

# Velocity gradient singularity and structure of the velocity profile in the Knudsen layer according to the Boltzmann equation

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Rarefied gas flow modeling presents significant challenges in the characterization of nanoscale devices and their applications. An important feature of such flows is the Knudsen layer, which is known to exhibit non-Newtonian viscosity behavior. Significantly, recent research has suggested that the effective viscosity at the surface is about half the standard dynamic viscosity. We examine these claims using numerical solutions of the linearized Boltzmann equation and direct simulation Monte Carlo calculations and discover that (i) the flow exhibits a striking power-law dependence on distance from the solid surface and (ii) the velocity gradient is singular at this surface. This finding contradicts these recent claims and has direct implications for gas flow modeling and the design of nanoscale devices.

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Micro- and nanoscale systems offer a vast array of potential applications in fields as diverse as biotechnology, microelectronics, medicine, materials science, and process engineering [1,2]. One such example is the Knudsen pump, which can generate a pressure differential on a micromachined chip without mechanical actuation [3,4]. Gas behavior in such systems is dominated by rarefaction effects, which arise because the mean free path of gas molecules is significant compared to the characteristic system dimensions. This leads to gas flow phenomena that are not manifested in macroscale flows [5,6]. While many aspects of such flows have been investigated [7–12], a complete understanding of rarefied flow phenomena in micro- and nanoscale systems is essential to fully realize the potential technological advances offered by such systems.

A characteristic feature of a gas flowing over a solid surface is the Knudsen layer, which is a rarefaction phenomenon that extends to a distance of about one mean free path from the surface and can dominate gas flow behavior at the nanoscale. The Knudsen layer exists because gas molecules interacting with the surface produce a nonequilibrium distribution of molecular velocities, and because molecules near the surface collide with the surface more frequently than they collide with each other. These effects have two important consequences: (1) The gas at the surface has a finite slip velocity relative to the surface, and (2) the gas near the surface exhibits non-Newtonian viscosity behavior [7].

The last 50 years have seen significant advances in the kinetic theory of gases [8–12], with many studies devoted to understanding the structure of the Knudsen layer. Recent research has focused on developing high-order hydrodynamic flow models that can capture such rarefaction effects and accurately describe the full spectrum of flow conditions, from the rarefied regime to near-equilibrium flow [6]. This is crucial for the development and characterization of nanoscale flows, where solution of the Boltzmann equation can pose a formidable challenge. Often, the accuracy of prospective hydrodynamic models is assessed by investigating their

ability to capture bulk flow phenomena, such as the Knudsen minimum in Poiseuille flow, instead of examining how accurately flow features such as the Knudsen layer are predicted. Indeed, few attempts have been made to study Knudsen layer structure with hydrodynamic flow models. One recent study [13] concluded that the Knudsen layer is poorly described by several high-order hydrodynamic flow models. This emphasizes the need for models that can accurately capture the essential physics and structure of the Knudsen layer and thus advance our understanding of rarefied gas flows.

Significantly, recent works by Lockerby *et al.* [14] and Fichman and Hetsroni [15] have investigated the non-Newtonian viscosity behavior in the Knudsen layer near a diffusely reflecting surface. Lockerby *et al.* [14] predicted an effective viscosity of  $0.59\mu_\infty$  at the surface, where  $\mu_\infty$  is the standard dynamic viscosity. Consistent with this result, Fichman and Hetsroni [15] predicted a value of  $\mu_\infty/2$ . In this paper, we critically examine these recent findings and resolve the detailed structure of the Knudsen layer for the Boltzmann equation with hard sphere molecules. In particular, we study the Knudsen layer using Kramers' problem (Fig. 1), which considers the unidirectional isothermal motion of a gas filling a half-space bounded by a planar solid surface. The only

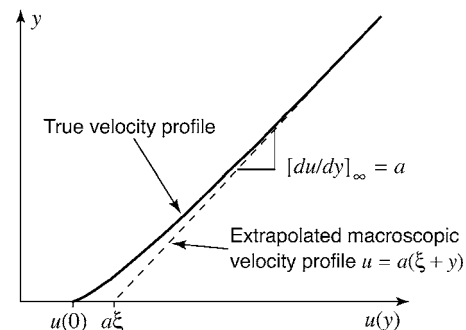


FIG. 1. Schematic of Kramers' problem.  $y$  is the normal distance from the stationary solid surface ( $y=0$ ) and  $u(y)$  is the bulk gas velocity in the direction parallel to the surface. The "macroscopic" slip velocity  $a\xi$  is extrapolated from the linear velocity gradient outside the Knudsen layer where  $y \rightarrow \infty$ , and differs from the true slip velocity  $u(0)$ .

