Comment on Cercignani's second-order slip coefficient

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Cercignani's second-order slip model has been neglected over the years, perhaps due to Sreekanth's claim that it cannot fit his experimental data. In this paper we show that Sreekanth's claim was based on an incorrect interpretation of this model. We also show that Cercignani's second-order slip model, when modified and used appropriately, is in good agreement with solutions of the Boltzmann equation for a hard-sphere gas for a wide range of rarefaction. Given its simplicity, we expect this model to be a valuable tool for describing isothermal micro- and nanoscale flows to the extent that the hard-sphere approximation is appropriate. © *2003 American Institute of Physics.*
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Accurate second-order slip coefficients are highly desirable because they allow the solution of flow problems using the continuum description that is significantly more efficient compared to molecular-based approaches. Even though the validity of Navier–Stokes is suspect beyond $\mathrm{Kn}\gtrsim 0.1$, in flows with high symmetry a second-order coefficient may be expected to give reasonable results for a few quantities of engineering interest such as the mean flow velocity.[1] For this reason significant effort has been expended in developing[1–4] and evaluating[4–6] second-order slip models.

One of the first second-order slip models to appear was the one by Cercignani.[1] He considers a steady flow alligned with the x direction and parallel to a stationary straight wall whose normal pointing into the fluid is aligned with the y direction. Using the BGK approximation he obtains

$$u|_{\mathrm{wall}}=1.016\theta\frac{\partial u}{\partial y}\bigg|_{\mathrm{wall}}-0.7667\theta^2\frac{\partial^2 u}{\partial y^2}\bigg|_{\mathrm{wall}},\tag{1}$$

where $\theta=\mu\sqrt{2RT}/P$. Here u is the gas velocity, μ is the gas viscosity, R is the gas constant, T is the temperature, P is the pressure and $|_{\mathrm{wall}}$ denotes evaluation at the wall. This result assumes that no gradients exist in directions other than the normal to the wall, that is, $\partial u/\partial z=\partial u/\partial x=0$. The same result was obtained by Sone and Onishi.[3]

This result has been overlooked over the years. It appears that one of the reasons for this is Sreekanth's paper[5] which claims that this model cannot fit his experimental data. In this paper we wish to point out that in his comparison Sreekanth misinterpreted the above model and overlooked Cercignani's suggestion to modify it such that it applies to the Maxwell gas model which is more appropriate for describing isothermal flows of real gases.[1] Below, we show that, when modified appropriately, Cercignani's slip model is in excellent agreement with solutions of the linearized Boltzmann equation for hard spheres, and DSMC simulations up to $\mathrm{Kn}\approx 0.4$. Agreement with experimental data is always subject to factors such as surface accommodation, and in pressure-driven flows, fluid acceleration due to compressibility. The neglect of the fluid acceleration and its effect on the flow profile and slip (recall that Cercignani's result requires $\partial u/\partial x=0$) is typically justified in internal flows through the use of the locally fully developed approximation. This is known to be a reasonable approximation for a number of flows of practical interest.[10] It is also generally accepted that the hard-sphere model is a reasonable approximation to real-gas behavior for isothermal flows. For comparisons between solutions of the linearized Boltzmann equation for hard spheres and experimental data see Refs. 4, 8.

Cercignani's correction amounts to multiplying the second-order slip coefficient by 2/3. The slip model for a Maxwell gas therefore becomes

$$u|_{\mathrm{wall}}=1.016\theta\frac{\partial u}{\partial y}\bigg|_{\mathrm{wall}}-0.511\theta^2\frac{\partial^2 u}{\partial y^2}\bigg|_{\mathrm{wall}}.\tag{2}$$

Given that the slip coefficients are fairly insensitive to the details of the intermolecular force law,[7] we can use a viscosity-based mean free path,

$$\lambda=\frac{\mu}{P}\sqrt{\frac{\pi RT}{2}},\tag{3}$$

to obtain the following *prediction* for the slip in a hard-sphere gas:

$$u|_{\mathrm{wall}}=1.1466\lambda\frac{\partial u}{\partial y}\bigg|_{\mathrm{wall}}-0.647\lambda^2\frac{\partial^2 u}{\partial y^2}\bigg|_{\mathrm{wall}}.\tag{4}$$

