Capturing Knudsen Layer Phenomena using a Lattice Boltzmann Model

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Abstract

In recent years, lattice Boltzmann methods have been increasingly used to simulate rarefied gas flows in micro- and nano-scale devices. This is partly due to the fact that the method is computationally efficient, particularly when compared to solution techniques like the direct simulation Monte Carlo approach. However, lattice Boltzmann models developed for rarefied gas flows have difficulty in capturing the nonlinear relationship between the shear stress and strain rate within the Knudsen layer. As a consequence, these models are equivalent to slip-flow solutions of the Navier-Stokes equations.

In this paper, we propose an *effective mean free path* to address the Knudsen layer effect, so that the capabilities of lattice Boltzmann methods can be extended beyond the slip-flow regime. The model has been applied to rarefied shear-driven and pressure-driven flows between parallel plates at Knudsen numbers between 0.01 and 1. Our results show that the proposed approach significantly improves the near-wall accuracy of the lattice Boltzmann method and provides a computationally economic solution technique over a wide range of Knudsen numbers.

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I. INTRODUCTION

Microsystems have developed rapidly since the concepts of 'lab-on-a-chip' and 'micro-Total-Analysis-Systems' were first introduced in the early 1990s. The benefits of miniaturization include increased chemical yields, lower reagent consumption, enhanced sensitivity, and reduced processing time. More importantly, miniaturization may offer enhanced functionality that cannot be achieved in conventional macro-scale devices. Recently, increasing numbers of miniaturized devices have been developed that require an understanding of the fundamental physics associated with rarefied gas flows in the slip- and transition-flow regimes. However, predicting such flows presents a significant modeling challenge due to the fact that gas microflows experience a range of non-equilibrium phenomena under standard operating conditions including velocity slip and temperature jump at solid boundaries, and a nonlinear stress/strain relationship within the Knudsen layer. Previously, these phenomena have only been encountered in macro-scale flows under extreme conditions [1].

Despite the major advances in microsystems technology, the current lack of fundamental understanding of micro- and nano-scale gas flows is hindering the systematic design of new miniaturized devices [2]. The Navier-Stokes equations with no-slip boundary conditions often fail to explain important experimental observations, e.g. that the measured flow rate is higher than expected while the drag and friction factor are lower than expected [3]. This is because the Navier-Stokes equations can only describe flows that are close to local thermodynamic equilibrium. When the mean free path of the gas molecules approaches the length scale of the device, the flow lacks scale separation and is unable to achieve local equilibrium [4]. The critical parameter is the Knudsen number, $Kn = l/H$, where l is the mean free path of the gas molecules and H is the characteristic length scale of the flow system. The Navier-Stokes equations with no-slip boundary conditions are only appropriate when $Kn < 0.001$. However, gas flows in miniaturized devices are often in the *slip regime* ($0.001 < Kn < 0.1$) or the *transition regime* ($0.1 < Kn < 10$). In these regimes, the gas can no longer be described as a continuous quasi-equilibrium fluid nor as a free molecular flow [5]. In practice, most devices will operate over a range of Knudsen numbers in different parts of the device; this makes it even more difficult to develop a general flow model.

The direct simulation Monte Carlo (DSMC) method (a statistical molecular dynamics approach) can successfully simulate high-speed transition flows [6]. In contrast, the flows

encountered in micro- and nano-scale systems typically involve low Mach numbers and low Knudsen numbers. Under these conditions, the DSMC approach is not computationally efficient due to the requirement to perform large amounts of data sampling in order to reduce the statistical scatter in the predicted flow fields. This makes current DSMC methods unsuitable for low speed, low Knudsen number flows [7]. Similar problems occur in hybrid DSMC/Navier-Stokes solvers for mixed-density flows [8] and direct solutions of the Boltzmann equation [9]. Significant effort has been made to extend the validity of continuum-based equations and develop higher-order equation sets, such as Grad's 13 moment method and the Burnett equations. However, these methods have generally failed to produce satisfactory results for low-speed flows in the transition regime, although significant progress has been made in coupling the Navier-Stokes equations with the BGK model [10]. The development of the Information Preservation (IP) method for DSMC [11, 12] appears to be a promising approach while Baker and Hadjiconstantinou [13] and Chun and Koch [14] have recently demonstrated that the statistical scatter associated with Monte Carlo methods can be reduced by considering only the deviation from equilibrium. However, there is currently no comprehensive and computationally efficient model that can simulate both low-speed and low Knudsen number gas flows for $0.1 \leq Kn \leq 1$.

