

A Critical Assessment of the Maxwell Slip Boundary Condition for Rarified Wall Bounded Flows

Abhimanyu Gavasane, Swapnil S. Sachdev, Bharat K. Mittal, Upendra V. Bhandarkar
and Amit Agrawal

Department of Mechanical Engineering, Indian Institute of Technology Bombay, India

ABSTRACT

The Maxwell slip boundary condition is widely used to compute the slip velocity at the wall under rarefied flow condition. In this paper, we apply the Direct Simulation Monte Carlo (DSMC) method on a Couette flow problem in order to evaluate this boundary condition. The computations are performed at different values of tangential momentum accommodation coefficient (between 0.1 and 1) and Knudsen numbers (Kn between 0.001 and 3), at 500 K for Argon, with the aim of comparing the ensuing slip length to that predicted by Maxwell's formula. It is found that the boundary condition is accurate up to a $Kn = 0.1$ but not at higher Knudsen numbers. Although it has been known that the slip boundary condition is valid only for small Knudsen numbers, the critical Knudsen number from where the deviation begins is not well documented. The present results indicate that such deviations occur at $Kn = 0.1$ in flows that are bounded by opposing walls. At higher Knudsen numbers, the Knudsen layers overlap and the collisions of molecules with walls dominate to change the boundary conditions significantly.

1. INTRODUCTION

It is well known that the no-slip boundary condition is not satisfied under rarefied flow condition – rather the gas slips at the solid walls. Maxwell proposed the following approach to calculate the slip velocity on a gas-solid interface under rarefied condition [1, 2]. On the assumption that a fraction σ of the molecules are reflected diffusively at the walls (i.e. their average tangential velocity corresponds to that of the wall, U_w), and the remaining $(1 - \sigma)$ of the molecules are reflected specularly (i.e. with the normal component of the velocity changing sign and the tangential component remaining the same), Maxwell obtained the following expression (in the absence of temperature gradients along the wall):

$$U_g - U_w = \frac{2 - \sigma}{\sigma} Kn \left(\frac{\partial U}{\partial n} \right)_w. \quad (1)$$

In the above equation, U stands for streamwise velocity, subscripts g and w refer to gas and wall respectively, σ is the tangential momentum accommodation coefficient (TMAC), and n is normal to the surface. A temperature gradient along the wall leads to a second term on the right hand side involving the temperature gradient. The TMAC can be related to the tangential momentum of the incident (τ_i) and reflected (τ_r) molecules using the following relation [2]:

$$\sigma = \frac{\tau_i - \tau_r}{\tau_i}. \quad (2)$$

Millikan [3] postulated that the slipping behaviour is due to “molecular inhomogeneities”, while Cao et al. [4] argued that the mechanism for momentum transfer between the wall and gas is due to trapping of gas molecules in the potential wells of the surfaces. The gas molecules may undergo several collisions and may escape after a residence time, during which momentum exchange between the fluid

*Corresponding author. Email: aagrawal.iitb@gmail.com

and wall is accomplished [4]. Therefore, σ can assume any value between 0 and 1, depending up on the nature of the gas and the surface, pressure of the gas, surface roughness, surface cleanliness, and temperature [5]. The extreme values of $\sigma = 1$ and 0 denote fully diffused and specular surface, respectively. The value of σ to be used for a pair of gas-solid interface and a given flow condition is not obvious; its value needs to be determined through experiments or calculated by some other means. From a detailed literature survey of experimentally available values, Agrawal and Prabhu [5] have proposed a value of 0.93 for all monatomic gases and commonly available surfaces.