Accurate numerical solutions of the Boltzmann equation in fact show[9] that for a hard-sphere gas the first-order slip coefficient is $\alpha=1.11$. This verifies that the slip coefficients are only mildly dependent on the interaction model. Given this information, we can improve the above prediction [Eq. (4)] by substituting the first-order term with the known value. We also propose to scale the second-order term by the square of 1.11/1.1466 since this ratio is representative of the difference in slip behavior between the Maxwell and hard-sphere molecules. (Rescaling the second-order term has a very small effect; the difference in slip velocity at $\mathrm{Kn}=0.4$ is of the order of 1%.) By applying those changes we obtain

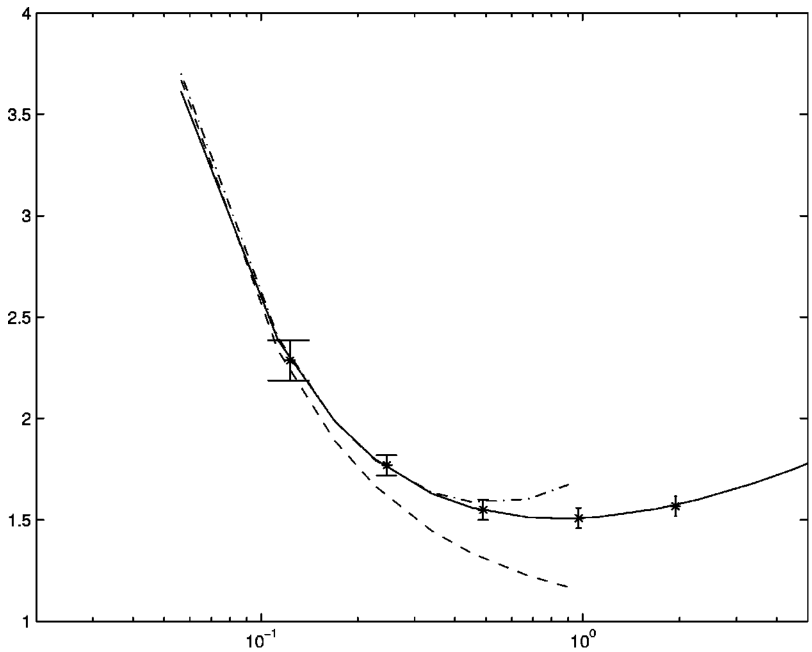

FIG. 1. Nondimensional flow rate as a function of the Knudsen number for fully developed flow. The solid line denotes $\overline{Q}$ as determined by a solution of the linearized Boltzmann equation for hard-sphere gases (Ref. 8), the dash–dotted line denotes Eq. (7), and the dashed line denotes a first-order slip model. The stars denote DSMC simulation results.

$$u|_{\mathrm{wall}}=\alpha\lambda\left.\frac{\partial u}{\partial y}\right|_{\mathrm{wall}}-\delta\lambda^2\left.\frac{\partial^2 u}{\partial y^2}\right|_{\mathrm{wall}}, \quad (5)$$

where $\delta\approx 0.61$.

As always, the slip-flow description is expected to be valid in the Navier–Stokes part of the flow, that is, away from the walls. The comparison of flow profiles is therefore not very meaningful for Kn>0.1, since the Knudsen layer covers a large part of the domain. As a result, attention is usually paid to the ability of the model to describe the flow rate through a duct. To do this, the contribution of the Knudsen layers to the flow rate, which is of the same order as the second-order slip, needs to be taken into account.

For flow in a two-dimensional channel $(\partial u/\partial x=\partial u/\partial z=0)$, the flow rate Q in the BGK approximation is given by

$$Q=\int_A\left[u+\xi\frac{\partial^2 u}{\partial y^2}\right]dA, \quad (6)$$

where the second term is the contribution of the Knudsen layer. Here A is the duct cross sectional area and $\xi=0.4665RT\mu^2/P^2$. According to Cercignani[1] the Knudsen layer contribution to the flow rate is largely independent of the molecular model and therefore ξ is *not* subject to the same correction as the second-order slip coefficient (multiplication by 2/3). We may thus assume that for a hard-sphere gas $\xi\simeq 0.4665RT\mu^2/P^2=0.296\lambda^2$.

