Slip length in a dilute gas

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We study the phenomenon of slip length using molecular dynamics and direct simulation Monte Carlo simulations of a dilute gas. Our work extends the range of Knudsen numbers that have been previously studied. In a recent paper, Bhattacharya and Lie [Phys. Rev. **43**, 761 (1991)] suggest a logarithmic dependence of slip length on Knudsen number. By a simple redefinition of the mean free path, we obtain good agreement between simulation results and Maxwell theory for slip length. The anomalies seen by Bhattacharya and Lie appear to be due to their definition of the mean free path.

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The velocity profile of a fluid very close to a wall (within a few mean free paths) exhibits a phenomenon known as slip. The velocity of the fluid $v(x)$ near the wall does not equal the wall's velocity even if the wall is perfectly thermalizing. A similar phenomenon, called jump, also occurs for temperature. The existence of velocity slip was first predicted by Maxwell [1]. Its effect is important in microscopic flows (e.g., flow between the write head and the platter on a hard disk) and in rarefied gas flows (e.g., very-high-altitude flight). In this short paper we address the question: Is slip a strictly local effect or does it depend on the entire flow field? Physical intuition suggest the former but recent computer experiments indicate the latter [2,3].

We define the slip length l_s, as the distance inside the wall at which the (extrapolated) fluid velocity would equal the wall's velocity [4]. The slip length may be written as

$$l_s \equiv \frac{v(x=0)}{(dv/dx)_{x=0}} = \frac{v_0}{\gamma_0} , \tag{1}$$

with the wall located at $x=0$. The dimensionless slip length l_s^* is defined as

$$l_s^* \equiv \frac{l_s}{L} , \tag{2}$$

where L is the characteristic length in the problem.

In this work we investigate how l_s^* varies with Knudsen number for planar Couette and Poiseuille flow. The Knudsen number is a dimensionless parameter defined as

$$\mathrm{Kn} = \frac{\lambda}{L} , \tag{3}$$

where λ is the mean free path. Maxwell theory predicts that the slip length is related to the mean free path as

$$l_s^* = \alpha \, \mathrm{Kn} , \tag{4}$$

where $\alpha \cong 1.15$ is the slip coefficient [5].

From basic kinetic theory we know that the mean free path λ_h, in a hard-sphere gas is

$$\lambda_h = \frac{m}{\sqrt{2}\pi d^2 \rho} , \tag{5}$$

where ρ is the fluid density, and m and d are the mass and diameter of the particles, respectively. Chapman-Enskog theory gives us the following expression for the viscosity η of a hard-sphere gas:

$$\eta = \tfrac{5}{16}\rho\lambda \left[\frac{2\pi k_B T}{m} \right]^{1/2} , \tag{6}$$

where T is the temperature and k_B is Boltzmann's constant.

For particles with extended potentials, the definition of the mean free path is problematic. Cercignani suggests the following operational definition for the mean free path [6]:

$$\lambda_v = \frac{\eta}{\rho} \left[\frac{\pi m}{2 k_B T} \right]^{1/2} . \tag{7}$$

Notice that λ_v is defined in terms of the viscosity. We define the hard-sphere and viscous Knudsen numbers as $\mathrm{Kn}_h = \lambda_h / L$ and $\mathrm{Kn}_v = \lambda_v / L$, respectively. For a hard-sphere gas at equilibrium, the two definitions of mean free path are equivalent [7]. Far from equilibrium they differ, since λ_v includes boundary effects.

The two definitions of the mean free path λ_h and λ_v are functions of density; the latter also depends on temperature. We computed the mean free path using the fluid density and temperature as measured near the wall. Using the average density and temperature instead had little effect on the results from our runs.

We measured slip length in two flow geometries. In planar Couette flow a fluid is confined between walls

moving in opposite directions with velocity v_w; the walls are located at $x=\pm L/2$. By conventional hydrodynamics [8], the steady-state velocity profile is

$$v(x)=\frac{2v_0}{L}x \ . \tag{8}$$

In planar Poiseuille flow, a fluid between stationary walls is acted on by an external force in a direction parallel to the walls; the velocity profile is

$$v(x)=\frac{\rho g}{2\eta}x^2+\left[v_0-\frac{\rho g L^2}{8\eta}\right] . \tag{9}$$

Note that by measuring the curvature of the profile we may obtain the viscosity of the fluid [9].

Since the phenomenon of slip occurs on a scale of only a few mean free paths, it is difficult to measure experimentally. In this respect, computer simulations are a useful tool for this problem. The two commonly used algorithms are molecular dynamics [10] (MD) and direct-simulation Monte Carlo [11] (DSMC). We simulated the flow of argon using both methods. In MD we used the Lennard-Jones potential (effective diameter $\sigma=3.405$ Å); in DSMC we used the variable hard-sphere potential [12]. Results from the two simulation methods for similar runs were in very close agreement.