It is worthwhile to point out that Maxwell proposed this model (Eq. 1) based on a referee's suggestion, and believed that the model can be further improved [1]. The $\partial U/\partial n$ term in Eq. 1 may be replaced by τ/μ (where τ is the shear stress at the wall and μ is the gas viscosity at the wall). This leads to an additional term ($\partial U_n/\partial x$, where U_n is the wall-normal velocity and x is the streamwise coordinate) in Eq. 1 [6, 7]. This additional term becomes particularly relevant with curved and rotating surfaces [7, 8, 9]. Similarly additional terms can also be introduced by considering second order effects. These can be obtained either by using a Taylor series expansion or just using the second derivative of the velocity with a pre-factor. In fact, the slip boundary condition has been established theoretically in a more general and rigorous form. More precisely, the slip boundary conditions are derived by a systematic asymptotic analysis of the Boltzmann equation for small Knudsen numbers based upon the Hilbert expansion and the analysis of the Knudsen layer. The results of this analysis are summarized in [6]. Alternate slip models also exist in the literature as reviewed in Refs. [10, 11, 12, 13].

In spite of the various issues noted above, the Maxwell's slip model (Eq. 1) continues to be extensively applied in a very large number of studies (see Refs. [7, 9, 13, 14, 15, 16, 17], among others). The purpose of this investigation is to evaluate this model using the direct simulation Monte Carlo (DSMC) technique. Specifically, the amount of slip predicted by DSMC is compared with that predicted by the model for different values of σ (between 0.1 and 1) and over a sufficiently large range of Knudsen number (between 0.001 and 3). The flow considered here is Couette flow, whereby fluid between two long parallel plates is dragged due to uniform motion of one plate while the other plate is held stationary. The present study is different from those in the literature in that the earlier studies presumed the behavior of the gas at the wall (such as diffuse reflection) and merely used a computational tool (molecular dynamics or DSMC) to compute the slip velocity at the wall (see Refs. [11, 18, 19, 20, 21], among others); this point is discussed further in Section 4. However, here, we allow the gas particles to undergo diffuse and specular reflections, in varying percentages, with the aim of evaluating Eq. 1.

2. NUMERICAL DETAILS

An in-house code was developed and employed to verify the Maxwell's model. The code uses the standard Direct Simulation Monte Carlo technique developed by Bird [22]. The flow domain is split into cells in the direction normal to the flow (with an infinite length along the flow direction). The technique assumes decoupling of molecular motion and molecular collisions. A certain number of simulated molecules N are initially divided equally among all the cells and each simulated molecule represents a number of real molecules. Initially, the molecules are given a velocity randomly from a Maxwellian distribution at the simulation temperature. The molecules travel for a time dt after which they undergo collisions. The collisions are considered by choosing random pairs from each cell using the null time counter method developed by Bird. To reduce computation time, each cell is further divided into sub-cells. The actual collision process is executed using a variable hard sphere model. Details are again available in the text by Bird [22]. The process of molecular motion followed by collisions is repeated till steady state is attained by macroscopic flow properties. A typical simulation involves 20,000 simulated molecules spread over 500 cells each of which is divided into four sub-cells. Depending on the conditions, these are varied such that the cell width is less than 1/4 of the mean free path of the molecules. The time dt is chosen so that it is much smaller than the mean collision time.

A random number is employed to determine whether a molecule will have specular or diffuse reflection from the wall. The random number is checked against the value of σ which is an input parameter for the code. The code is validated by comparing the results with those from Pan et al. [18];

for all noble gases the results were found to compare within $\pm 6\%$ [23]. More detailed calculations as described in the next section were performed only with Argon.

3. RESULTS

The calculations were carried out for Knudsen numbers of 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1 and 3, thus spanning from the continuum regime ($Kn < 0.001$) to the border of free molecular flow regime ($Kn > 10$). For each value of Kn , the TMAC (σ) was varied from 0.1 to 1 in steps of 0.1 (80 computations in total). Note that theoretically, $\sigma = 0$ implies total specular reflection at the walls and corresponds to infinite amount of slip (see Eq. 1).