The lattice Boltzmann method offers an attractive technique for micro- and nano-scale fluidic applications where the microscopic and macroscopic behavior are coupled. The method retains a computational efficiency comparable to Navier-Stokes solvers but is potentially a more accurate model for gas flows, over a broad range of Knudsen numbers, because its origins lie in kinetic theory. Since Nie *et al.* [15] and Lim *et al.* [16] first applied the lattice Boltzmann method to simulate rarefied gas flows, many publications have emerged which demonstrate that velocity slip and temperature jump phenomena can be captured by the lattice Boltzmann equation (LBE) approach [17–26]. However, the foregoing work focused on developing new boundary conditions for the velocity slip and temperature jump rather than constructing new LBE models that conserve symmetry for the higher-order moments (an essential requirement to obtain quantitative results for high Knudsen number flows). Consequently, these lattice Boltzmann models are still working within the Navier-Stokes slip-flow regime and are therefore restricted to very low Knudsen numbers i.e. $Kn \leq 0.1$. In other words, these models fail to capture the flow characteristics in the Knudsen layer where the Navier-Stokes equations are not valid. However, Sbragaglia and Succi [27] have

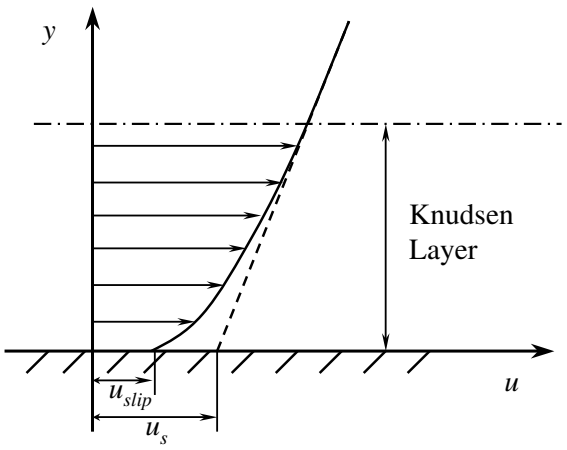

FIG. 1: Schematic diagram showing the microscopic slip (u_{slip}) and macroscopic slip (u_s) for Kramers' problem [30]. Actual velocity profile (—) and velocity profile predicted using Navier-Stokes and LBE models (– –) within the Knudsen layer.

recently argued that the LBE method should be able to provide a reasonable description of rarefied gas flows beyond the hydrodynamic slip-flow limit and up to $Kn \sim \mathcal{O}(1)$.

One of the most important tests for any transition-regime model is whether it can capture the nonlinear flow characteristics in the Knudsen layer. In order to simulate high Kn flows, where temperature and density variations play an important role, one possible solution is to develop more advanced LBE models for the high-order moments. Recently, Shan *et al.* [28] have shown that higher-order LBE models, based on an expansion of the Boltzmann distribution function, can be constructed. In contrast, Benzi *et al.* [29] have proposed a phenomenological pseudo-potential to describe molecular interactions at the surface. This approach could offer a way of constructing a more comprehensive near-wall treatment to capture nonlinear phenomena. However, no definitive results have yet been produced to demonstrate that either of these approaches can capture Knudsen layer effects. In this paper, we propose an alternative and computationally efficient method to extend the range and validity of the LBE method into the transition regime.

II. CAPTURING KNUDSEN LAYERS

The Knudsen layer, or kinetic boundary layer, is a region near a solid wall with a thickness of a few mean free paths where the usual linear relationship between the stress and rate of

strain is no longer valid, i.e. the Navier-Stokes equations become inappropriate in this layer. Figure 1 illustrates the velocity profile in the Knudsen layer for the particular case of Kramers' problem - a gas bounded by a single planar wall, subjected to a uniform and constant shear stress. As illustrated in Fig. 1, the flow behavior in the Knudsen layer is very different from that predicted by the Navier-Stokes equations and LBE models which over-estimate the velocity slip at the wall.

