 \left. \frac{\partial^2 u}{\partial y^2} \right|_{wall}, \quad (23)$$

where u_s is the slip velocity, A_1 and A_2 are the first order and second order slip coefficients, respectively. In order to achieve the second order slip boundary condition, if one chooses the combination coefficients as the following forms (Eq.24 to Eq.26), the three kinds of combined forms are identical in a parametric range, and the discrete effects caused by boundary conditions can be eliminated(see RBR, RMB and RMR in Fig.5 and Fig.6).

Figure 5: Velocity profiles with TMAC=0.8[99]

Figure 6: Relative error of velocity slip vs Kn with TMAC=0.8[99]

$$\sigma = \left\{ 1 - \sqrt{\frac{\pi}{6}} \left[A_1 + \left(A_2 + \frac{8}{\pi} \right) Kn \right] + \frac{3\pi^{1/2}\Delta^2}{8\sqrt{6}Kn} \right\}^{-1}, \quad (24)$$

$$r = 2 - \left\{ \frac{1}{2} - \sqrt{\frac{\pi}{6}} \left[\frac{A_1}{2} + \left(\frac{A_2}{2} + \frac{4}{\pi} \right) Kn \right] + \frac{3\pi^{1/2}\Delta^2}{8\sqrt{6}Kn} \right\}^{-1}, \quad (25)$$

$$\chi = \left\{ \frac{1}{2} - \sqrt{\frac{\pi}{6}} \left[\frac{A_1}{2} + \left(\frac{A_2}{2} + \frac{4}{\pi} \right) Kn \right] + \frac{3\pi^{1/2}\Delta^2}{8\sqrt{6}Kn} \right\}^{-1}. \quad (26)$$

From the above description, LBM can be viewed as an alternative form of slip N-S equation. However, it should be noted that, in Maxwell's original paper, the author used a phenomenological argument to derive slip boundary conditions[100]. This is evident in the fact that the "momentum accommodation coefficients" for each particular gas/surface combination are required in Maxwell-type slip boundary conditions. Typically, the accommodation coefficients can only be inferred from experimental results, rather than directly measured. As a result, the boundary slip observed from combined forms are more phenomenological than physical compared to those from other methods such as DSMC and Boltzmann equation [95] [101], and therefore this fails to demonstrate the physical kinetic nature of the LBM, which has been claimed a distinguishing feature of LBM than other CFD methods. To enable the LBM with combined from boundary conditions to be a predictive tool, Sbragaglia and Succi[53] suggested that a micro-scale simulation, such as MD needs to be used to obtain the values of coefficients corresponding to a given intermolecular potential, prior to the LB simulations at a larger scale which is not accessible by micro-scale simulations.

2.2.5. Langmuir slip boundary (LSB)

Another slip boundary used in the LBM is based on Langmuir slip model. The Langmuir slip model has been developed by Eu et al.[102] and Myong [103]. The slip velocity can be expressed as:

$$u_s = \alpha u_w + (1 - \alpha)u_g, \quad (27)$$

where, u_g denotes the velocity adjacent to the wall, α is the fraction of surface covered by adsorbed atoms at thermal equilibrium which varies with the type of gas and the nature of wall material. For monatomic gases and diatomic gases α can be expressed by:

$$\alpha|_{mon} = \frac{\beta p}{1 + \beta p}; \alpha|_{di} = \frac{\sqrt{\beta p}}{1 + \sqrt{\beta p}}, \quad (28)$$

311 with:

$$\beta = \frac{A\lambda/Kn}{k_bT} \exp\left(\frac{D_e}{K_bT}\right) = \frac{1}{4\omega Kn}, \quad (29)$$

312 where, k_b represents the Boltzmann constant, A is the mean area of a site, D_e
 313 is the potential adsorption parameter and T is the temperature. Compared to
 314 Maxwell slip model, in which the slip coefficient is a free parameter from the
 315 concept of diffusive reflection, the major advantage of Langmuir slip model is
 316 to utilize a physical coefficient of heat and gas particle interaction potential,
 317 ω [103], Nevertheless, Langmuir slip model still has the same difficulty in
 318 determining the value of the coefficient as the Maxwell slip model[104].

319 The LB model with Langmuir slip boundary condition was firstly used
 320 to study gas bearing problems[105]. Later, Chen and Tian [106] implement
 321 Langmuir slip boundary by non-equilibrium extrapolation scheme to study
 322 gas flow in the micro-channel, with an approximation that the local gas
 323 density at the wall equals to gas density at the nearby cell, the distribution
 324 functions for wall boundary nodes can be expressed as:

$$f_i(\mathbf{x}_b) \approx \alpha[f_i^{eq}(\rho(\mathbf{x}_f), u(\mathbf{x}_b)) - f_i^{eq}(\rho(\mathbf{x}_f), u(\mathbf{x}_f))] + f(\rho(\mathbf{x}_f), u(\mathbf{x}_f)), \quad (30)$$

325 where, $\mathbf{x}_b$ is the boundary node and $\mathbf{x}_f$ is the nearest node to the boundary
 326 node.

327 2.3. Capture the Knudsen layer effect

328 For micro-gaseous flow simulation, Once $Kn > 0.1$, presence of Knud-
 329 sen layer near the solid boundary cannot be ignored. Inside of the Knud-
 330 sen layer, the intermolecular collisions become insufficient and the quasi
 331 thermodynamic-equilibrium assumption, upon which the N-S equation de-
 332 pends, does not hold. The standard LBM with a slip boundary condition
 333 captures a few low-order moments of the solutions of the Boltzmann equation,
 334 and is only accurate at the N-S level[107]. Thus, just like N-S equation, the
 335 standard LBM fails to describe the gas motion within the Knudsen layer(See
 336 Fig.7). To improve the capability of the LBM for high- Kn flows in the
 337 transition flow regime, some lattice Boltzmann schemes have been proposed
 338 recently.

Figure 7: Schematic of the Knudsen layer

2.3.1. Effective viscosity/mean free path model

The dynamic viscosity μ of a fluid plays a critical role in its dynamic behaviour, and thus is an important consideration for fluid flow simulation. The viscosity describes the internal friction between moving fluid layers and the spanwise momentum conductivity. Furthermore, it determines the relaxation time τ and τ_s used in the BGK-LB model and MRT-LB model, respectively. With an increase in Knudsen number, especially when the mean free path becomes comparable with the characteristic length, the local mean free path is significantly affected by the wall boundaries, which are much smaller than that defined in unbounded systems[95][108]. Since the viscosity and the mean free path are interrelated[109], by introducing an effective relaxation time that corresponds to the effective mean free path or effective viscosity to reflect the gas molecular/wall interactions, the LB models are able to capture the effects of the Knudsen layer for high Knudsen numbers.

2.3.1.1. Relations of relaxation time with Kn . By introducing an empirical parameter a , Nie et al.[87] built a linear relationship of Kn with relaxation time τ . The problem of this model is that the artificial parameter, a needs to be determined by comparing simulation results with that obtained from experiments, and therefore it cannot be directly used in other situations[52]. To improve this, other attempts have been proposed in the literature, and it has been confirmed that the relaxation time can be related to Kn by multiplying a certain microscopic velocity. The choice of this velocity is rather diverse in the literature(see Table 2), and most recently, Zhang et

al.[110] and Guo et al.[57] argued that to satisfy a “consistent requirement”, this certain microscopic velocity must be chosen as $\sqrt{\pi RT/2}$, and τ can be given as:

$$\tau = HKn/(\delta x \sqrt{\pi/6}) + 0.5. \quad (31)$$

Table 2: Relationships of relaxation time with Kn

Nie et al. [87]	$\tau = HKn/a + 0.5$
Lim et al. [88]	$\tau = HKn/\delta x$
Lee and Lin [51]	$\tau = HKn/\delta x + 0.5$
Niu et al. [52]	$\tau = HKn/(c\sqrt{6/\gamma\pi}) \approx HKn$
Tang et al. [66]	$\tau = (HKn)/(\delta x \sqrt{8/3\pi}) + 0.5$
Zhang et al.[56] Guo et al.[57]	$\tau = HKn/(\delta x \sqrt{\pi/6}) + 0.5$

2.3.1.2. Wall function approach. One way to capture the Knudsen layer is to modify the mean free path by implementing a “geometry dependent” correction function to reflect the wall confinement as:

$$\lambda_e = \lambda J(r, \lambda), \quad (32)$$

where, $J(r, \lambda)$ is the correction function which considers the effect of wall surface on the mean free path λ , and r is distance from the wall. Wall function approach has been widely used to study micro-channel and micro-tube flows[68][60][63], whist it is a phenomenological approach like that of Maxwell’s slip model[111]. Despite the fact that by introducing an effective wall function approach with a more complex collision operator, the LBM can predict the flow behaviour up to the upper end of the transition flow regime[68], the existing wall functions themselves are only accurate in a finite range of Kn . The different correction functions for parallel walls situations and their valid Kn are listed in Table 3.