The system consisted of 1000 atoms enclosed in a rectangular box of size $L\times A$, where A is the cross-sectional area. The distance between the walls was constant at $L=30\sigma$, while the cross section varied from $A=81\sigma^2$ to $40\,000\sigma^2$. The boundaries in the y and z directions were periodic and the boundaries in the x direction were thermal walls. When a particle reaches a thermal wall, the particle's velocity is reset randomly from the biased Maxwell-Boltzmann distribution with temperature $T_w=450$ K.

For the Poiseuille runs, the systems were subjected to an acceleration field of magnitude $g=2.27\times10^{15}$ cm/s^2 in MD runs and $g=2.27\times10^{14}$ cm/s^2 in the DSMC runs. For Couette flow, the thermal wall moved in opposite directions with speeds of $\pm4.36\times10^4$ cm/s.

The effective viscosity was obtained from the shear stress P_{xy} at the thermal wall. The shear stress was calculated as the net change of momentum of particles at the walls per unit per unit time. The effective viscosity is computed from

$$P_{xy}=-\eta\gamma_0 \ . \tag{10}$$

In the Poiseuille runs, the effective viscosity was also computed from the velocity profile [see Eq. (9)] and the two methods gave similar values.

Bhattacharya and Lie [2,3] reported that for large Knudsen number (>0.05) they observed a significant reduction in the expected slip length. Their analysis employed the simple, hard-sphere definition for the mean free path. Using Kn_h, we reproduce their results in both Couette and Poiseuille flow (see Fig. 1). They suggested that the slip coefficient may vary as $l_s^*\propto\ln(\mathrm{Kn}_h)$. Our runs extend the range of Knudsen number to lower values, and we find good agreement with Eq. (4) for $\mathrm{Kn}_h<0.05$.

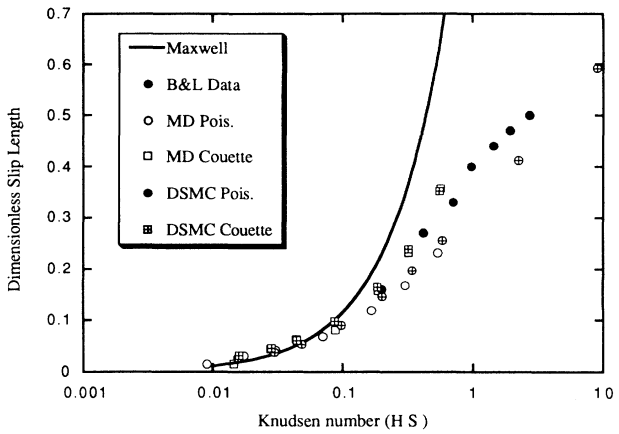

FIG. 1. Dimensionless slip length l_s^* vs hard-sphere (HS) Knudsen number Kn_h. The closed circles are from the Ref. [3]. The open circles and squares are our molecular-dynamics Poiseuille and Couette data, respectively. The cross-hatched circles and squares are our DSMC Poiseuille and Couette data, respectively. The solid line is given by (4) with $\alpha=1.15$; this linear relation appears as a curve in this graph due to the semi-log scale.

Using the viscous definition for mean free path, we find that the slip length is accurately given by Maxwell theory for the entire range of Knudsen numbers (see Fig. 2). A least-squares fit of the data gives the value $\alpha=0.97$ for the slip coefficients; for just the low-Knudsen-number data ($\mathrm{Kn}_v<0.05$) we obtain the slightly higher value of $\alpha=1.04$. Given an estimated relative error in λ_v of about 10%, the data are in reasonable agreement with theory.

There remains the question of why the two definitions of mean free path give similar results at low Knudsen number but differ dramatically when the separation between the walls is small. Maxwell theory was originally formulated for the semi-infinite geometry, i.e., a fluid bounded by a single wall. It should not be surprising that the theory needs some modification when there is a second boundary nearby.

The hard-sphere definition for the mean free path only

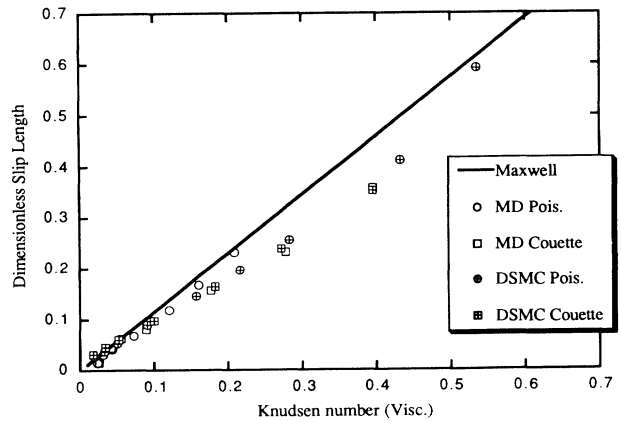

FIG. 2. Dimensionless slip length l_s^* vs viscous Knudsen number Kn_v. See Fig. 1 caption for details.

depends on the density and the particle diameter. On the other hand, the viscous mean free path also depends on the distance between the walls, since the effective viscosity decreases with increasing Knudsen number [4]. Heuristically, the viscous mean free path is the *effective* distance traveled by a particle between collisions with particles *or* walls. It would be interesting to develop this point of view along more rigorous lines.

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