Unlike the DSMC method, the mean free path must be prescribed through the Knudsen number in LBE simulations of rarefied gas flow. However, the presence of a solid boundary will have a significant impact on the distance a gas molecule can travel between successive collisions, especially in the near-wall region. As a consequence, the mean free path will be smaller than that observed in the bulk flow. We therefore propose an *effective mean free path*, which is defined as the average distance a gas molecule will travel between consecutive collisions with either another gas molecule or the solid wall. This adjustment to the mean free path will only apply in the Knudsen layer and, for isothermal rarefied gas flow at low speed, the correction can be obtained from well documented work on the velocity defect in the Knudsen layer for Kramers' problem [30].

The velocity defect, the difference between the actual velocity and that predicted by the Navier-Stokes equations, increases as the wall is approached. This particular problem has been investigated experimentally and numerically for gas flows at the incompressible and isothermal limit. Despite the lack of a universally accepted description of the Knudsen layer, there is clear evidence to suggest that the velocity defect decreases rapidly away from a solid boundary and is virtually zero outside the Knudsen layer, as illustrated in Fig. 1. For diffuse scattering of the gas molecules, Cercignani [31, 32] has shown that the velocity profile in the Knudsen layer for Kramers' problem is given by:

$$u(y) = k\left[y + \zeta - l\, I\left(\frac{y}{l}\right)\right], \tag{1}$$

where k is the velocity gradient in the bulk flow, $\zeta = 1.1466\, l$ is the slip coefficient, y is the distance normal to the wall, and I is a function that represents the velocity defect in the Knudsen layer. The mean free path in the bulk flow, l, is defined as $(\mu/p)\sqrt{\pi k_B T/2m}$, where μ is the viscosity, p is the pressure, k_B is Boltzmann's constant, T is the absolute temperature, and m is the molecular mass. Tabulated values for the velocity defect have previously been reported [31, 33–35] and compared with experimental data [36].

More recently, Lockerby *et al.* [37, 38] developed several expressions to approximate the Knudsen layer, including an empirical expression, $I(y/l) \approx 7/20(1 + y/l)^{-2}$, and an alternative formulation for the velocity profile given by

$$u(y) = k\left[y + l\sqrt{\frac{2}{\pi}} + \frac{7}{10C}l\left(1 - e^{-Cy/l}\right)\right], \tag{2}$$

where C is a constant (see [38] for a more detailed description). For Kramers' problem, $C = 1$ leads to a velocity profile that is very close to that obtained from both the linearized Boltzmann equation and DSMC simulations.

To enable the Navier-Stokes equations to capture the velocity profile in the Knudsen layer, an *effective viscosity* has been proposed by Lockerby *et al.* [37]. However, to incorporate Knudsen layer effects in lattice Boltzmann models, it is necessary to redefine the wall function in terms of an *effective mean free path*, l_e. From kinetic theory, the viscosity is related to the mean free path via $\mu = \phi\bar{c}\rho l$, where $\bar{c}$ is the mean molecular speed and ϕ is taken to be a constant with a value of 0.499 [39]. For an isothermal, incompressible flow the mean free path is proportional to the viscosity and therefore the effective mean free path, l_e, can be obtained from

$$l_e = \frac{l}{1 + 0.7e^{-Cy/l}}. \tag{3}$$

Equation (3) represents a *wall function* that can provide a correction to the mean free path. Outside the Knudsen layer, the effective mean free path in Eq. (3) approaches the mean free path in the bulk flow, l. However, at the wall ($y = 0$), the effective mean free path is 1.7 times smaller than in the bulk flow. Although the wall function defined in Eq. (3) is based on Kramers' problem, the velocity defect within the Knudsen layer is a universal phenomenon found in all rarefied flows. In the present study, the wall function approach is incorporated into a D2Q9 LBE model and applied to a range of shear- and pressure-driven flows.