Table 3: Summarize of different correction functions

	J		Kn
Stops [112]	$1 + \frac{1}{2}$	$\begin{aligned} & (r/\lambda - 1)\exp(-r/\lambda) \\ & + ((H - r)/\lambda - 1)\exp(-(H - r)/\lambda) \\ & - (r/\lambda)^2 E_i(r/\lambda) \\ & - ((H - r)/\lambda)^2 E_i((H - r)/\lambda) \end{aligned}$	≈ 0.2
Zhang et al. [85]		$\frac{1}{1+0.7[\exp(-Cr/\lambda)+\exp(-C(H-r)/\lambda)]}$	≈ 1
Arlemark et al. [113]	$1 - \frac{1}{82}$	$\begin{aligned} & \exp\left(-\frac{H/2+y}{\lambda}\right) + \exp\left(-\frac{H/2-r}{\lambda}\right) \\ & + 4 \sum_{i=1}^7 \exp\left(-\frac{H/2+r}{\lambda \cos\left[\frac{(2i-1)\pi}{28}\right]}\right) \\ & + 4 \sum_{i=1}^7 \exp\left(-\frac{H/2-r}{\lambda \cos\left[\frac{(2i-1)\pi}{28}\right]}\right) \\ & + 2 \sum_{i=1}^6 \exp\left(-\frac{H/2+r}{\lambda \cos\left[\frac{i\pi}{14}\right]}\right) \\ & + 2 \sum_{i=1}^6 \exp\left(-\frac{H/2-r}{\lambda \cos\left[\frac{i\pi}{14}\right]}\right) \end{aligned}$	≈ 0.2
Dongari et al. [108]	$1 - \frac{1}{96}$	$\begin{aligned} & \left(1 + \frac{r}{\lambda}\right)^{-2} + \left(1 + \frac{H-r}{\lambda}\right)^{-2} \\ & + 4 \sum_{i=1}^8 \left(1 + \frac{r}{\lambda \cos\left[\frac{(2i-1)\pi}{32}\right]}\right)^{-2} \\ & + 4 \sum_{i=1}^8 \left(1 + \frac{H-r}{\lambda \cos\left[\frac{(2i-1)\pi}{32}\right]}\right)^{-2} \\ & + 2 \sum_{i=1}^7 \left(1 + \frac{r}{\lambda \cos\left[\frac{i\pi}{16}\right]}\right)^{-2} \\ & + 2 \sum_{i=1}^7 \left(1 + \frac{H-r}{\lambda \cos\left[\frac{i\pi}{16}\right]}\right)^{-2} \end{aligned}$	≈ 2

378 A general problem of wall functions is that it has been derived based on
379 the distance to the wall and therefore it is difficult to deal with complex
380 geometries and the Knudsen layer overlap effect[63]. To solve this problem,
381 an approximate Stop's expression is proposed by Guo et al.[57] as:

$$J(Kn) = \frac{2}{\pi} \arctan(\sqrt{2}Kn^{-3/4}). \quad (33)$$

382 It can be seen that this correction function is not related to the distance
383 from the wall. In other words, with this formulation it is possible to tackle
384 the problem of Knudsen layer interference in more complex geometry by
385 computing the average of all effective mean free paths.

386 *2.3.1.3. Bosanquet-type effective viscosity approach.* The larger the Knudsen
387 number, the closer the mean free path to the characteristic length H . In the
388 case $\lambda \gg H$, the effective mean free path equals H and the viscosity, $\mu_\infty =$
389 $a_\infty \rho \bar{c} H$ with a_∞ being a numerical constant. Michalis et al.[114] observed
390 that the effective viscosity can be approximated by the terms μ and μ_∞ .
391 They conducted micro-flow simulations with the Direct Simulation Monte
392 Carlo(DSMC) method to investigate the rarefaction effects on the viscosity
393 in the transition regime. The calculated densities and velocity profiles were
394 used to compute the actual viscosity of the fluid. With these results Michalis
395 et al.[114] showed that the Bosanquet-type of approximation describes quite
396 satisfactorily the Kn-dependence of the viscosity over the entire transition
397 flow regime and it can be expressed as:

$$\mu_e \approx \frac{\mu}{1 + aKn}, \quad (34)$$

398 where, a is the rarefaction factor and $a = a_0/a_\infty$. Because the Bosanquet-
399 type effective viscosity considers the overall rarefaction effect on gas viscosity
400 such as the approximate wall function approach proposed by Guo et al.[57],
401 it can be utilized in rarefied flow simulations in porous media. However,
402 the choice of a is still an open question. Beskok and Karniadakis[19] used
403 $a = 2.2$ together with their general slip boundary condition to simulate fluid
404 flow in channels. Later, Sun and Chan[115] used $a = 2$ in estimating effective
405 viscosity at different Knudsen number in channels with aspect ratio between
406 15 and 20. They found the results of effective viscosity is reasonable when
407 compared with that obtained from the DSMC method. Michalis et al.[114]
408 observed that the value of a depends on the Knudsen number and it varies
409 slightly over the majority of the transition flow regime. Recently, Kalarakis
410 et al.[116] suggested $a = 3.4$ based on a study in which authors estimated
411 permeability using LB method and then compared the results with that from
412 DSMC for porous media with porosity equal to 0.7 and 0.8.

413 *2.3.2. High-order lattice Boltzmann model*

414 While the effective viscosity/mean free path model is one way of extend-
415 ing slip LB models into the non-equilibrium gas flow, developing high-order
416 LB models has also attracted significant recent interest. Since the LB equa-
417 tion is a discrete approximation to the continuous Boltzmann equation which
418 is capable of describing gas flow in a wide range of Knudsen number, some ef-
419 forts have been made to design higher-order LB models by increasing discrete

420 velocities to achieve its approximation accuracy to the continuous Boltzmann
421 equation[93][107][117][118][119][120].

422 It has been shown that the high-order LB models can improve the predic-
423 tions for non-equilibrium flows and the simulation results are qualitatively
424 agree with previous studies[93][107][118], Ansumali et al.[117] presented ana-
425 lytical solutions of the discrete velocity Boltzmann equation for Couette flow
426 using the so-called D2Q9 and D2Q16 schemes and showed that the increase
427 of order in the GaussHermite quadrature results in a much more accurate
428 treatment of finite Kn flows. However, no systematic study on the quadrature
429 set higher than D2Q16 were discussed by them. Later, Kim et al.[74] com-
430 pared several high-order models including D2Q12, D2Q16, D2Q21, D2Q25
431 and D2Q36 models, and they concluded that the accuracy of the higher-order
432 LB models does not increase monotonically with the increase of the order of
433 Gauss-Hermite quadrature and cannot guarantee an improved accuracy for
434 microscale gas flow with the Kn up to $O(1)$. This was further confirmed by
435 Meng and Zhang[121] with a study of D2Q16, D2Q25 D2Q36 D2Q49 and
436 D2Q64 LB models. Kim et al.[74] also reported that the Knudsen layer can
437 be observed with the minimum of D2Q16 discrete velocities even this partic-
438 ular higher-order LB model fails to reproduce the Knudsen minima correctly.
439 In fact, numerical studies suggest that a very high-order LB model is needed
440 to reproduce the Knudsen paradox phenomena[74][121]. In addition to the
441 inconsistencies at higher Kn, large computational costs hinder the applica-
442 tions of high-order LB models in the simulation of more complex flow. Meng
443 and zhang[122] compared the computational costs associated with D2Q25
444 and D2Q400 models for a quasi-steady standing-shear-wave problem, and
445 they found D2Q400 is more than 240 times slower than D2Q25 while the
446 difference of two simulation results is less than 3%. Recently, Suga and
447 coworkers[71][123][124] compared D2Q9/D3Q19 with D2Q21/D3q39 in the
448 simulation of fluid flow in micro-porous media with a porosity around 0.9
449 at Kn ranges from 0.04 to 0.24. They concluded that the flow field results
450 provided by D2Q9/D3Q19 are less accurate than D2Q21/D3Q39. However,
451 the deficiency is not significant in the complex flow fields, and MRT-LB mod-
452 els almost perfectly overlap with those of the high-order LB models, which
453 also means that a higher-order lattice may not be significantly important for
454 predicting general flow profiles in micro porous media.