The slip length is calculated using the data close to any wall. Ensemble averaging is carried out for the last 1000 time steps; detailed tests indicated that this is adequate for convergence. Table 1 lists the values of slip coefficients (for a Kn of 0.01 and σ varying from 0.1 to 1) calculated using three methods: our numerical calculations, from Maxwell's original theoretical relation (third column) and from the modified relation using kinetic theory as described by Barber and Emerson [10] (fifth column). The Maxwell's theoretical slip length (S_v) is related to TMAC through the following relation:

$$S_v = \frac{2-\sigma}{\sigma} KnL. \quad (3)$$

where L is the characteristic length for the flow (distance between the two plates). Further, the slip coefficient (S_{th}) can be defined as:

$$S_{th} = Kn \left(\frac{2-\sigma}{\sigma} \right). \quad (4)$$

The modified relation assumes a pre-factor of 1.1466 [10]. The fourth and the last columns in the table correspond to the ratio of the slip coefficients (Maxwell to numerical and modified Maxwell to numerical respectively). As can be noted, the values from the numerical simulations are consistently around 10% higher than that predicted by Maxwell's formula (this is consistent with [11]). However, the modified Maxwell relation using a prefactor of 1.1466 is within $\pm 5\%$ of the DSMC results (except for an anomalous point at a TMAC of 0.8 where it is off by around 10%). It can therefore be assumed that the modified Maxwell's relation for the slip is valid at $Kn = 0.01$.

The value of the slip ratios (modified Maxwell's relation to DSMC simulations) for all the Knudsen numbers is plotted in Fig. 1. As apparent from the figure, the ratio is close to unity till a Knudsen number of 0.1 after which it deviates significantly. At higher Knudsen numbers, the values obtained from the numerical simulations are lesser than those obtained theoretically. Our attempts at evaluating a second-order slip boundary condition did not yield much difference in the results (not shown). Arguably, this is because the second order terms can bring a relatively small change in the value of slip velocity and cannot account for the rather large ($> 100\%$) deviation observed at $Kn > 0.3$ (see Fig. 1).

We have also carried out simulations at a different temperature (100 K). The main difference expected at lower temperatures is the way the gas molecules interact with the wall. At lower temperatures, molecules are expected to spend a longer time in the potential well of the wall, where they equilibrate with the wall and thus are reflected diffusively with a higher probability. Thus fundamentally, the main change at lower temperature is that the value of TMAC may change [4, 5]. No difference in the results is noted [23] because the value of σ is a parameter that is input to the simulations, and as long as the method for handling gas-gas and wall-gas collisions remain the same the results should remain invariant with temperature. In our present simulations, we have not included means of calculating the dependence of σ on temperature, and therefore these results are to be expected. Similarly, calculations performed using different monatomic gases also showed similar results [23], since again σ is just a parameter and we are not studying how σ varies with the gas-wall combination. A molecular dynamics simulation (as has been carried out in Refs. [4, 21] for example) which involves the gas wall potential is however capable of handling both the temperature effect as well as the gas-wall combination.

Table 1. Variation with TMAC of the numerical (S_{DSMC}) and theoretical (S_{th} and $S_{th,mod}$) slip coefficients, for argon at $Kn = 0.01$. The theoretical value of slip coefficient has been calculated from Eq. 4 (as $S_{th} = \frac{2-\sigma}{\sigma} Kn$). The modified theoretical value is calculated as per

Ref. 10 with a pre-factor of 1.1466 (i.e., $S_{th,mod} = 1.1466S_{th}$). The temperature is fixed at 500 K for these simulations.

σ	S_{DSMC}	S_{th} (Present work)	Ratio (= S_{th}/S_{DSMC})	$S_{th,mod}$ (Ref. 10)	Ratio (= $S_{th,mod}/S_{DSMC}$)
0.1	0.20554	0.19	0.9244	0.21785	1.0599
0.2	0.09855	0.09	0.9132	0.10319	1.0471
0.3	0.06159	0.05667	0.9201	0.06497	1.0550
0.4	0.04381	0.04	0.9130	0.04586	1.0468
0.5	0.03386	0.03	0.8860	0.03440	1.0159
0.6	0.02623	0.02333	0.8894	0.02675	1.0198
0.7	0.02075	0.01857	0.8952	0.02129	1.0264
0.8	0.01903	0.015	0.7882	0.01720	0.9037
0.9	0.01407	0.01222	0.8687	0.01401	0.9961
1.0	0.01177	0.01	0.8497	0.01147	0.9743