III. LATTICE BOLTZMANN FORMULATION

To demonstrate the present approach, we consider the lattice Bhatnagar-Gross-Krook (BGK) model with an external forcing term F_i as proposed by He *et al.* [40]:

$$\frac{\partial f_k}{\partial t} + e_{ki}\frac{\partial f_k}{\partial x_i} = -\frac{f_k - f_k^{eq}}{\lambda} + \frac{(e_{ki} - u_i)F_i}{c_s^2\rho}f_k^{eq}, \tag{4}$$

where f_k is the velocity distribution function, f_k^{eq} is the distribution function at equilibrium, e_{ki} is the lattice velocity, u_i is the macroscopic velocity, c_s is the sound speed of the lattice fluid, ρ is the density, and λ is the relaxation time. For a two dimensional, nine-velocity lattice model (D2Q9), the equilibrium distribution function can be expressed as:

$$\begin{aligned} f_k^{eq} &= \rho\omega_k \left[1 + \frac{e_{ki}u_i}{c_s^2} + \frac{(e_{ki}u_i)^2}{2c_s^4} - \frac{u_i u_i}{2c_s^2}\right] , \\ \omega_0 = \frac{4}{9} \quad ; \quad \omega_k &= \frac{1}{9} , \; k = 1,2,3,4 \quad ; \quad \omega_k = \frac{1}{36} , \; k = 5,6,7,8, \end{aligned} \tag{5}$$

where the lattice velocities, e_k, are given by

$$\begin{aligned} e_0 &= 0 , \\ e_k &= \left[\cos\left(\frac{(k-1)\pi}{2}\right), \sin\left(\frac{(k-1)\pi}{2}\right)\right] c , \qquad k = 1,2,3,4, \\ e_k &= \left[\cos\left(\frac{(k-5)\pi}{2} + \frac{\pi}{4}\right), \sin\left(\frac{(k-5)\pi}{2} + \frac{\pi}{4}\right)\right] \sqrt{2}\, c , \quad k = 5,6,7,8, \end{aligned} \tag{6}$$

where $c = \sqrt{3RT}$ (R is the gas constant). After discretizing Eq. (4), we obtain

$$f_k(\mathbf{x} + \mathbf{e}_k\delta t, t + \delta t) - f_k(\mathbf{x}, t) = -\frac{1}{\tau}[f_k(\mathbf{x}, t) - f_k^{eq}(\mathbf{x}, t)] + \delta t \frac{(e_{ki} - u_i)F_i}{c_s^2 \rho} f_k^{eq}(\mathbf{x}, t), \tag{7}$$

where $\tau = \lambda/\delta t$ is the nondimensional relaxation time and δt is the time step.

Zhang *et al.* [20] have shown that the Knudsen number in a D2Q9 lattice BGK model can be related to the relaxation time as follows:

$$Kn = \sqrt{\frac{8}{3\pi}} \frac{(\tau - 0.5)}{N_H} , \tag{8}$$

where $N_H = H/\delta x$ is the number of lattice sites, δx is the lattice length, and H is the height of the channel. Substituting the effective mean free path from Eq. (3) allows the nondimensional relaxation time to be written as

$$\tau = \sqrt{\frac{3\pi}{8}} \left(\frac{KnN_H}{1 + 0.7e^{-Cy/l}}\right) + 0.5 . \tag{9}$$

Recent work applying lattice Boltzmann methods to rarefied gas flows has focused on the development of slip boundary conditions and currently there are many approaches to capture slip effects at the wall. Examples include bounce-back, specular reflection, or a combination of the two [15, 16, 19, 23, 41], kinetic theory boundary conditions [17, 42, 43],

and a virtual wall collision scheme [24]. In the present investigation, a kinetic boundary condition [17, 42, 44] has been used with the assumption of fully diffuse molecular reflection:

$$|(\mathbf{e}_k - \mathbf{u}_w)\cdot\mathbf{n}|\, f_k = \sum_{(\mathbf{e}_{k'}-\mathbf{u}_w)\cdot\mathbf{n}<0} |(\mathbf{e}_{k'} - \mathbf{u}_w)\cdot\mathbf{n}|\, R_f(\mathbf{e}_{k'} \rightarrow \mathbf{e}_k) f_{k'}, \tag{10}$$

where k' and k are the incident and reflected directions of the particles, $\mathbf{u}_w$ and ρ_w are the velocity and density at the wall, $\mathbf{n}$ is the unit normal, and R_f is the the scattering kernel given by

$$R_f(\mathbf{e}_{k'} \rightarrow \mathbf{e}_k) = \frac{A_N}{\rho_w}[(\mathbf{e}_k - \mathbf{u}_w)\cdot\mathbf{n}] f_k^{eq}\,|_{\mathbf{u}=\mathbf{u}_w}\,. \tag{11}$$