3. Simulation of fluid/gas flow in shale gas Reservoirs with the LBM

Shale gas reservoirs are considered unique because of its complex petrophysical properties and its inherent multiscale nature, with details at the microscale affecting the overall operation of macroscopic gas production. Generally, theoretical treatments of flow in porous shale are usually associated with three different length scales: pore-(microscopic), representative elementary volume(REV)- and stimulated reservoir volume (SRV)-scales. The SRV-scale is the largest scale, which includes tight matrix and multi-scale fracture networks[125]. One of the critical issues in SRV-scale simulation of shale gas reservoir is how to handle fracture flow and fracture/matrix interactions. Compared to LBM, traditional CFD methods such as FEM[126][127][128] and FDM[125][129] are currently primary simulation tools on SRV- scale simulation in dealing with multiple flow mechanism and rock deformation despite the fact that they are still far behind the industry’s demand[125]. Pore scale is the smallest scale where the flow is studied on pore geometries. Pore scale results can provide quantities such as permeability, porosity at various locations. With these results, some fundamental issues such as medium variability can be quantitatively assessed and REV can be quantified. The REV scale is larger than the pore scale but much smaller than the field scale, within the range of an REV, the macroscopic variables (such as permeability and porosity) do not change with the magnitude of the averaging volume. As an image based simulation tool, the LBM has been developed to simulate fluid/gas flow in porous shale on pore scale and REV scale.

3.1. Pore scale simulation

At the pore scale, the flow of fluid through the pores of shale reservoir is directly simulated by the LBM. Initially, standard LBM is developed with non-slip boundary conditions to study continuum flow in porous media. As gas flow in shale is involved with different flow regimes, recently, some attempts have been made to extend standard LBM to capture non-continuum phenomenon.

3.1.1. Estimation of intrinsic permeability

Under the continuum assumption, standard LBM can be easily applied to complex boundary geometries due to its kinetic nature and a simple bounce-back rule for non-slip boundary condition. This particular feature makes

the LBM superior to classical numerical techniques (e.g., finite differences and finite elements) and other simplified network models for studying flow in realistic porous media. Moreover, as the incompressible N-S equation can be obtained in the nearly incompressible limit of the LB model, LBM is widely used to estimate the intrinsic permeability of shale along with tomography techniques[130][131] [132]. For example, Chen et al.[133] generated 3D FIB-SEM images of shale samples and estimated intrinsic permeability and tortuosity with standard LBM. Later the same techniques were applied but the computation was carried out using a pore-scale GPU-accelerated LB simulator (GALBS) which increases the computing speed (1000 times faster than the serial code and 10 times faster than the paralleled code run on a standalone CPU)[134]. The relative permeability of shale was also studied by Cantisano et al.[135] and Nagarajan et al.[136]. Nagarajan et al.[136] calculated the gas-oil relative permeability of Liquid Rich Shale (LRS) with the LBM and compared their results with laboratory studies. The authors observed that standard LBM can give similar remaining oil saturation to that of the experimental observations, however, significant difference exists in the relative permeability curves.

3.1.2. Estimation of apparent permeability

When continuum hypothesis breaks down, the gas molecules tend to “slip” on the solid surface, and the measured gas permeability through a porous media is higher than that of intrinsic permeability due to gas slippage. To estimate the gas apparent permeability(k_a) of shale, several approaches have been proposed from the literature.

3.1.2.1. Klinkenberg model based LBM. In Klinkenberg model, the apparent permeability is calculated based on a linear correlation factor(f_c) for correcting the intrinsic permeability (k_0):

$$k_a = k_0 f_c, \quad (35)$$

where, f_c is a correction factor and is given by [137]:

$$f_c = (1 + \frac{b_k}{p}), \quad (36)$$

with a slip factor b_k which depends on Kn . Later, it is confirmed that Klinkenberg’s correlation is only first order accurate. Beskok and Karniadakis [19] proposed a second-order correlation by considering the different

521 flow regimes from continuum flow to free molecular flow:

$$f_c = [1 + \alpha(Kn)Kn] \left[1 + \frac{4Kn}{1 - bKn} \right], \quad (37)$$

522 where, slip coefficient b equals to -1 for slip flow, and $\alpha(Kn)$ is a rarefac-
 523 tion coefficient which is given by Florence et al.[22] for a purely diffusive
 524 (TMAC=1) situation as:

$$\alpha(Kn) = \frac{128}{15\pi^2} \tan^{-1}[4Kn^{0.4}]. \quad (38)$$

525 Allan and Mavko[138] used the combination of Beskok and Karniadakis-
 526 Florence's correlation along with a 3D incompressible LB model to estimate
 527 the k_a for a shale image with a $167nm$ length in each dimension. In their
 528 study, the intrinsic permeability k_0 was predicted by standard LBM. Further,
 529 the adsorption gas was induced in their model as an immobile phase which
 530 affects permeability in two manners: decreasing the gas permeability and
 531 changing the TMAC. Moreover, they pointed out that a supercritical phase
 532 transition may take place during the pressure depression and diffusive flow
 533 mechanisms becomes a negligible mass transport mechanism when gas is in
 534 a supercritical phase (see Fig. 8).

535 Allan and Mavko's work appears to be the first to apply the LBM to
 536 quantify the effect of slip and adsorption on micro-porous shale rock transport
 537 properties. With an average Kn which is derived from flux weighted average
 538 pore width, however, the realistic gas flow through the pore space cannot
 539 be obtained. Also, the surface diffusion of adsorption gas is not considered
 540 in their model, and no further discussions are provided on the influence of
 541 adsorption gas on TMAC.

Figure 8: The difference between the total permeability and the continuum permeability as a function of pore pressure. For comparison, two curves are presented corresponding to a gaseous phase (dot-dashed curve), and to a fluid phase that undergoes a supercritical transition (solid curve). The horizontal dotted line marks that the total permeability is equal to the continuum permeability when adsorption layer is not considered.

542 *3.1.2.2. Dusty gas model (DGM) based LBM.* The dusty gas model is based
 543 on the superposition of convection and molecular spatial diffusion(Knudsen
 544 diffusion):

$$J = -\frac{\rho k_a}{\mu} = J_d + J_k = -\frac{\rho k_d}{\mu} \nabla p + -\frac{\rho}{p} D_{eff} \nabla p, \quad (39)$$

545 where, J is the mass flux per unit area, J_d is the viscous flow flux and J_k is
 546 the Knudsen diffusion flux. D_{eff} is the effective Knudsen diffusivity. Based
 547 on Eq.39, the apparent permeability can be calculated as:

$$k_a = k_0 \left(1 + \frac{D_{eff} \mu}{p k_0} \right). \quad (40)$$

548 Very recently, a DGM based LB model was proposed by Chen et al.[139]
 549 to calculate the apparent permeability of shale. In this model a MRT-LBM
 550 for fluid flow and a SRT-LBM for mass transport were used to estimate
 551 intrinsic permeability k_0 and effective Knudsen diffusivity D_{eff} , respectively.
 552 In order to account for the variation of local Knudsen diffusivity with local

553 pore diameter, the relaxation time used in the LBM transport model was
 554 modified based on:

$$\tau_g = \frac{d_p}{d_{p,ref}}(\tau_{p,ref} - 0.5) + 0.5, \quad (41)$$

555 where d_p is local pore diameter, $d_{p,ref}$ is a reference pore size which is chosen
 556 as 25 nm in their simulation, and $\tau_{p,ref}$ is set as 1.0.

557 The DGM based LB model developed by Chen et al.[139] was adopted
 558 to estimate the tortuosity and the gas apparent permeability of four recon-
 559 structed shale samples form Sichuan Basin (China). Their simulation results
 560 indicate that commonly used Bruggeman equation greatly underestimates
 561 tortuosity of shale, and DGM based LB model can give a comparable results
 562 of apparent permeability as that given by Beskok and Karniadakis-Civan's
 563 correction[140](see Fig.9).

Figure 9: Correction factors predicted by the LBM and empirical correlations under different Kn

564 Later, the same techniques were applied by them to estimate the appar-
 565 ent permeability of 250 reconstructed kerogen samples using a reconstructed
 566 method called overlapping sphere method, with a porosity ranging from 0.1
 567 to 0.55, and a mean diameter of 30, 45, and 60 nm[141]. The simulation

568 results further confirm the high tortuosity of kerogen pores and Beskok
 569 and Karniadakis-Civan's correlation for calculating apparent permeability
 570 of shale matrix.

571 To our best knowledge, Chen et al.'s work[139][141] is the first study of nu-
 572 merically investigating the effective Knudsen diffusivity based on real porous
 573 structures of shale with the LBM. The advantage of this method is ease
 574 of implementation. In their DGM based LBM, gas adsorption and surface
 575 diffusion are not considered, and the Knudsen diffusion term used in DGM
 576 contains the assumption of fully diffusive boundary condition (TMAC=1)
 577 which underestimates the mass flux in the transition regime[142].

578 *3.1.2.3. Slip N-S model based LBM.* Slip N-S model based LBM is the direct
 579 simulation of gas flow through pore structure with the use of appropriate
 580 slip boundary conditions and effective relaxation time(See section 2). A few
 581 attempts have been made in the literature by applying slip LBM to shale
 582 gas flow through kerogen pores. In these applications, additional physical
 583 properties are added into slip boundary conditions and LB model to reflect
 584 the adsorption gas and/or surface diffusion effect.