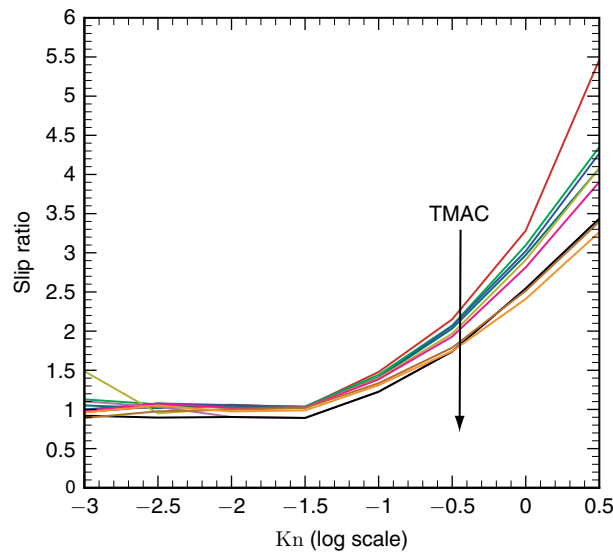


Figure 1. Plot of slip ratio (theoretical to numerical) versus Knudsen number (\log_{10} scale) for TMAC ranging from 0.1–1.0 in steps of 0.1. The theoretical values are calculated using the *modified* Maxwell's relation.

4. DISCUSSION

The deviation at larger Knudsen numbers may be explained as follows. In Maxwell's derivation [1], it is assumed that the molecules hitting a wall have a distribution corresponding to some bulk distribution where the molecules are at equilibrium due to collisions amongst themselves. However, as seen in the present case, as the Knudsen number increases, a molecule arriving from a distance larger than a mean free path is actually arriving more or less after colliding with the other wall (theoretically at a Knudsen number of one, the mean free path is equal to the distance between the two walls). Hence the molecule carries information from the other wall rather than from the bulk that corresponds to an equilibrium within the molecules themselves. This effect is strong and can be seen by viewing the velocity profiles between the two plates for Knudsen numbers of 0.001 and 3 (see Fig. 2, with the vertical axis denoted

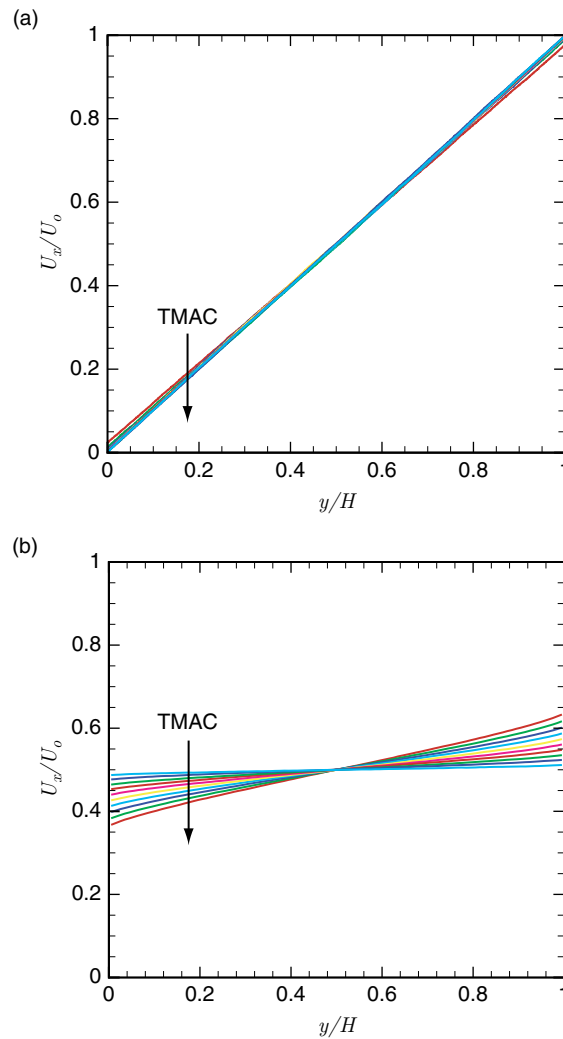


Figure 2. Plot of velocity profile for TMAC ranging from 0.1–1.0 for (a) $Kn = 0.001$ and (b) $Kn = 3$. The value of U_0 employed in these simulations is 0.7 times the speed of sound. The results are independent of the value of U_0 in the range of 0.05 to 0.7 times the speed of sound.