The coefficient, A_N, in Eq. (11) is given by

$$A_N = \rho_w \frac{\sum_k |(\mathbf{e}_k - \mathbf{u}_w)\cdot\mathbf{n}|\, f_k}{|(\mathbf{e}_k - \mathbf{u}_w)\cdot\mathbf{n}|\, f_k^{eq}\,|_{\mathbf{u}=\mathbf{u}_w}\, \sum_k |(\mathbf{e}_{k'} - \mathbf{u}_w)\cdot\mathbf{n}|\, f_{k'}}. \tag{12}$$

IV. RAREFIED FLOW BETWEEN PARALLEL PLATES

The present wall function technique for the effective mean free path is based on Kramers' problem: namely, a gas bounded by a single planar wall and subjected to a uniform and constant shear stress. However, this technique can be applied to more complex geometries by assuming that the influence of overlapping Knudsen layers is additive. For example, if the distance between the parallel plates is H, then the effective mean free path in the overlapping Knudsen layers can be assumed to be

$$l_e = \frac{l}{1 + 0.7(e^{-Cy/l} + e^{-C(H-y)/l})}, \tag{13}$$

where y is the distance from one wall and $H - y$ is the distance from the other wall. In this section, we test whether this approach can provide accurate predictions over a range of Knudsen numbers up to $Kn \sim \mathcal{O}(1)$.

A. Planar Couette flow

The model was initially tested on a planar Couette problem consisting of a moving upper plate and a stationary lower plate. The kinetic boundary conditions given in Eqs. (10, 11, 12) were used to describe the molecular interactions with the solid walls, while periodic boundary conditions were implemented at the inlet and outlet. Figure 2 illustrates

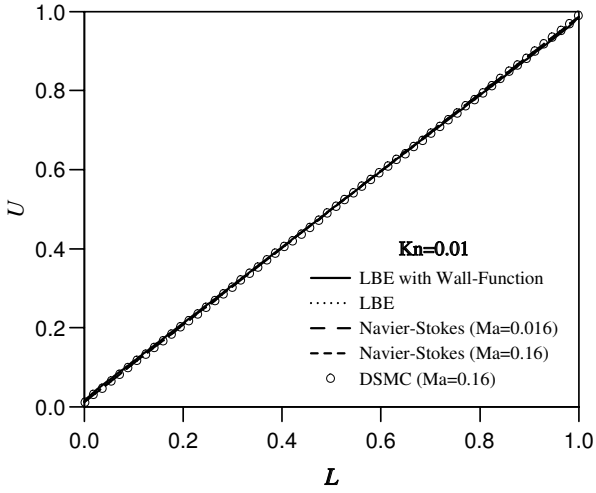

FIG. 2: Nondimensional velocity profiles for planar Couette flow at a Knudsen number of 0.01. Comparison of LBE solution with the wall-function approach (—), LBE solution without the wall-function approach ($\cdots$), Navier-Stokes slip-flow solution at $Ma = 0.016$ (— —), Navier-Stokes slip-flow solution at $Ma = 0.16$ (– – –), and DSMC data at $Ma = 0.16$ ($\circ$).

the predicted velocity profiles for a planar Couette flow at a Knudsen number of 0.01. For this problem, the nondimensional velocity, U, is defined as $U = u/U_{plate}$ while the nondimensional distance is defined as $L = y/H$. To validate the LBE wall function technique, the results have been compared to DSMC data and a first-order slip-flow solution of the Navier-Stokes equations. The DSMC method is often used as an independent numerical test and it is generally accepted that the method provides an accurate description of the flow characteristics within the Knudsen layer. In the present study, the DSMC simulations were performed using the computational scheme developed by Bird [6] and the gas-surface interactions were modeled using a Maxwellian diffuse reflection boundary condition.