585 Fathi and Akkutlu [143] developed a LB-Langmuir isotherm model in
 586 which LSB was used to capture the velocity slip. To consider the impact of
 587 surface diffusion, u_w in Eq.27 was calculated based on:

$$u_w = u_a = \frac{D_s}{D_k \rho_a} \left[\rho_g \mu_g \frac{K C_{\mu s}}{(1 + K C)^2} \right], \quad (42)$$

588 where, C is the free gas density, $C_{\mu s}$ is the maximum adsorption capacity,
 589 D_k is the tortuosity-corrected coefficient of molecular diffusion, D_s is surface
 590 diffusion coefficient, ρ_a is the adsorbed-phase density, and K is the equilib-
 591 rium partition (or distribution) coefficient. Interestingly, the pseudopotential
 592 model proposed by Shan and Chen[144] was also employed in their LB model
 593 to consider the non-ideal gas effect and the interactions between solid and
 594 gas, however, it is argued that this treatment may lead to a double consider-
 595 ation of the gas-solid interactions[145] as pseudopotential model and slip LB
 596 are parallel in capturing gas slippage[82][83][84].

597 Based on BR and Langmuir isotherm model, Ren et al.[146] proposed a
 598 different form of LB slip boundary condition, in which the surface diffusion
 599 of adsorption gas is modelled as a moving wall. In their model, the transport
 600 rate of adsorbed gas is independent of D_k as mentioned in Eq.42 and can be

601 expressed as:

$$u_a = -D_s \frac{\rho_s M}{\rho_a V_{std}} \frac{q_L p_L}{(p_L + p_{free})^2} \frac{\partial p_{free}}{\partial x}, \quad (43)$$

602 where, M is the molecular weight of the gas, ρ_s is the organic solid density,
 603 V_{std} is the gas volume per mole at standard temperature and pressure, q_L ,
 604 p_L and p_{free} are Langmuir volume, Langmuir pressure, and free-gas pres-
 605 sure, respectively. They demonstrated that their model can predict more
 606 reasonable physical behaviour compared to that in Fathi and Akkutlu[143],
 607 however, no validation is provided when considering the adsorption gas and
 608 surface diffusion effect. The non-ideal gas effect was also studied by Ren et
 609 al.[146](see Fig.10), and they demonstrated the necessity to use LB under
 610 real gas conditions instead of the one under ideal gas conditions as large
 611 difference exists between the simulation results for ideal and non-ideal gas.

Figure 10: Comparison of free-gas velocity profiles in Kerogen pores using the LB under ideal and non-ideal gas conditions

612 Slip N-S based LBM gets rid of the usage of empirical or semi-empirical
 613 correlations, and it is believed that it can provide accurate simulation re-
 614 sults comparable with experimental studies. The main advantage of this
 615 method is that detailed local information of the flow (such as velocity field
 616 and pressure field) can be obtained and the local information can be used to
 617 study macroscopic relations. The slip N-S based LBM is, however, still in
 618 its infancy, and its applications in shale are limited to single channel flow.

Also current complex boundary treatments prevent its further application in porous media[82][94].

3.2. REV scale simulation

Due to the huge computational cost, pore-scale LBM is impractical to perform REV-scale simulations of porous shale. Therefore, several alternative approaches are proposed to apply the LBM on REV scale[36][147][148][149].

To apply the LBM for REV scale flow simulation, Guo et al.[36] proposed a generalized LB model, in which the forcing term(Eq.6) was related to the porosity of porous media:

$$F_i = (1 - \frac{1}{2\tau})\omega_i[\frac{\mathbf{c}_i - \mathbf{u}}{c_s^2} + \frac{\mathbf{c}_i \cdot \mathbf{u}}{\varepsilon c_s^4}\mathbf{c}_i] \cdot \mathbf{F}, \quad (44)$$

with

$$\mathbf{F} = -\frac{\varepsilon\mu}{k_0}\mathbf{u} - \frac{\varepsilon\rho F_\varepsilon}{\sqrt{k_0}}|\mathbf{u}|\mathbf{u} + \varepsilon\rho\mathbf{G}, \quad (45)$$

where, F_ε is the geometry function and k_0 is the intrinsic permeability. Both F_ε and k_0 need to be estimated based on the empirical relationships with porosity, ε .

Chen et al.[150] further extended this generalized LBM for slip flow by considering Klinkenberg's effect on REV scale, and this was achieved by the usage of apparent permeability, k_a instead of k_0 . Beskok and Karniadakis-Civan's correlation [20] was adopted to calculate k_a :

$$k_a = k_0 \left[1 + \frac{1.358}{1 + 0.17Kn^{-0.4348}}Kn \right] \left[1 + \frac{4Kn}{1 + Kn} \right], \quad (46)$$

where, k_0 is calculated based on Kozeny-Carman (KC) equation[151], and the local characteristic pore radius for the calculation of Kn was estimated by[152]:

$$r = 0.08886\sqrt{\frac{k_0}{\varepsilon}}. \quad (47)$$

Chen et al.[150] performed several analysis based on a heterogeneous shale matrix with natural fractures, organic matter and inorganic minerals., Later the same technique were used by them to quantify the permeability of reconstructed shale matrix[153]. Their simulation results qualitatively and quantitatively confirm the increase in permeability induced by Klinkenberg's

effect. Moreover, Chen et al's study provides a framework of applying the LBM on REV scale for further research, within this framework, other physical effects (such as adsorption and surface diffusion) can be easily integrated by modifying the local apparent permeability.

4. Discussions and Conclusions

The LB method has gone through significant improvements over the years and has become a viable and efficient substitute for N-S solver for many flow problems. Because of the underlying kinetic nature, LB equation has attracted a huge interest in its extension to mimic micro-gaseous flows. In this paper we presented a general review of the LBM with an emphasis on boundary conditions, treatments for relaxation time and application of the LBM in isothermal fluid/gas flow simulation in shale gas reservoir.

It has been found that the LBM is an effective method for simulating micro gas flow in continuum to slip flow regime. For example, through the Chapman-Enskog expansion, lattice Boltzmann equation can be proved to recover the macroscopic continuity and momentum (N-S) equations. In slip flow regime, the Knudsen layer takes a small portion of the channel height, which can be neglected by extrapolating the bulk gas flow towards the wall. In this case, with the implementation of proper relaxation time and combination coefficients for various boundaries such as BB, SR or MD, the LB equation can give similar results to that of N-S equation with slip boundary conditions for pressure driven/force driven micro-channel flow and micro-Couette flow.

In transition flow regime, the Knudsen layer effect is significant, and the N-S equation with first-order slip boundary breaks down. Second-order or high-order slip boundary conditions are needed, and the change of the local mean free path/Knudsen number inside of the Knudsen layer has to be considered. The validation with MD or DSMC simulation results indicates that the LBM can be extended to simulate gas flow in transition flow regimes with high-order velocity sites and/or using wall function approach or approximated viscosity approach. However, because current effective viscosity models are only accurate with a moderate range of Knudsen number and the degree of freedom in the momentum space is very limited, difficulties still exist in studying non-equilibrium gas flow with high Knudsen numbers using LBM.

Several LB approaches are proposed to study gas transport in shale gas reservoir both on pore scale and REV scale. Pore scale simulation is an effective way to improve the understanding of different flow mechanisms. Application of the LBM to study shale gas transport on pore scale depends very much on its ability to capture micro-gaseous flow and the transport of adsorption gas. Slip N-S based LBM has the potential to provide accurate simulation results comparable with experimental studies with small Knudsen number. Existing slip N-S based LB models are premature to accurately estimate micro-flow properties in porous shale, and Klinkenberg model or DGM based LBM provide an alternative way to simulate gas flow on pore scale. The development of REV scale based LBM enable us to simulate gas flow on a larger scale, however, the simulation study should be complemented by laboratory studies on core samples. Increase in efficiency of these methods for simulation of micro-gaseous flow have the potential for applications in evaluating shale gas reservoirs.

The LBM still has a number of limitations in studying micro-gaseous flow, such as capturing the gas-solid interactions and non-ideal gas effect. Compared to other methods such as MD and DSMC, most of the previous applications of the LBM are more phenomenological than physical. For gas flow in shale gas reservoir, studies based on experiments, MD and DSMC are recommended to be carried out before using the LBM.

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6. References

- [1] R. G. Loucks, R. M. Reed, S. C. Ruppel, D. M. Jarvie, Morphology, genesis, and distribution of nanometer-scale pores in siliceous mudstones of the mississippian barnett shale, *Journal of Sedimentary Research* 79 (12) (2009) 848–861.