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flow gradient is in the bulk velocity component  $u$  parallel to the surface. The gradient in  $u$  is normal to the surface and tends to a constant value  $a$  as the normal distance  $y$  tends to infinity, see Fig. 1. The effective viscosity  $\mu$  is defined by  $\mu(y) = |\tau(du/dy)^{-1}|$  where the shear stress  $\tau$  is constant in Kramers' problem. To determine the effective viscosity at the surface, previous work [14,15] implicitly assumed that the velocity field is analytic at  $y=0$ , i.e., its derivative exists. Here we show that this assumption is not valid.

To solve Kramers' problem and resolve the detailed structure of the Knudsen layer, we must solve the Boltzmann equation, which provides a rigorous description of a dilute gas. The nonlinear integrodifferential form of the Boltzmann equation presents formidable analytical difficulties and complete closed-form solutions have not been found, even for simple flows such as Kramers' problem. The primary difficulty is due to the collision term, which may be linearized for weakly nonequilibrium flows to give the linearized Boltzmann equation (LBE). Here, we reanalyze published LBE solutions of Kramers' problem for monatomic hard sphere molecules with a diffusely reflecting surface. To verify the results of this LBE analysis, we solve the full nonlinear Boltzmann equation using an established computational technique, Bird's direct simulation Monte Carlo (DSMC) method [16].

For Kramers' problem in a monatomic gas, the LBE is

$$2av_y(v_x - ay) + v_y\partial_y h = \mathcal{L}h,$$

where  $(v_x, v_y, v_z) = \mathbf{v}$  is the molecular velocity with components  $v_x$  parallel to  $u$ ,  $v_y$  parallel to  $y$ , and  $v_z$  orthogonal to  $v_x$  and  $v_y$ . The function

$$h(y, \mathbf{v}) = f(y, \mathbf{v})/f_0 - 1$$

is the deviation of the molecular velocity distribution function  $f$  from the absolute Maxwellian distribution  $f_0$  and  $\mathcal{L}h$  is the linearized collision term [17]. We present gas flow velocities in terms of the reduced velocity  $\tilde{u}$ ,

$$\tilde{u}(\tilde{y}) = u(\tilde{y})/(a\lambda),$$

where  $\tilde{y} = y/\lambda$  and  $\lambda$  is the mean free path for hard sphere molecules given by

$$\lambda = (\sqrt{2}n\pi d^2)^{-1},$$

where  $n$  is the molecular number density and  $d$  is the hard sphere diameter.

Our investigations focus on the LBE numerical solutions of Ohwada *et al.* [18], Loyalka and Hickey [19,20], and Siewert [21]. These solutions are presented in Fig. 2 as  $\tilde{y}$  versus  $\tilde{u} - \tilde{u}(0)$  on a log-log scale. Importantly, these independent solutions display excellent agreement. From Fig. 2 it is also clear that on a log-log scale, the velocity profile is linear to a high degree of accuracy for  $\tilde{y} \lesssim 1$ , even at a distance of only  $\lambda/45$  from the surface. Since  $\lambda$  is the only natural length scale in a dilute gas flow, these numerical results demonstrate that the flow velocity in this region follows the distinct power-law dependence

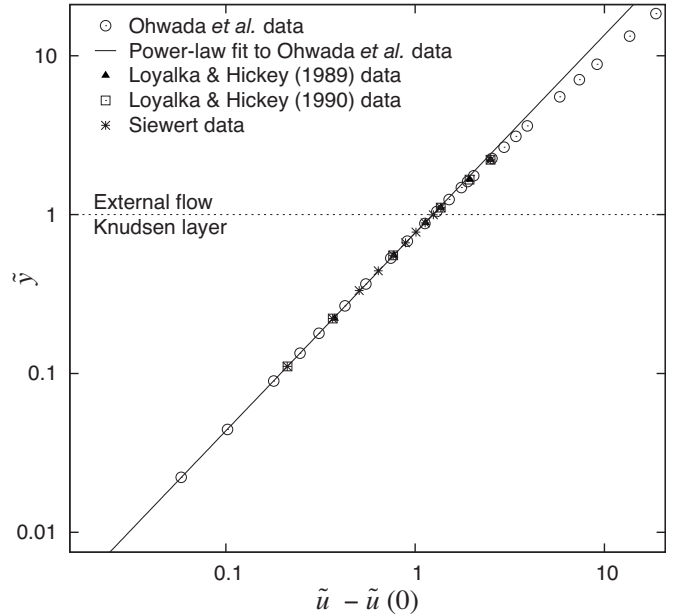


FIG. 2. Comparison of published LBE solutions for Kramers' problem. The power-law fit to the solution of Ohwada *et al.* [18] is shown because it has the highest resolution near  $\tilde{y}=0$ . Fits to the other published LBE solutions are indistinguishable from this fit.