as U_x/U_0 where x is the flow direction and U_0 is the velocity of the upper moving plate). At a Knudsen number of 0.001, the normalized velocity profile varies approximately linearly from zero to unity at the upper plate. Small values of slip are observed at lower values of TMAC, which is to be expected. At $Kn = 3$, we see that the velocity profile is considerably flattened with a large amount of slip. Since the molecules collide with the walls more frequently than with other molecules, the information with the molecules is the average of the information at the two walls; hence the ratio (U_x/U_0) is closer to 0.5 everywhere, rather than only at the mid-plane.

Some experimental data [12, 14, 15, 16, 24] are also available for rarefied gas flows. The experimental data is typically analyzed by comparing against the Navier-Stokes solution with slip boundary condition. For example, in an experimental study undertaken by Sreekanth [12], the pressure at nine locations were measured in a long tube. The pressure in the tube was related to the slip coefficients using theory (based on continuum integral momentum equation) also derived in that paper. Sreekanth noted that comparison between his experimental data and theory improves by changing the value of slip coefficients (a second-order slip model was employed in this study) from 1 and 0 for $Kn \leq 0.03$, to 1.1466 and 0 for $0.03 < Kn < 0.13$, and further to 1.1466 and 0.14 for $Kn \geq 0.13$. One

can therefore employ a higher-order slip boundary condition in conjunction with experimental or appropriately tuned slip coefficients in order to analyze the flow at higher Knudsen number [9, 13, 17]. In spite of modifications in the value of slip coefficient, a disagreement in the results from Navier-Stokes and Boltzmann equation is still obtained for Knudsen number greater than unity [9, 13]. The mismatch can either be due to the breakdown of the continuum assumption fundamental in the derivation of the Navier-Stokes equations or failure of the Maxwell's model, or both. Typically the mismatch is attributed to the inability of Navier-Stokes in making predictions at high Knudsen numbers. The present results indicate that the Maxwell boundary conditions themselves are not applicable beyond a critical Knudsen number of 0.1 and the fault does not entirely lie on the non-applicability of the continuum hypothesis.

Alternate to using the Navier-Stokes equations (which are of order Knudsen number and higher order terms are neglected when deriving these equations using the Chapman-Enskog expansion), the Burnett equations which are of order Knudsen square have also been employed to a limited extent. These equations are prone to instabilities and therefore difficult to solve. Nonetheless, some successful attempts at solving them with Couette flow have also been reported in the literature [25, 26, 27]. The linearized Boltzmann equation has also been solved for rarefied flows [6, 28, 29, 30]. Another approach to attack the problem is to differentiate the flow into a bulk flow regime and a Knudsen layer close to the wall and apply the Navier-Stokes relations in the bulk [6, 31, 32]. The Knudsen layer can be solved analytically [6] or modelled using a wall function [33]. Presently these approaches do not consider the overlap of the Knudsen layers when two walls are present. Such an overlap starts occurring as the Knudsen number increases beyond 0.1 which is where the deviation from the theoretical value is stark. The overlap of the Knudsen layers will need a further analysis. It must be noted that the Maxwell's boundary condition is not required in the above approaches; however these studies do not explicitly compare their slip velocities with that predicted using Maxwell's condition.

The present work has attempted to directly test the Maxwell's slip boundary conditions (along with some of the modifications suggested in the literature) and suggest inapplicability of these equations beyond a Knudsen number of 0.1. It is also clear from Fig. 1 that results are not offset by a constant factor and therefore a simple correction by a factor is not applicable. Probably a rigorous mathematical treatment of overlapping Knudsen layers may address this issue.