- 712 [2] C. H. Sondergeld, K. E. Newsham, J. T. Comisky, M. C. Rice, C. S. Rai,
713 Petrophysical considerations in evaluating and producing shale gas re-
714 sources, in: SPE Unconventional Gas Conference, Society of Petroleum
715 Engineers, 2010.
- 716 [3] F. Javadpour, D. Fisher, M. Unsworth, Nanoscale gas flow in shale gas
717 sediments, *Journal of Canadian Petroleum Technology* 46 (10) (2007)
718 55–61.
- 719 [4] S. M. Kang, E. Fathi, R. J. Ambrose, I. Y. Akkutlu, R. F. Sigal, Carbon
720 dioxide storage capacity of organic-rich shales, *SPE Journal* 16 (04)
721 (2011) 842–855.
- 722 [5] C. Freeman, G. Moridis, T. Blasingame, A numerical study of mi-
723 croscale flow behavior in tight gas and shale gas reservoir systems,
724 *Transport in Porous Media* 90 (1) (2011) 253–268.
- 725 [6] D. Luffel, C. Hopkins, S. P.D., Matrix permeability measurement of
726 gas productive shales, in: SPE Annual Technical Conference and Ex-
727 hibition, Society of Petroleum Engineers, 1993.
- 728 [7] A. Tinni, E. Fathi, R. Agarwal, C. H. Sondergeld, I. Y. Akkutlu, C. S.
729 Rai, Shale permeability measurements on plugs and crushed samples,
730 in: SPE Canadian Unconventional Resources Conference, Society of
731 Petroleum Engineers, 2012.
- 732 [8] J. Zhang, G. W. Scherer, Permeability of shale by the beam-bending
733 method, *International Journal of Rock Mechanics and Mining Sciences*
734 53 (2012) 179–191.
- 735 [9] Y. M. Metwally, C. H. Sondergeld, Measuring low permeabilities of gas-
736 sands and shales using a pressure transmission technique, *International*
737 *Journal of Rock Mechanics and Mining Sciences* 48 (7) (2011) 1135–
738 1144.
- 739 [10] A. Ghanizadeh, A. Amann Hildenbrand, M. Gasparik, Y. Gensterblum,
740 B. M. Krooss, R. Littke, Experimental study of fluid transport pro-
741 cesses in the matrix system of the european organic-rich shales: Ii. posi-
742 donia shale (lower toarcian, northern germany), *International Journal*
743 *of Coal Geology* 123 (2014) 20–33.

- 744 [11] R. Heller, J. Vermilyen, M. Zoback, Experimental investigation of ma-
745 trix permeability of gas shales, AAPG Bulletin 98 (5) (2014) 975–995.
- 746 [12] A. Mehmani, M. Prodanović, F. Javadpour, Multiscale, multiphysics
747 network modeling of shale matrix gas flows, Transport in Porous Media
748 99 (2) (2013) 377–390.
- 749 [13] Y. Yuan, N. G. Doonechaly, S. Rahman, An analytical model of ap-
750 parent gas permeability for tight porous media, Transport in Porous
751 Media (2015) 1–22.
- 752 [14] B. Li, A. Mehmani, J. Chen, D. T. Georgi, G. Jin, The condition
753 of capillary condensation and its effects on adsorption isotherms of
754 unconventional gas condensate reservoirs, in: SPE Annual Technical
755 Conference and Exhibition, Society of Petroleum Engineers, 2013.
- 756 [15] J. Chen, A. Mehmani, B. Li, D. Georgi, G. Jin, Estimation of total
757 hydrocarbon in the presence of capillary condensation for unconven-
758 tional shale reservoirs, in: SPE Middle East Oil and Gas Show and
759 Conference, Society of Petroleum Engineers, 2013.
- 760 [16] G. Jin, H. G. Pérez, G. Agrawal, M. R. Khodja, A. Z. Ali, S. R.
761 Hussaini, Z. Z. Jangda, The impact of gas adsorption and composition
762 on unconventional shale permeability measurement, in: SPE Middle
763 East Oil & Gas Show and Conference, Society of Petroleum Engineers,
764 2015.
- 765 [17] L. Zhang, D. Li, D. Lu, T. Zhang, A new formulation of apparent
766 permeability for gas transport in shale, Journal of Natural Gas Science
767 and Engineering 23 (2015) 221–226.
- 768 [18] K. Wu, X. Li, C. Wang, W. Yu, Z. Chen, Model for surface diffu-
769 sion of adsorbed gas in nanopores of shale gas reservoirs, Industrial &
770 Engineering Chemistry Research 54 (12) (2015) 3225–3236.
- 771 [19] A. Beskok, G. E. Karniadakis, Report: a model for flows in channels,
772 pipes, and ducts at micro and nano scales, Microscale Thermophysical
773 Engineering 3 (1) (1999) 43–77.
- 774 [20] F. Civan, Effective correlation of apparent gas permeability in tight
775 porous media, Transport in Porous Media 82 (2) (2010) 375–384.

- 776 [21] F. Civan, C. S. Rai, C. H. Sondergeld, Shale gas permeability and
777 diffusivity inferred by improved formulation of relevant retention and
778 transport mechanisms, *Transport in Porous Media* 86 (3) (2011) 925–
779 944.
- 780 [22] F. A. Florence, J. Rushing, K. E. Newsham, T. A. Blasingame, Im-
781 proved permeability prediction relations for low permeability sands,
782 in: *Rocky Mountain Oil & Gas Technology Symposium*, Society of
783 Petroleum Engineers, 2007.
- 784 [23] X. Xiong, D. Devegowda, M. Villazon, G. German, R. F. Sigal,
785 F. Civan, A fully-coupled free and adsorptive phase transport model for
786 shale gas reservoirs including non-darcy flow effects, in: *SPE Annual
787 Technical Conference and Exhibition*, Society of Petroleum Engineers,
788 2012.
- 789 [24] H. Singh, F. Javadpour, A. Ettehadtavakkol, H. Darabi, Nonempirical
790 apparent permeability of shale, *SPE Reservoir Evaluation & Engineer-
791 ing* 17 (03) (2014) 414–424.
- 792 [25] K. Wu, Apparent permeability for gas flow in shale reservoirs cou-
793 pling effects of gas diffusion and desorption, in: *Unconventional Re-
794 sources Technology Conference (URTEC)*, Society of Petroleum Engi-
795 neers, 2014.
- 796 [26] J. Klaver, G. Desbois, J. L. Urai, R. Littke, Bib-sem study of the pore
797 space morphology in early mature posidonia shale from the hils area,
798 germany, *International Journal of Coal Geology* 103 (2012) 12–25.
- 799 [27] J. Klaver, G. Desbois, R. Littke, J. L. Urai, Bib-sem characterization of
800 pore space morphology and distributions in postmature to overmature
801 samples from the haynesville and bossier shales, *Marine and Petroleum
802 Geology* 59 (2015) 451–466.
- 803 [28] R. M. Slatt, N. R. O’Brien, Pore types in the barnett and woodford
804 gas shales: Contribution to understanding gas storage and migration
805 pathways in fine-grained rocks, *AAPG bulletin* 95 (12) (2011) 2017–
806 2030.
- 807 [29] M. Milner, R. McLin, J. Petriello, Imaging texture and porosity in mud-
808 stones and shales: Comparison of secondary and ion-milled backscatter

- sem methods, in: Canadian Unconventional Resources and International Petroleum Conference, Society of Petroleum Engineers, 2010.
- [30] M. E. Curtis, R. J. Ambrose, C. H. Sondergeld, Structural characterization of gas shales on the micro-and nano-scales, in: Canadian Unconventional Resources and International Petroleum Conference, Society of Petroleum Engineers, 2010.
- [31] G. R. McNamara, G. Zanetti, Use of the boltzmann equation to simulate lattice-gas automata, *Physical Review Letters* 61 (20) (1988) 2332–2335.
- [32] F. Higuera, J. Jimenez, Boltzmann approach to lattice gas simulations, *EPL (Europhysics Letters)* 9 (7) (1989) 663–668.
- [33] X. He, L. Luo, A priori derivation of the lattice boltzmann equation, *Physical Review E* 55 (6) (1997) R6333–R6336.
- [34] X. He, L. Luo, Theory of the lattice boltzmann method: From the boltzmann equation to the lattice boltzmann equation, *Physical Review E* 56 (6) (1997) 6811–6817.
- [35] A. Nabovati, E. W. Llewellyn, A. Sousa, A general model for the permeability of fibrous porous media based on fluid flow simulations using the lattice boltzmann method, *Composites Part A: Applied Science and Manufacturing* 40 (6) (2009) 860–869.
- [36] Z. Guo, T. Zhao, Lattice boltzmann model for incompressible flows through porous media, *Physical Review E* 66 (3) (2002) 036304.
- [37] C. Pan, M. Hilpert, C. Miller, Lattice-boltzmann simulation of two-phase flow in porous media, *Water Resources Research* 40 (1) (2004) w01501.
- [38] A. K. Gunstensen, D. H. Rothman, Lattice-boltzmann studies of immiscible two-phase flow through porous media, *Journal of Geophysical Research: Solid Earth* (1978–2012) 98 (B4) (1993) 6431–6441.
- [39] S. Succi, E. Foti, F. Higuera, Three-dimensional flows in complex geometries with the lattice boltzmann method, *EPL (Europhysics Letters)* 10 (5) (1989) 433–438.