$$\tilde{u}(\tilde{y}) = \tilde{u}(0) + C\tilde{y}^\alpha \quad (1)$$

with the corresponding effective viscosity

$$\mu(\tilde{y}) = \mu_\infty \tilde{y}^{1-\alpha}/(\alpha C).$$

For these published LBE solutions, the parameters  $C$  and  $\alpha$  were obtained by linear regression of the log-log data for  $\tilde{y} \leq 1$ , and are presented in Table I. Note that for all these LBE solutions, the parameter  $\alpha$  is distinctly less than unity, violating the tacit assumption of analyticity in the velocity field that would result in an integer power exponent. It necessarily follows from this that at the surface ( $\tilde{y}=0$ ) the velocity gradient is infinite and the effective viscosity is zero.

Our prediction of an infinite velocity gradient for the Boltzmann equation is consistent with the logarithmic singularity previously observed for the (approximate) linearized Bhatnagar, Gross, and Krook (BGK) equation [12,22]. Importantly, these findings refute the recent results of Lockerby *et al.* [14] and Fichman and Hetsroni [15]. Other recent hy-

TABLE I. Fit parameters for power-law velocity profile  $\tilde{u} = \tilde{u}(0) + C\tilde{y}^\alpha$  in the Knudsen layer where  $\tilde{y} < 1$ . The LBE solutions are also closely approximated by the power-law  $\tilde{u} = \beta + (1/\beta)\tilde{y}^\beta$  where  $\beta=0.8$ .

Solution	$\xi/\lambda$	$\tilde{u}(0)$	$C$	$\alpha$
Ohwada <i>et al.</i> [18]	1.1113	0.8054	1.2378	0.8027
Loyalka and Hickey [19]	1.0906	0.7998	1.2466	0.7978
Loyalka and Hickey [20]	1.0940	0.7927	1.2275	0.7992
Siewert [21]	1.0937	0.7927	1.2413	0.8083
DSMC	1.11	0.81	1.24	0.82

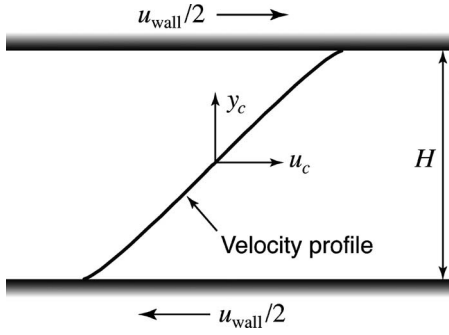


FIG. 3. Simulation domain for DSMC calculations of Couette flow.  $u_c$  is the bulk flow velocity parallel to the wall and  $y_c$  is the displacement from the midplane where  $y_c=0$ . The walls are at  $y_c = \pm H/2$ .

hydrodynamic models [13] for the velocity profile in the Knudsen layer also do not capture this behavior and possess a finite velocity gradient at the surface.

Importantly, at  $\tilde{y}=1$ , the velocity predicted by Eq. (1) is only 1.9% lower than the velocity from the LBE solutions, while the extrapolated macroscopic velocity  $\tilde{u}=\xi/\lambda+\tilde{y}$  is only 2.5% higher than the velocity from the LBE solutions. The entire velocity profile for Kramers' problem is therefore accurately described by

$$\tilde{u}(\tilde{y}) = \begin{cases} \tilde{u}(0) + C\tilde{y}^\alpha & (\tilde{y} < 1, \text{ within Knudsen layer}) \\ \xi/\lambda + \tilde{y} & (\tilde{y} > 1, \text{ outside Knudsen layer}). \end{cases}$$

Such flow behavior is not predicted by any current hydrodynamic model and hence the validity of approximating the full nonlinear Boltzmann equation with the LBE must be confirmed to make a definitive statement. To solve the full Boltzmann equation for Kramers' problem computationally, we used the DSMC method [16]. This method considers the discrete molecular character of gases and models macroscopic gas behavior by considering a set of simulator particles, representative of the real gas molecules, as they undergo simulated intermolecular collisions, interact with solid surfaces, and move through physical space. Probabilistic rather than deterministic procedures are used to simulate molecular collision processes.