5. CONCLUDING REMARKS

This paper focuses on evaluating the Maxwell's slip model, which is the most popular model for computing the slip velocity at the gas-wall interface, under high Knudsen number flow situations. The existing studies in the literature do not verify the validity of Maxwell's model. They merely assume the validity of Maxwell's model and deduce the value of σ or some other parameter relevant to that work. An independent verification of the model was therefore required and this need has been fulfilled to an extent through this study. A detailed test of the model for a sufficiently large range of Knudsen number and TMAC values is undertaken here, using the direct simulation Monte Carlo technique. This method has proved itself extremely useful because a direct experimental verification of the model appears rather difficult.

The results of the present study indicate that Maxwell's equation is valid for low Knudsen numbers ($K_n < 0.1$). At higher values of K_n , the effect of the second wall becomes significant and molecules collide more with either walls than amongst themselves and hence carry velocity information that is an average of the information available at the two walls. The present results elucidate the effect of two proximate walls on gas-wall interaction at relatively high Knudsen numbers which results in overlapping of Knudsen layers. Probably in cases where only one wall is present, such as in the boundary layer of re-entry vehicles at high altitudes, Maxwell's equations can still be applied. For most applications of current interest which revolve around microchannels, fluid is surrounded by walls on all its lateral sides. In these latter and related situations caution is advised in applying Maxwell's equation beyond a Knudsen number of 0.1. Our results are expected to be of interest to practitioners of rarefied gas dynamics as well as those in the field of vacuum science and gas flow in micro/nano-channels.

REFERENCES

- [1] Maxwell, J.C., On the stresses in rarified gases arising from inequalities of temperature, *Philosophical Transactions of the Royal Society*, 1879, 170, 231–256.
- [2] Kennard, E.H., *Kinetic theory of gases with an introduction to statistical mechanics*, Allied Pacific, Bombay, 1962.
- [3] Millikan, R.A., coefficients of slip in gases and the law of reflection of molecules from the surfaces of solids and liquids, *Physical Review*, 1923, 21, 217–238.
- [4] Cao, B.Y., Chen, M., and Guo, Z.Y., Temperature dependence of the tangential momentum accommodation coefficient for gases, *Applied Physics Letters*, 2005, 86, 091905.
- [5] Agrawal, A., and Prabhu, S.V., A survey on measurement of tangential momentum accommodation coefficient, *Journal of Vacuum Science and Technology A*, 2008, 26, 634–645.
- [6] Sone, Y., *Molecular gas dynamics : theory, techniques and applications*, Birkhauser, Boston, 2007.
- [7] Lockerby, D.A., Reese, J.M., Emerson, D.R., and Barber, R.W., Velocity boundary condition at solid walls in rarefied gas calculations, *Physical Review E*, 2004, 70, 017303.
- [8] Einzel, D., Panzer, P., and Liu, M., Boundary condition for fluid flow: Curved or rough surfaces, *Physical Review Letters*, 1990, 64, 2269–2272.
- [9] Agrawal, A., and Prabhu, S.V., Deduction of slip coefficient in slip and transition regimes from existing cylindrical Couette flow data, *Experimental Thermal and Fluid Sciences*, 2008, 32, 991–996.
- [10] Barber, R.W. and Emerson, D.R., Challenges in Modeling Gas-Phase Flow in Microchannels: From Slip to Transition, *Heat Transfer Engineering*, 2004, 27, 3–12.
- [11] Karniadakis, G.E., Beskok, A., and Aluru, N., *Microflows and Nanoflows - Fundamentals and simulations*, Springer-Verlag, New York, 2005.
- [12] Sreekanth, A.K., Slip flow through long circular tubes, in Ed: L. Trilling and H.Y. Wachman, *Proceedings of the sixth international symposium on Rarefied Gas Dynamics*. 667–676 (1969), Academic press.
- [13] Dongari, N., Agrawal, A., and Agrawal, A., Analytical solution of gaseous slip flow in long microchannels, *International Journal of Heat and Mass Transfer*, 2007, 50, 3411–3421.
- [14] Arkilic, E.B., Breuer, K.S., and Schmidt, M.A., Mass flow and tangential momentum accommodation in silicon micromachined channels, *Journal of Fluid Mechanics*, 2001, 437, 29–43.
- [15] Maurer, J., Tabeling, P., Joseph, P., and Willaime, H., Second-order slip laws in microchannels for helium and nitrogen, *Physics of Fluids*, 2003, 15, 2613–2621.
- [16] Ewart, T., Perrier, P., Graur, I.A., and Meolans, J.G., Mass flow rate measurements in a microchannel, from hydrodynamic to near free molecular regimes, *Journal of Fluid Mechanics*, 2007, 584, 337–356.
- [17] Dongari, N., Sambasivam, R., and Durst, F., Extended Navier-Stokes Equations and Treatments of Micro-Channel Gas Flows, *Journal of Fluid Science and Technology*, 2009, 4, 454–467.
- [18] Pan, L.S., Liu, G.R. and Lam, K.Y., Determination of slip coefficient for rarefied gas flows using direct simulation Monte Carlo, *Journal of Micromechanics and Microengineering*, 1999, 9 89.
- [19] Xue, H., Fan, Q., and Shu, C., Prediction of micro-channel flows using direct simulation Monte Carlo, *Probabilistic Engineering Mechanics*, 2000, 15, 213–219.
- [20] Montanero, J.M., Santos, A., and Garzo, V., Monte Carlo simulation of nonlinear Couette flow in a dilute gas, *Physics of Fluids*, 2000, 12, 3060–3073.
- [21] Bhattacharya, D.K. and Lie, G.C., Molecular-dynamics simulations of nonequilibrium heat and momentum transport in very dilute gases, *Physical Review Letters*, 1989, 62, 897–900.
- [22] Bird G.A., *Molecular gas dynamics and the direct simulation of gas molecules*, Oxford University Press, Oxford, 1994.