- [40] Q. Kang, D. Zhang, S. Chen, X. He, Lattice boltzmann simulation of chemical dissolution in porous media, *Physical Review E* 65 (3) (2002) 036318.
- [41] Q. Kang, P. C. Lichtner, D. Zhang, Lattice boltzmann pore-scale model for multicomponent reactive transport in porous media, *Journal of Geophysical Research: Solid Earth* (1978–2012) 111 (B5) (2006) B05203.
- [42] M. L. Porter, M. G. Schaap, D. Wildenschild, Lattice-boltzmann simulations of the capillary pressure–saturation–interfacial area relationship for porous media, *Advances in Water Resources* 32 (11) (2009) 1632–1640.
- [43] S. Ramaswamy, M. Gupta, A. Goel, U. Aaltosalmi, M. Kataja, A. Koponen, B. Ramarao, The 3d structure of fabric and its relationship to liquid and vapor transport, *Colloids and Surfaces A: Physicochemical and Engineering Aspects* 241 (1) (2004) 323–333.
- [44] T. Koido, T. Furusawa, K. Moriyama, An approach to modeling two-phase transport in the gas diffusion layer of a proton exchange membrane fuel cell, *Journal of Power Sources* 175 (1) (2008) 127–136.
- [45] L. Wang, B. Afsharpoya, Modeling fluid flow in fuel cells using the lattice-boltzmann approach, *Mathematics and Computers in Simulation* 72 (2) (2006) 242–248.
- [46] N. S. Martys, H. Chen, Simulation of multicomponent fluids in complex three-dimensional geometries by the lattice boltzmann method, *Physical Review E* 53 (1) (1996) 743–751.
- [47] B. Ferreol, D. H. Rothman, Lattice-boltzmann simulations of flow through fontainebleau sandstone, in: *Multiphase Flow in Porous Media*, Springer, 1995, pp. 3–20.
- [48] E. S. Boek, M. Venturoli, Lattice-boltzmann studies of fluid flow in porous media with realistic rock geometries, *Computers & Mathematics with Applications* 59 (7) (2010) 2305–2314.
- [49] M. Coles, R. Hazlett, E. Muegge, K. Jones, B. Andrews, B. Dowd, P. Siddons, A. Peskin, P. Spanne, W. Soll, Developments in synchrotron x-ray microtomography with applications to flow in porous

- media, in: SPE Annual Technical Conference and Exhibition, Society of Petroleum Engineers, 1996.
- [50] B. Li, D. Kwok, Li and kwok reply:, Physical Review Letters 92 (2004) 139402.
- [51] T. Lee, C. Lin, Rarefaction and compressibility effects of the lattice-boltzmann-equation method in a gas microchannel, Physical Review E 71 (4) (2005) 046706.
- [52] X. Niu, C. Shu, Y. Chew, A lattice boltzmann bgk model for simulation of micro flows, EPL (Europhysics Letters) 67 (4) (2004) 600–606.
- [53] M. Sbragaglia, S. Succi, Analytical calculation of slip flow in lattice boltzmann models with kinetic boundary conditions, Physics of Fluids (1994-present) 17 (9) (2005) 093602.
- [54] S. Succi, Mesoscopic modeling of slip motion at fluid-solid interfaces with heterogeneous catalysis, Physical Review Letters 89 (6) (2002) 064502.
- [55] G. Tang, W. Tao, Y. He, Lattice boltzmann method for simulating gas flow in microchannels, International Journal of Modern Physics C 15 (02) (2004) 335–347.
- [56] Y. Zhang, R. Qin, D. R. Emerson, Lattice boltzmann simulation of rarefied gas flows in microchannels, Physical Review E 71 (4) (2005) 047702.
- [57] 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.
- [58] F. Verhaeghe, L. Luo, B. Blanpain, Lattice boltzmann modeling of microchannel flow in slip flow regime, Journal of Computational Physics 228 (1) (2009) 147–157.
- [59] A. Homayoon, A. Isfahani, E. Shirani, M. Ashrafizadeh, A novel modified lattice boltzmann method for simulation of gas flows in wide range of knudsen number, International Communications in Heat and Mass Transfer 38 (6) (2011) 827–832.

- 903 [60] Z. Guo, C. Zheng, B. Shi, Lattice boltzmann equation with multiple
904 effective relaxation times for gaseous microscale flow, *Physical Review*
905 *E* 77 (3) (2008) 036707.
- 906 [61] C. Zhuo, C. Zhong, Filter-matrix lattice boltzmann model for mi-
907 crochannel gas flows, *Physical Review E* 88 (5) (2013) 053311.
- 908 [62] Q. Li, Y. He, G. Tang, W. Tao, Lattice boltzmann modeling of
909 microchannel flows in the transition flow regime, *Microfluidics and*
910 *Nanofluidics* 10 (3) (2011) 607–618.
- 911 [63] G. Tang, Y. Zhang, X. Gu, D. Emerson, Lattice boltzmann modelling
912 knudsen layer effect in non-equilibrium flows, *EPL (Europhysics Let-*
913 *ters)* 83 (4) (2008) 40008.
- 914 [64] H. Shokouhmand, A. Meghdadi Isfahani, An improved thermal lattice
915 boltzmann model for rarefied gas flows in wide range of knudsen num-
916 ber, *International Communications in Heat and Mass Transfer* 38 (10)
917 (2011) 1463–1469.
- 918 [65] X. Niu, C. Shu, Y. Chew, Numerical simulation of isothermal micro
919 flows by lattice boltzmann method and theoretical analysis of the dif-
920 fuse scattering boundary condition, *International Journal of Modern*
921 *Physics C* 16 (12) (2005) 1927–1941.
- 922 [66] G. Tang, W. Tao, Y. He, Lattice boltzmann method for gaseous mi-
923 croflows using kinetic theory boundary conditions, *Physics of Fluids*
924 17 (5) (2005) 058101.
- 925 [67] L. Luo, Comment on”heat transfer and fluid flow in microchannels and
926 nanochannels at high knudsen number using thermal lattice-boltzmann
927 method”, *Physical Review E* 84 (2011) 048301.
- 928 [68] A. Norouzi, J. A. Esfahani, Two relaxation time lattice boltzmann
929 equation for high knudsen number flows using wall function approach,
930 *Microfluidics and Nanofluidics* (2014) 1–10.
- 931 [69] J. A. Esfahani, A. Norouzi, Two relaxation time lattice boltzmann
932 model for rarefied gas flows, *Physica A: Statistical Mechanics and its*
933 *Applications* 393 (2014) 51–61.

- 934 [70] X. Zhang, L. Xiao, X. Shan, L. Guo, Lattice boltzmann simulation of
935 shale gas transport in organic nano-pores, *Scientific reports* 4.
- 936 [71] K. Suga, Lattice boltzmann methods for complex micro-flows: appli-
937 cability and limitations for practical applications, *Fluid Dynamics Re-*
938 *search* 45 (3) (2013) 034501.
- 939 [72] C. K. Aidun, J. R. Clausen, Lattice-boltzmann method for complex
940 flows, *Annual Review of Fluid Mechanics* 42 (2010) 439–472.
- 941 [73] Z. Guo, C. Zheng, B. Shi, Discrete lattice effects on the forcing term in
942 the lattice boltzmann method, *Physical Review E* 65 (4) (2002) 046308.
- 943 [74] S. H. Kim, H. Pitsch, I. D. Boyd, Accuracy of higher-order lattice
944 boltzmann methods for microscale flows with finite knudsen numbers,
945 *Journal of Computational Physics* 227 (19) (2008) 8655–8671.
- 946 [75] A. P. Randles, V. Kale, J. Hammond, W. Gropp, E. Kaxiras, Perfor-
947 mance analysis of the lattice boltzmann model beyond navier-stokes,
948 in: *Parallel & Distributed Processing (IPDPS)*, 2013 IEEE 27th Inter-
949 national Symposium, IEEE, 2013.
- 950 [76] P. L. Bhatnagar, E. P. Gross, M. Krook, A model for collision pro-
951 cesses in gases. i. small amplitude processes in charged and neutral
952 one-component systems, *Physical Review* 94 (3) (1954) 511–525.
- 953 [77] P. Lallemand, L.-S. Luo, Theory of the lattice boltzmann method: Dis-
954 persion, dissipation, isotropy, galilean invariance, and stability, *Physi-*
955 *cal Review E* 61 (6) (2000) 6546–6562.
- 956 [78] L. Luo, W. Liao, X. Chen, Y. Peng, W. Zhang, Numerics of the lattice
957 boltzmann method: Effects of collision models on the lattice boltzmann
958 simulations, *Physical Review E* 83 (5) (2011) 056710.
- 959 [79] I. Ginzburg, Equilibrium-type and link-type lattice boltzmann models
960 for generic advection and anisotropic-dispersion equation, *Advances in*
961 *Water resources* 28 (11) (2005) 1171–1195.
- 962 [80] D. C. Tretheway, C. D. Meinhardt, Apparent fluid slip at hydrophobic
963 microchannel walls, *Physics of Fluids (1994-present)* 14 (3) (2002) L9–
964 L12.