Following Bird [23], we used precise DSMC calculations of Couette flow to capture Kramers' problem with the simulation geometry shown in Fig. 3. We simulated monatomic hard sphere molecules, with diffuse reflection at the walls. A convergence analysis was performed to determine suitable values for the wall separation  $H$ , the relative wall speed  $u_{\text{wall}}$ , the simulation time step  $\Delta t$ , and the number of computational cells. This consisted of a systematic series of DSMC calculations in which these parameters were modified until there was no significant variation in the results. This provided  $H = \lambda/0.06$ , which was large enough to eliminate interference between Knudsen layers near each wall. We used  $u_{\text{wall}} = 30$  m/s, giving a Mach number of 0.097 and ensuring incompressible flow conditions. Consistent with standard DSMC procedures [16],  $\Delta t$  was set to a value significantly smaller than the mean time between intermolecular collisions. Our  $\Delta t$  was 10% of the mean time between collisions

TABLE II. DSMC simulation details.

$d=3.638 \times 10^{-10}$ m	Sample interval= $\Delta t$
$m=6.634 \times 10^{-26}$ kg	Samples/cell= $10^9$
$n=1.507 \times 10^{25}/\text{m}^3$	Simulated collisions $\approx 50 \times 10^9$
Mean particles/cell=100	Particle moves $\approx 10^{12}$

for hard sphere molecules, given by  $\Delta t = \frac{1}{10}\lambda/[8kT_{\text{wall}}/(\pi m)]^{1/2}$ , where  $k$  is Boltzmann's constant, the wall temperature  $T_{\text{wall}}=273$  K, and  $m$  is the molecular mass. The convergence analysis also showed that 1000 cells were sufficient, which were arranged in a regular grid. Other simulation details are summarized in Table II. The density and temperature variations in the DSMC solution were both about 0.05%, thus confirming that the incompressible and isothermal flow conditions necessary to capture Kramers' problem were achieved with excellent accuracy. The statistical error in the velocity from the DSMC solution was  $\pm 0.14$  m/s, using a 99% confidence interval. To analyze Kramers' problem with our DSMC Couette flow solution, we used the mean Couette flow velocities  $\tilde{u}_c = \frac{1}{2}[u_c(y_c) - u_c(-y_c)]$  that were transformed to the reference frame of Kramers' problem.

A nonlinear regression fit to the DSMC solution with the power-law form of Eq. (1) was used, yielding the parameters shown in Table I. This DSMC solution is compared to the LBE solution of Ohwada *et al.* in Fig. 4. Significantly, our DSMC solution shows close agreement with the LBE solution, thus verifying the accuracy of the LBE description of Kramers' problem, confirming the power-law dependence of the velocity profile within the Knudsen layer and the effective viscosity of zero at the surface.

To explore the applicability of these findings to molecular

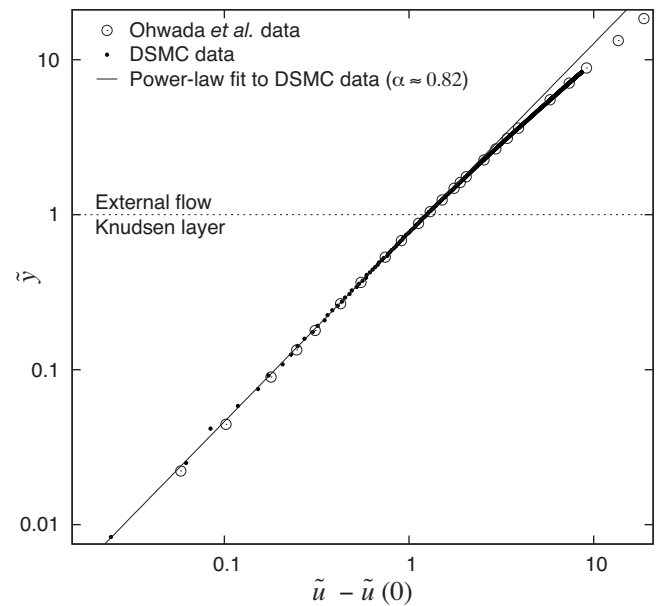


FIG. 4. DSMC solution of Kramers' problem compared to the LBE solution of Ohwada *et al.* [18]. The DSMC data points are located at the center of each computational cell and extend from  $\tilde{y}=1/120$  to  $\tilde{y}=25/3$  from the wall.