Using the above, we find that the mean velocity, $\overline{u}$, for a fully developed $(\partial u/\partial x=0)$ pressure-driven flow of a hard-sphere gas in a two-dimensional channel $(\partial u/\partial z=0)$ is given by

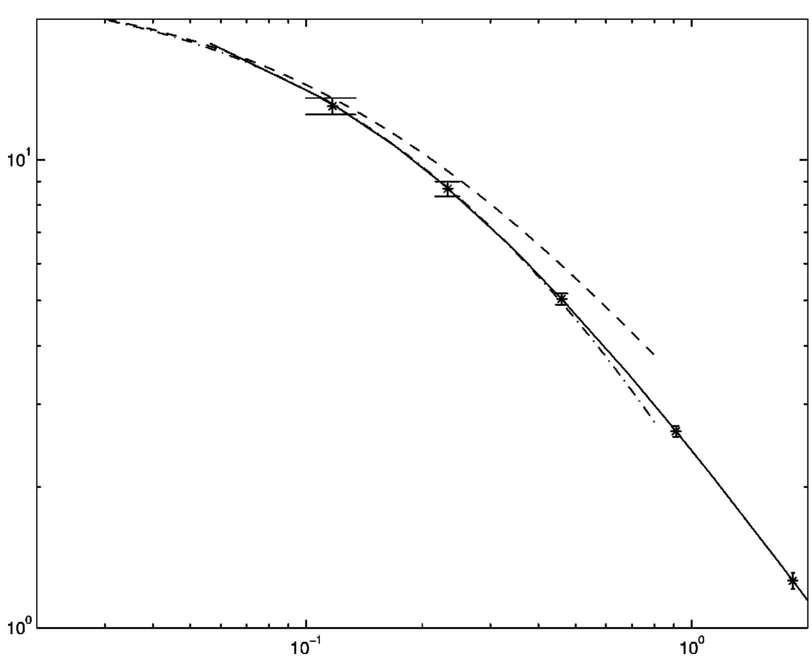

FIG. 2. The skin friction coefficient as a function of the Knudsen number for fully developed flow. The solid line denotes Eq. (10) and the dash–dotted line denotes the second-order slip result [Eq. (8)]. The dashed line denotes a first-order slip model and the stars denote DSMC simulation results.

$$\overline{u}=-\frac{H^2}{2\mu}\frac{dP}{dx}\left(\frac{1}{6}+\alpha\,\mathrm{Kn}+2\beta\,\mathrm{Kn}^2\right). \tag{7}$$

The skin friction coefficient is given by

$$C_f=\frac{\tau_w}{1/2\rho\overline{u}^2}=\frac{24}{(1+6\alpha\,\mathrm{Kn}+12\beta\,\mathrm{Kn}^2)\mathrm{Re}}, \tag{8}$$

where τ_w is the wall shear stress and $\mathrm{Re}=\rho\overline{u}2H/\mu$ is the Reynolds number. Here $\beta=0.61-0.296\approx0.31$ is the second-order slip coefficient which includes the contribution of the Knudsen layer. It is interesting to note that Sreekanth found $\beta=0.14$ to fit his experimental data best. However, Sreekanth was using a first-order slip coefficient of 1.1466; the difference between his best-fit values and the model proposed above is thus small and within the acceptable limits of experimental and modeling error.

These two results are compared below to hard-sphere DSMC simulations for $\mathrm{Re}\,H/L<O(1)$ and solutions of the linearized Boltzmann equation for hard spheres.[8] The results for the flow rate (Fig. 1) are presented in terms of the nondimensional flow rate per unit depth $\overline{Q}=\overline{Q}(\mathrm{Kn})$,

$$\overline{Q}=\frac{\overline{u}}{-\frac{1}{P}\frac{dP}{dx}\sqrt{\frac{RT}{2}}H}, \tag{9}$$

as a function of the Knudsen number. The skin-friction coefficient for arbitrary Knudsen numbers in fully developed flow can be written[10] in terms of $\overline{Q}$ as

$$C_f=\frac{32}{5\sqrt{\pi}\,\mathrm{Re}\,\mathrm{Kn}\,\overline{Q}}. \tag{10}$$

A comparison between the second-order model, this result and DSMC simulations is given in Fig. 2. Note that the wall shear stress in our DSMC simulations was evaluated from direct momentum exchange with the wall and not from the pressure gradient.