- 965 [81] J. C. Harley, Y. Huang, H. H. Bau, J. N. Zemel, Gas flow in micro-
966 channels, *Journal of Fluid Mechanics* 284 (1995) 257–274.
- 967 [82] L. Zhu, D. Tretheway, L. Petzold, C. Meinhart, Simulation of fluid
968 slip at 3d hydrophobic microchannel walls by the lattice boltzmann
969 method, *Journal of Computational Physics* 202 (1) (2005) 181–195.
- 970 [83] J. Harting, C. Kunert, H. J. Herrmann, Lattice boltzmann simulations
971 of apparent slip in hydrophobic microchannels, *EPL (Europhysics Let-
972 ters)* 75 (2) (2006) 328.
- 973 [84] R. Benzi, L. Biferale, M. Sbragaglia, S. Succi, F. Toschi, Mesoscopic
974 two-phase model for describing apparent slip in micro-channel flows,
975 *EPL (Europhysics Letters)* 74 (4) (2006) 651.
- 976 [85] Y. Zhang, X. Gu, R. W. Barber, D. R. Emerson, Capturing knudsen
977 layer phenomena using a lattice boltzmann model, *Physical Review E*
978 74 (4) (2006) 046704.
- 979 [86] S. Succi, *The Lattice-Boltzmann Equation*, Oxford university press,
980 Oxford, 2001.
- 981 [87] X. Nie, G. D. Doolen, S. Chen, Lattice-boltzmann simulations of fluid
982 flows in mems, *Journal of Statistical Physics* 107 (1-2) (2002) 279–289.
- 983 [88] C. Lim, C. Shu, X. Niu, Y. Chew, Application of lattice boltz-
984 mann method to simulate microchannel flows, *Physics of Fluids* (1994-
985 present) 14 (7) (2002) 2299–2308.
- 986 [89] Z. Chai, Z. Guo, L. Zheng, B. Shi, Lattice boltzmann simulation of
987 surface roughness effect on gaseous flow in a microchannel, *Journal of
988 Applied Physics* 104 (1) (2008) 014902.
- 989 [90] S. Tao, Z. Guo, Boundary condition for lattice boltzmann modeling
990 of microscale gas flows with curved walls in the slip regime, *Physical
991 Review E* 91 (4) (2015) 043305.
- 992 [91] D. Technischen, Lattice boltzmann simulations in the finite knudsen
993 number range within the peano framework, Ph.D. thesis, University
994 At Munchen (2011).

- 995 [92] S. Ansumali, I. V. Karlin, Kinetic boundary conditions in the lattice
996 boltzmann method, *Physical Review E* 66 (2) (2002) 026311.
- 997 [93] X. Niu, S. A. Hyodo, T. Munekata, K. Suga, Kinetic lattice boltz-
998 mann method for microscale gas flows: Issues on boundary condition,
999 relaxation time, and regularization, *Physical Review E* 76 (3) (2007)
1000 036711.
- 1001 [94] Z. Chai, B. Shi, Z. Guo, J. Lu, Gas flow through square arrays of
1002 circular cylinders with klinkenberg effect: a lattice boltzmann study,
1003 *Communications in Computational Physics* 8 (5) (2010) 1052.
- 1004 [95] Z. Guo, C. Zheng, Analysis of lattice boltzmann equation for microscale
1005 gas flows: relaxation times, boundary conditions and the knudsen layer,
1006 *International Journal of Computational Fluid Dynamics* 22 (7) (2008)
1007 465–473.
- 1008 [96] Z. Guo, B. Shi, T.-S. Zhao, C. Zheng, Discrete effects on boundary
1009 conditions for the lattice boltzmann equation in simulating microscale
1010 gas flows, *Physical Review E* 76 (5) (2007) 056704.
- 1011 [97] P. Neumann, T. Rohrmann, Lattice boltzmann simulations in the slip
1012 and transition flow regime with the peano framework, *Open Journal of*
1013 *Fluid Dynamics* 2 (2012) 101–110.
- 1014 [98] X. He, Q. Zou, L. Luo, M. Dembo, Analytic solutions of simple flows
1015 and analysis of nonslip boundary conditions for the lattice boltzmann
1016 bgk model, *Journal of Statistical Physics* 87 (1-2).
- 1017 [99] L. Zheng, Z. Guo, B. Shi, Microscale boundary conditions of the lattice
1018 boltzmann equation method for simulating microtube flows, *Physical*
1019 *Review E* 86 (1) (2012) 016712.
- 1020 [100] J. C. Maxwell, On stresses in rarified gases arising from inequalities of
1021 temperature, *Philosophical Transactions of the royal society of London*
1022 170 (1879) 231–256.
- 1023 [101] W. Zhang, G. Meng, X. Wei, A review on slip models for gas microflows,
1024 *Microfluidics and Nanofluidics* 13 (6) (2012) 845–882.

- 1025 [102] B. C. Eu, R. E. Khayat, G. D. Billing, C. Nyeland, Nonlinear trans-
 1026 port coefficients and plane couette flow of a viscous, heat-conducting
 1027 gas between two plates at different temperatures, Canadian Journal of
 1028 Physics 65 (9) (1987) 1090–1103.
- 1029 [103] R. Myong, A generalized hydrodynamic computational model for rar-
 1030 eified and microscale diatomic gas flows, Journal of Computational
 1031 Physics 195 (2) (2004) 655–676.
- 1032 [104] Q. Yang, H. Zhang, Discussion on the gaseous slip model based on
 1033 langmuir adsorption isotherm, Physics Procedia 32 (2012) 179–183.
- 1034 [105] H. M. Kim, D. Kim, W. T. Kim, P. Seung Chung, M. S. Jhon, Lang-
 1035 muir slip model for air bearing simulation using the lattice boltzmann
 1036 method, Magnetics, IEEE Transactions on 43 (6) (2007) 2244–2246.
- 1037 [106] S. Chen, Z. Tian, Simulation of microchannel flow using the lattice
 1038 boltzmann method, Physica A: Statistical Mechanics and its Applica-
 1039 tions 388 (23) (2009) 4803–4810.
- 1040 [107] X. Shan, X. Yuan, H. Chen, Kinetic theory representation of hydro-
 1041 dynamics: a way beyond the navier–stokes equation, Journal of Fluid
 1042 Mechanics 550 (2006) 413–441.
- 1043 [108] N. Dongari, Y. Zhang, J. M. Reese, Modeling of knudsen layer effects
 1044 in micro/nanoscale gas flows, Journal of Fluids Engineering 133 (7)
 1045 (2011) 071101.
- 1046 [109] C. Cercignani, A. Daneri, Flow of a rarefied gas between two parallel
 1047 plates, Journal of Applied Physics 34 (12) (1963) 3509–3513.
- 1048 [110] Y. Zhang, R. Qin, Y. Sun, R. Barber, D. Emerson, Gas flow in
 1049 microchannels—a lattice boltzmann method approach, Journal of Sta-
 1050 tistical Physics 121 (1-2) (2005) 257–267.
- 1051 [111] L. O’Hare, D. A. Lockerby, J. M. Reese, D. R. Emerson, Near-wall
 1052 effects in rarefied gas micro-flows: some modern hydrodynamic ap-
 1053 proaches, International journal of heat and fluid flow 28 (1) (2007)
 1054 37–43.