models beyond simple hard spheres, we also analyzed the DSMC solution of Couette flow provided by Lockerby *et al.* [13]. This calculation used the variable soft sphere molecular model [24], which approximates an intermolecular interaction having a repulsive force that is proportional to an inverse power of the intermolecular separation. For this DSMC solution, we found that the velocity profile for  $\bar{y} \lesssim 1$  was also accurately described by a power law with the form of Eq. (1) and  $\alpha=0.8$ . This result indicates that the power-law description of the velocity profile in the Knudsen layer given in Eq. (1) applies beyond the simple hard sphere model. To make a definitive statement about the general applicability of the power-law model in real gases, however, detailed solutions of the Boltzmann equation using a range of realistic molecular models, validated by accurate experimental measurements, are required. For gas mixtures containing molecules that possess rotational energy, such as air, the DSMC method is the only practical tool for solving the Boltzmann equation and will form an integral part of such investigations. The power-law velocity profile reported here using numerical computations has significant implications for future analytical work on the Boltzmann equation and Knudsen layer structure.

In summary, we have investigated the detailed structure of

the Knudsen layer for hard sphere molecules according to the Boltzmann equation, and found that it exhibits a striking power-law dependence on distance from the solid surface. This finding establishes that the velocity gradient is infinite at the surface where the effective viscosity is zero, contradicting recent results [14,15]. Importantly, this singular nature of the velocity profile has been completely overlooked in recent works. Our finding is therefore expected to be of particular value in developing hydrodynamic models of rarefied flow beyond the Boltzmann equation and thus aid in the design and characterization of micro- and nanoscale gas flows. Significantly, no current hydrodynamic model captures the essential physics of the Knudsen layer with its nonanalytic power-law structure reported here, which in turn casts serious doubts on their underlying validity. The fundamental knowledge presented in this paper is therefore expected to provide strong stimulus for the future development of such models.

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- [1] H. G. Craighead, *Science* **290**, 1532 (2000).
- [2] S. E. Lyshevski, *Nano- and Micro-Electromechanical Systems*, 2nd ed. (CRC, Boca Raton, 2005).
- [3] Y. Sone, *Annu. Rev. Fluid Mech.* **32**, 779 (2000).
- [4] S. McNamara, and Y. B. Gianchandani, *J. Microelectromech. Syst.* **14**, 741 (2005).
- [5] M. Gad-el-Hak, *J. Fluids Eng.* **121**, 5 (1999).
- [6] J. M. Reese, M. A. Gallis, and D. A. Lockerby, *Philos. Trans. R. Soc. London, Ser. A* **361**, 2967 (2003).
- [7] V. Garzó and A. Santos, *Kinetic Theory of Gases in Shear Flows: Nonlinear Transport* (Kluwer Academic, Dordrecht, 2003).
- [8] M. N. Kogan, *Rarefied Gas Dynamics* (Plenum, New York, 1969).
- [9] C. Bardos, R. E. Caflisch, and B. Nicolaenko, *Commun. Pure Appl. Math.* **39**, 323 (1986).
- [10] F. Sharipov and V. Seleznev, *J. Phys. Chem. Ref. Data* **27**, 657 (1998).
- [11] C. Cercignani, *Rarefied Gas Dynamics* (Cambridge University Press, Cambridge, England 2000).
- [12] Y. Sone, *Kinetic Theory and Fluid Dynamics* (Birkhäuser, Boston, 2002).
- [13] D. A. Lockerby, J. M. Reese, and M. A. Gallis, *Phys. Fluids* **17**, 100609 (2005).
- [14] D. A. Lockerby, J. M. Reese, and M. A. Gallis, *AIAA J.* **43**, 1391 (2005).
- [15] M. Fichman and G. Hetsroni, *Phys. Fluids* **17**, 123102 (2005).
- [16] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Clarendon Press, Oxford, 1994).
- [17] C. Cercignani, *The Boltzmann Equation and Its Applications* (Springer-Verlag, New York, 1988).
- [18] T. Ohwada, Y. Sone, and K. Aoki, *Phys. Fluids A* **1**, 1588 (1989).
- [19] S. K. Loyalka and K. A. Hickey, *Phys. Fluids A* **1**, 612 (1989).
- [20] S. K. Loyalka and K. A. Hickey, *ZAMP* **41**, 245 (1990).
- [21] C. E. Siewert, *ZAMP* **54**, 273 (2003).
- [22] D. R. Willis, *Phys. Fluids* **5**, 127 (1962).
- [23] G. A. Bird, *Proceedings of the 10th International Symposium on Rarefied Gas Dynamics*, edited by J. L. Potter [*Prog. Astronaut. Aeronaut.* **51**, 323 (1977)].
- [24] K. Koura and H. Matsumoto, *Phys. Fluids A* **3**, 2459 (1991).