The current LBE model is only valid in the isothermal/incompressible limit, and therefore the simulations are restricted to low speed flow. Unfortunately, the DSMC approach is computationally expensive at low Mach numbers, due to the requirement to perform large amounts of sampling to reduce the statistical scatter. It is therefore necessary to choose a Mach number that minimizes compressibility effects in the LBE model while reducing the computational burden of the DSMC simulations. For a Knudsen number of $Kn = 0.01$, two Mach numbers have been considered, $Ma = 0.016$ and 0.16, respectively. Figure 2 shows that the Navier-Stokes slip-flow solutions at these two flow speeds are almost indistinguishable,

demonstrating that compressibility is negligible below a Mach number of 0.16. Moreover, the LBE solution is in excellent agreement with both the DSMC data and the Navier-Stokes solutions, confirming that the proposed wall function approach has minimal effect at low Knudsen numbers.

Figure 3 illustrates the growing influence of the Knudsen layer as Kn is increased beyond the slip-flow regime. For these results, the DSMC simulations were performed at a Mach number of 0.16 to reduce the computational cost. As expected, the LBE predictions without the wall function are almost identical to the Navier-Stokes slip-flow solution. Both the Navier-Stokes and lattice Boltzmann methods overpredict the slip at the wall, with the velocity increasing linearly from the stationary lower plate to the moving upper plate. As the Knudsen number is increased, the predicted velocity profiles are shown to depart further from the DSMC data. However, when the wall function is incorporated into the LBE model, the accuracy of the predictions is significantly improved and the proposed model is clearly able to capture the nonlinear flow behavior in the Knudsen layer.