Both figures show that the agreement for $\mathrm{Kn}\lesssim0.4$ is excellent. Similarly to applications of practical interest, the flow in our DSMC simulations was caused by a pressure gradient applied at the ends of the channel, leading to some fluid acceleration due to the axial pressure drop. Despite this, the locally fully developed approximation appears to be reasonable for $\mathrm{Re}\,H/L<O(1)$.

Equation (5) performs reasonably well by leading to a flowfield which satisfactorily captures the flow profile inside the channel although, as explained above, this comparison is less meaningful[11] for $\mathrm{Kn}>0.1$. The maximum discrepancy in the velocity profile away from the walls for $\mathrm{Kn}\lesssim0.3$ is of the order of 5% and typically less. Given its great simplicity (the alternatives are molecular simulation or numerical solution of the Boltzmann equation) and the relatively good predictive power of the hard-sphere model in isothermal flows, this model should be of great use, and in particular in situations where the flow rate is of interest.[12–14]

For flows with velocity gradients in the plane normal to the flow direction (only $\partial u/\partial x=0$), Cercignani finds that the only modification required within the BGK approximation is the replacement of $\partial^2u/\partial y^2$ with $\partial^2u/\partial y^2+\partial^2u/\partial z^2$ in Eqs. (1) and (6). [It follows that Eqs. (2), (4) and (5) will be similarly modified.] Further work is required to ensure that this generalization can be reliably used for other interaction models.[15]

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[1] C. Cercignani, ‘‘Higher order slip according to the linearized Boltzmann equation,’’ Institute of Engineering Research Report AS-64-19, University of California, Berkeley, 1964.
[2] R. G. Deissler, ‘‘An analysis of second-order slip flow and temperature–jump boundary conditions for rarefied gases,’’ Int. J. Heat Mass Transfer **7**, 681 (1964).
[3] Y. Sone and Y. Onishi, ‘‘Kinetic theory of evaporation and condensation-hydrodynamic equation and slip boundary condition,’’ J. Phys. Soc. Jpn. **44**, 1981 (1978).
[4] A. Beskok and G. E. Karniadakis, ‘‘A model for flows in channels and ducts at micro and nano scales,’’ Microscale Thermophys. Eng. **3**, 43 (1999).
[5] A. K. Sreekanth, ‘‘Slip flow through long circular tubes,’’ *Proceedings of the 6th International Symposium on Rarefied Gas Dynamics*, edited by L. Trilling and H. Wachman (Academic, Cambridge, MA, 1969).
[6] C. Aubert and S. Colin, ‘‘High-order boundary conditions for gaseous flows in rectangular microducts,’’ Microscale Thermophys. Eng. **5**, 41 (2001).
[7] C. Cercignani, *The Boltzmann Equation and its Applications* (Springer-Verlag, New York, 1988).
[8] T. Ohwada, Y. Sone, and K. Aoki, ‘‘Numerical analysis of the Poiseuille and thermal transpiration flows between parallel plates on the basis of the Boltzmann equation for hard-sphere molecules,’’ Phys. Fluids A **1**, 2042 (1989).
[9] T. Ohwada, Y. Sone, and K. Aoki, ‘‘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,’’ Phys. Fluids A **1**, 1588 (1989).
[10] N. G. Hadjiconstantinou and O. Simek, ‘‘Constant-wall-temperature Nusselt number in micro and nano channels,’’ J. Heat Transfer **124**, 356 (2002).
[11] Y. Zheng, A. L. Garcia, and B. J. Alder, ‘‘Comparison of kinetic theory and hydrodynamics for Poiseuille flow,’’ J. Stat. Phys. **109**, 495 (2002).
[12] S. Fukui and R. Kaneko, ‘‘Analysis of ultra thin gas film lubrication based on linearized Boltzmann equation: First report-derivation of a generalized lubrication equation including thermal creep flow,’’ J. Tribol. **110**, 253 (1988).
[13] N. G. Hadjiconstantinou, ‘‘Sound wave propagation in transition-regime micro- and nanochannels,’’ Phys. Fluids **14**, 802 (2002).
[14] N. G. Hadjiconstantinou, ‘‘Dissipation in small scale gaseous flows,’’ to appear in the J. Heat Transfer.
[15] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Clarendon, Oxford, 1994).