- 1055 [112] D. Stops, The mean free path of gas molecules in the transition regime,
1056 Journal of Physics D: Applied Physics 3 (5) (1970) 685–696.
- 1057 [113] E. J. Arlemark, S. K. Dadzie, J. M. Reese, An extension to the navier–
1058 stokes equations to incorporate gas molecular collisions with bound-
1059 aries, Journal of Heat Transfer 132 (4) (2010) 041006.
- 1060 [114] V. K. Michalis, A. N. Kalarakis, E. D. Skouras, V. N. Burganos, Rar-
1061 efaction effects on gas viscosity in the knudsen transition regime, Mi-
1062 crofluidics and Nanofluidics 9 (4-5) (2010) 847–853.
- 1063 [115] Y. Sun, W. Chan, Analytical modeling of rarefied poiseuille flow in mi-
1064 crochannels, Journal of Vacuum Science & Technology A 22 (2) (2004)
1065 383–394.
- 1066 [116] A. Kalarakis, V. Michalis, E. Skouras, V. Burganos, Mesoscopic simu-
1067 lation of rarefied flow in narrow channels and porous media, Transport
1068 in Porous Media 94 (1) (2012) 385–398.
- 1069 [117] S. Ansumali, I. Karlin, S. Arcidiacono, A. Abbas, N. Prasianakis, Hy-
1070 drodynamics beyond navier-stokes: Exact solution to the lattice boltz-
1071 mann hierarchy, Physical Review Letters 98 (12) (2007) 124502.
- 1072 [118] R. Zhang, X. Shan, H. Chen, Efficient kinetic method for fluid simu-
1073 lation beyond the navier-stokes equation, Physical Review E 74 (4)
1074 (2006) 046703.
- 1075 [119] S. S. Chikatamarla, I. V. Karlin, Entropy and galilean invariance of lat-
1076 tice boltzmann theories, Physical Review Letters 97 (19) (2006) 190601.
- 1077 [120] L. Szalmás, Knudsen layer theory for high-order lattice boltzmann
1078 models, Europhysics Letters 80 (2) (2007) 24003.
- 1079 [121] J. Meng, Y. Zhang, Gauss-hermite quadratures and accuracy of lattice
1080 boltzmann models for nonequilibrium gas flows, Physical Review E
1081 83 (3) (2011) 036704.
- 1082 [122] J. Meng, Y. Zhang, Accuracy analysis of high-order lattice boltzmann
1083 models for rarefied gas flows, Journal of Computational Physics 230 (3)
1084 (2011) 835–849.

- 1085 [123] K. Suga, S. Takenaka, T. Ito, M. Kaneda, T. Kinjo, S. Hyodo, Evalu-
1086 ation of a lattice boltzmann method in a complex nanoflow, *Physical*
1087 *Review E* 82 (1) (2010) 016701.
- 1088 [124] K. Suga, S. Takenaka, T. Ito, M. Kaneda, T. Kinjo, S. Hyodo, Lattice
1089 boltzmann flow simulation in micro-nano transitional porous media, in:
1090 2010 14th International Heat Transfer Conference, American Society
1091 of Mechanical Engineers, 2010, pp. 321–329.
- 1092 [125] Y. Wu, J. Li, D. Ding, C. Wang, Y. Di, A generalized framework model
1093 for the simulation of gas production in unconventional gas reservoirs,
1094 *SPE Journal* 19 (05) (2014) 845–857.
- 1095 [126] Y. Li, Y. Jiang, J. Zhao, C. Liu, L. Zhang, Extended finite element
1096 method for analysis of multi-scale flow in fractured shale gas reservoirs,
1097 *Environmental Earth Sciences* 73 (10) (2015) 6035–6045.
- 1098 [127] M. Sheng, G. Li, S. N. Shah, X. Jin, Extended finite element modeling
1099 of multi-scale flow in fractured shale gas reservoirs, in: *SPE Annual*
1100 *Technical Conference and Exhibition*, Society of Petroleum Engineers,
1101 2012.
- 1102 [128] N. Gholizadeh Doonechaly, R. Abdel Azim, S. S. Rahman, Evaluation
1103 of recoverable energy potential from enhanced geothermal systems: A
1104 sensitivity analysis in a poro-thermo-elastic framework, *Geofluids*.
- 1105 [129] Z. Pan, L. D. Connell, Reservoir simulation of free and adsorbed gas
1106 production from shale, *Journal of Natural Gas Science and Engineering*
1107 22 (2015) 359–370.
- 1108 [130] C. J. Landry, Matrix-fracture connectivity in eagle ford shale, in: *Un-*
1109 *conventional Resources Technology Conference (URTEC)*, Society of
1110 Petroleum Engineers, 2014.
- 1111 [131] P. Tiwari, M. Deo, C. Lin, J. Miller, Characterization of oil shale pore
1112 structure before and after pyrolysis by using x-ray micro ct, *Fuel* 107
1113 (2013) 547–554.
- 1114 [132] J. Ma, A multi-scale framework for digital core analysis of gas shale at
1115 millimeter scales, in: *Unconventional Resources Technology Conference*
1116 *(URTEC)*, Society of Petroleum Engineers, 2014.

- 1117 [133] C. Chen, D. Hu, D. Westacott, D. Loveless, Nanometer-scale charac-
 1118 terization of microscopic pores in shale kerogen by image analysis and
 1119 pore-scale modeling, *Geochemistry, Geophysics, Geosystems* 14 (10)
 1120 (2013) 4066–4075.
- 1121 [134] C. Chen, D. Hu, V. N. Martysevich, Applications of high-resolution
 1122 imaging and high-performance parallel computing in unconventional
 1123 energy recovery, in: *Abu Dhabi International Petroleum Exhibition*
 1124 *and Conference*, Society of Petroleum Engineers, 2014.
- 1125 [135] M. T. Cantisano, Relative permeability in a shale formation in colombia
 1126 using digital rock physics, in: *Unconventional Resources Technology*
 1127 *Conference (URTEC)*, Society of Petroleum Engineers, 2013.
- 1128 [136] N. Nagarajan, Critical role of rock and fluid-impact on reservoir per-
 1129 formance on unconventional shale reservoirs, in: *Unconventional Re-*
 1130 *sources Technology Conference (URTEC)*, Society of Petroleum Engi-
 1131 neers, 2013.
- 1132 [137] L. Klinkenberg, The permeability of porous media to liquids and gases,
 1133 in: *Drilling and Production Practice*, American Petroleum Institute,
 1134 1941.
- 1135 [138] A. M. Allan, G. Mavko, The effect of adsorption and knudsen diffu-
 1136 sion on the steady-state permeability of microporous rocks, *Geophysics*
 1137 78 (2) (2013) D75–D83.
- 1138 [139] L. Chen, L. Zhang, Q. Kang, J. Yao, W. Tao, Nanoscale simulation of
 1139 shale transport properties using the lattice boltzmann method: perme-
 1140 ability and diffusivity, *Scientific Reports*.
- 1141 [140] A. S. Ziarani, R. Aguilera, Knudsen permeability correction for tight
 1142 porous media, *Transport in Porous Media* 91 (1) (2012) 239–260.
- 1143 [141] L. Chen, Q. Kang, R. Pawar, Y.-L. He, W. Tao, Pore-scale prediction of
 1144 transport properties in reconstructed nanostructures of organic matter
 1145 in shales, *Fuel* 158 (0) (2015) 650–658.
- 1146 [142] M. Kazemi, A. Takbiri-Borujeni, An analytical model for shale gas
 1147 permeability, *International Journal of Coal Geology* 146 (2015) 188–
 1148 197.

- 1149 [143] E. Fathi, A. Tinni, I. Y. Akkutlu, Correction to klinkenberg slip theory
1150 for gas flow in nano-capillaries, International Journal of Coal Geology
1151 103 (2012) 51–59.
- 1152 [144] X. Shan, H. Chen, Lattice boltzmann model for simulating flows with
1153 multiple phases and components, Physical Review E 47 (3) (1993)
1154 1815–1820.
- 1155 [145] Z. Li, T. Min, L. Chen, Q. Kangd, Y.-L. He, W.-Q. Tao, Investiga-
1156 tion of methane adsorption and its effect on gas transport in shale
1157 matrix through microscale and mesoscale simulations, arXiv preprint
1158 arXiv:1503.07445.
- 1159 [146] J. Ren, P. Guo, Z. Guo, Z. Wang, A lattice boltzmann model for sim-
1160 ulating gas flow in kerogen pores, Transport in Porous Media (2014)
1161 1–17.
- 1162 [147] O. Dardis, J. McCloskey, Lattice boltzmann scheme with real num-
1163 bered solid density for the simulation of flow in porous media, Physical
1164 Review E 57 (4) (1998) 4834.
- 1165 [148] M. A. Spaid, F. R. Phelan Jr, Lattice boltzmann methods for model-
1166 ing microscale flow in fibrous porous media, Physics of Fluids (1994-
1167 present) 9 (9) (1997) 2468–2474.
- 1168 [149] Q. Kang, D. Zhang, S. Chen, Unified lattice boltzmann method for flow
1169 in multiscale porous media, Physical Review E 66 (5) (2002) 056307.
- 1170 [150] L. Chen, W. Fang, Q. Kang, J. D. Hyman, H. S. Viswanathan, W.-
1171 Q. Tao, Generalized lattice boltzmann model for flow through tight
1172 porous media with klinkenberg’s effect, Physical Review E 91 (3) (2015)
1173 033004.
- 1174 [151] P. Carman, Fluid flow through granular beds, Chemical Engineering
1175 Research and Design 75 (1997) S32–S48.
- 1176 [152] J. Heid, J. McMahon, R. Nielsen, S. Yuster, Study of the permeability
1177 of rocks to homogeneous fluids, in: Drilling and production practice,
1178 American Petroleum Institute, 1950.

- 1179 [153] L. Chen, Q. Kang, Z. Dai, H. S. Viswanathan, W. Tao, Permeability
1180 prediction of shale matrix reconstructed using the elementary building
1181 block model, Fuel 160 (2015) 346–356.