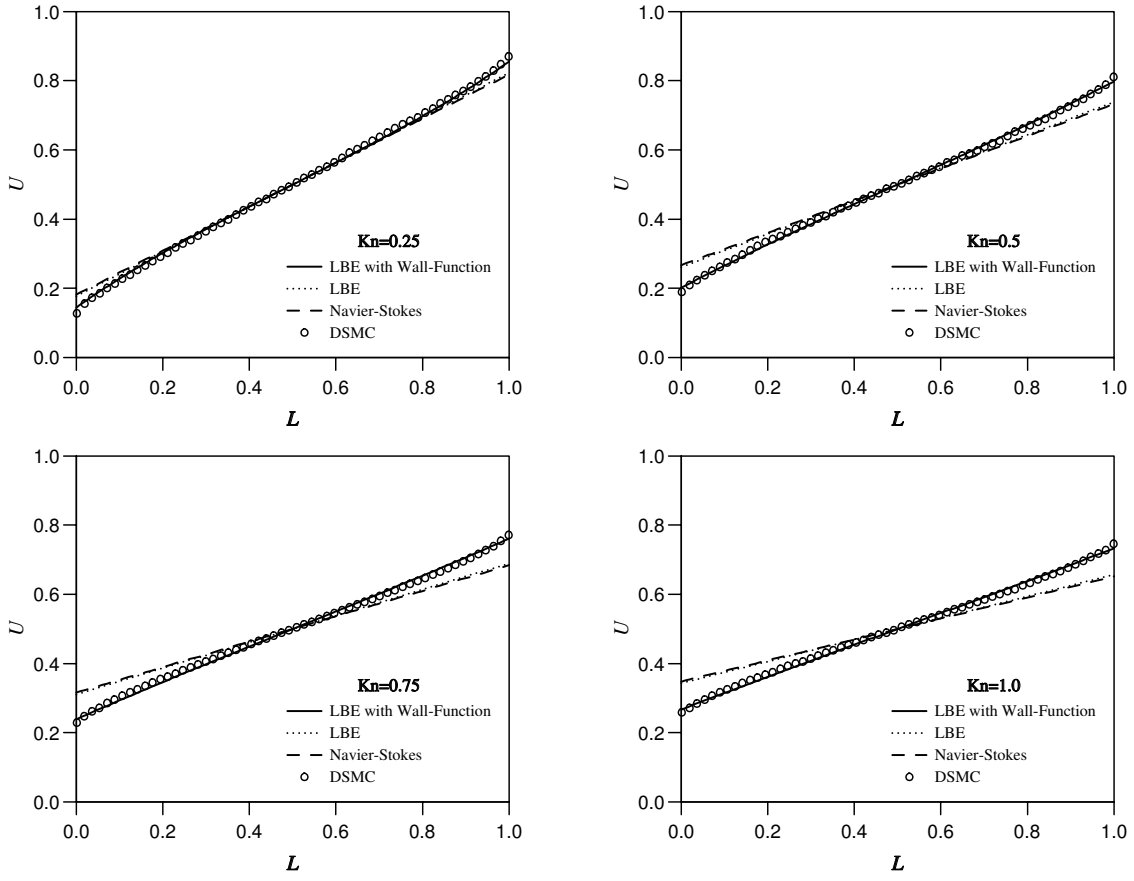

FIG. 3: Nondimensional velocity profiles for planar Couette flow at Knudsen numbers of 0.25, 0.5, 0.75, and 1.0. Comparison of LBE solution with the wall-function approach (—), LBE solution without the wall-function approach ($\cdots$), Navier-Stokes slip-flow solution (— —), and DSMC data ($\circ$).

B. Pressure-driven flow

The second test case considers fully-developed pressure driven (Poiseuille) flow between parallel plates. To validate the wall-function approach, the lattice Boltzmann results are compared with data obtained by Ohwada *et al.* [45] using a direct solution of the linearized Boltzmann equation. Ohwada *et al.* assumed the applied pressure gradient in the streamwise direction was small, so that the flow could be considered incompressible. In the lattice Boltzmann simulations, a uniform pressure gradient was applied in the streamwise direction while periodic velocity boundary conditions were used at the inlet and outlet.

Figure 4 illustrates the predicted velocity profiles across the channel for various Knudsen