- [23] Sachdev, S.S., *Study of rarefied gas flows using direct simulation Monte Carlo*, M.Tech. thesis, Department of Mechanical Engineering, Indian Institute of Technology Bombay (2008).
- [24] Verma, B., Demsis, A., Agrawal, A., and Prabhu, S.V., Semiempirical correlation for the friction factor of gas flowing smooth microtubes, *Journal of Vacuum Science and Technology A*, 2009, 27, 584–590.
- [25] Xue, H., Ji, H.M., and Shu, C., Analysis of micro-Couette flow using the Burnett equations, *International Journal of Heat and Mass Transfer*, 2001, 44, 4139–4146.
- [26] Lockerby, D.A. and Reese, J.M., High-resolution Burnett simulations of micro Couette flow and heat transfer, *Journal of Computational Physics*, 2003, 188, 333–347.
- [27] Bao, F.B., Lin, J.Z., and Shi, X., Burnett simulation of flow and heat transfer in micro Couette flow using second-order slip coefficients, *Heat and Mass Transfer*, 2007, 43, 559–566.
- [28] Cercignani, C., and Daneri, A., Flow of a rarefied gas between two parallel plates, *Journal of Applied Physics*, 1963, 34, 3509–3513.
- [29] Cercignani, C., Lampis, M., and Lorenzani, S., Variational approach to gas flows in microchannels, *Physics of Fluids*, 2004, 16 3426–3437.
- [30] Sharipov, F., Application of the Cercignani-Lampis scattering kernel to calculations of rarefied gas flows. I. Plane flow between two parallel plates, *European Journal of Mechanics B*, 2002, 21 113–123.
- [31] Hadjiconstantinou, N.G., Comment on Cercignani's second order slip coefficient, *Physics of Fluids*, 2003, 15, 2352–2354.
- [32] Ohwada T., Sone Y. and Aoki K., Numerical analysis of the shear and thermal creep flows of a rarefied gas over a plane wall on the basis of the linearized Boltzmann equation for hard sphere molecules, *Physics of Fluids A*, 1989, 1, 1588–1599.
- [33] O'Hare L., Lockerby D. A., Reese J. M. and Emerson D. R., Near-wall effects in rarefied gas micro-flows: some modern hydrodynamic approaches, *International Journal of Heat and Fluid Flow*, 2007, 28, 37–43.