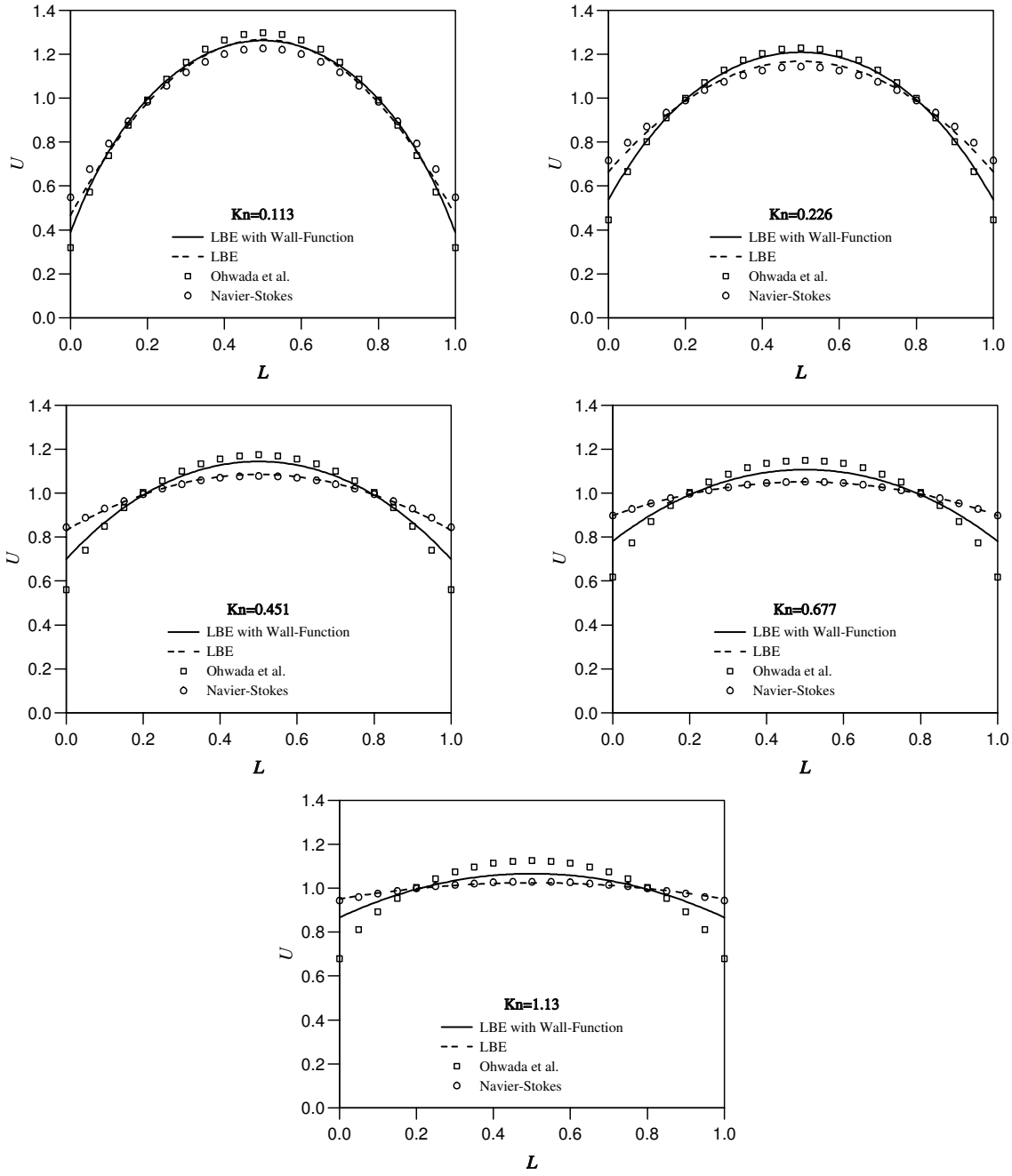

FIG. 4: Nondimensional velocity profiles for planar Poiseuille flow at Knudsen numbers of 0.113, 0.226, 0.451, 0.677, and 1.13. Comparison of LBE solution with the wall-function approach (—), LBE solution without the wall-function approach (– – –), Ohwada *et al.*'s solution [45] of the linearized Boltzmann equation (square), and the Navier-Stokes slip-flow solution (○).

numbers between 0.113 and 1.13. For this problem, the nondimensional velocity, U, is defined as $U = u/\overline{U}$, where $\overline{U}$ is the mean velocity in the channel. The lattice Boltzmann simulations without the wall-function are almost identical to the Navier-Stokes slip-flow solution and the discrepancy between these predictions and Ohwada *et al.*'s linearized Boltzmann solution clearly increases with Knudsen number. However, adopting the wall-function approach leads to a significant improvement in the LBE predictions up to $Kn \sim 0.5$.

In pressure driven flows, the pressure gradient causes a heat flux in the streamwise direction despite the uniform temperature of the gas [45]. This higher-order rarefaction effect cannot be captured using the current wall function approach and causes the LBE model to increasingly depart from Ohwada *et al.*'s predictions as the Knudsen number is increased. For $Kn > 0.5$, the wall function does provide an improved description of the velocity profile but, in its current form, is unable to capture the full nonlinearity associated with the Knudsen layer.

V. CONCLUSIONS

A wall-function approach for the *effective mean free path* has been proposed that enables lattice Boltzmann methods to be extended beyond the slip-flow regime. For planar Couette flow, the results indicate that the method significantly improves the accuracy of lattice Boltzmann models, especially in the near-wall region, and it has been shown that the method provides a reasonable description of the nonlinear flow characteristics in the Knudsen layer up to $Kn \sim \mathcal{O}(1)$. In the case of pressure-driven flow, the wall function approach provides a significant improvement for Knudsen numbers up to 0.5 but the method is currently unable to capture the full effect of the Knudsen layer for $Kn > 0.5$. This approach has been implemented without sacrificing the computational efficiency of the lattice Boltzmann method. However, the present wall-function is based on phenomenological observations for Kramers' problem and this needs to be improved in the future. The next stage of the investigation is to extend the wall-function technique to incorporate additional effects, such as surface curvature and temperature variations, and address deficiencies in the prediction of pressure-driven flow at higher Knudsen numbers.

VI. ACKNOWLEDGMENTS

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