Velocity boundary condition at solid walls in rarefied gas calculations

Duncan A. Lockerby
Department of Mechanical Engineering, King's College London, London WC2R 2LS, United Kingdom

Jason M. Reese
Department of Mechanical Engineering, Strathclyde University, Glasgow G1 1XJ, United Kingdom

David R. Emerson and Robert W. Barber
Centre for Microfluidics, CLRC Daresbury Laboratory, Warrington WA4 4AD, United Kingdom
(Received 15 October 2003; revised manuscript received 22 December 2003; published 26 July 2004)

Maxwell's famous slip boundary condition is often misapplied in current rarefied gas flow calculations (e.g., in hypersonics, microfluidics). For simulations of gas flows over curved or moving surfaces, this means crucial physics can be lost. We give examples of such cases. We also propose a higher-order boundary condition based on Maxwell's general equation and the constitutive relations derived by Burnett. Unlike many other higher-order slip conditions these are applicable to any form of surface geometry. It is shown that these "Maxwell-Burnett" boundary conditions are in reasonable agreement with the limited experimental data available for Poiseuille flow and can also predict Sone's thermal-stress slip flow—a phenomenon which cannot be captured by conventional slip boundary conditions.

DOI: 10.1103/PhysRevE.70.017303 PACS number(s): 47.27.Lx, 47.45.Gx

I. INTRODUCTION

In 1879, Maxwell published a paper on the viscous stresses arising in rarefied gases [1]. At the time, a reviewer commented that it also might be useful if Maxwell could use his theoretical findings to derive a velocity boundary condition for rarefied gas flows at solid surfaces. Consequently, in an appendix to the paper, Maxwell proposed his now-famous velocity slip boundary condition. This boundary condition was successful in predicting two prior experimental observations: (a) that a rarefied gas could slide over a surface and (b) that inequalities in temperature could give rise to a force tending to make the gas slide over a surface from colder to hotter regions (which had been discovered by Reynolds and was known as "thermal transpiration"—now more commonly known as "thermal creep"). What has subsequently been overlooked by many current researchers is the general form of the slip expression derived by Maxwell, and this has some substantial consequences for modern simulations of, e.g., hypersonic aerodynamics and gas flows in microsystems.

Maxwell related the tangential gas velocity slip $\vec{u}_{\text{slip}}$ to the tangential shear stress $\vec{\tau}$ and heat flux $\vec{q}$. Written in tensor form so that it is easily applicable to flows over three-dimensional surfaces (a nontensorial expression can be found in, e.g., Ref. [2]) Maxwell's expression is

$$\vec{u}_{\text{slip}} = -\frac{(2-\sigma)}{\sigma\mu}\lambda\vec{\tau} - \frac{3}{4}\frac{N_{\text{Pr}}(\gamma-1)}{\gamma p}\vec{q}, \qquad (1)$$

where $\vec{\tau}=(\vec{i}_n\cdot\mathbf{\Pi})\cdot(\mathbb{1}-\vec{i}_n\vec{i}_n)$, $\vec{q}=\vec{Q}\cdot(\mathbb{1}-\vec{i}_n\vec{i}_n)$, an arrow denotes a vector quantity, σ is the momentum accommodation coefficient (equal to 1 for surfaces that reflect all incident molecules diffusely and 0 for purely specular reflection), μ is the gas viscosity at the wall, λ is the molecular mean free path at the wall, N_{Pr} is the Prandtl number, γ is the specific heat ratio, p is the gas pressure at the wall, $\vec{i}_n$ is a unit vector normal and away from the wall, $\mathbf{\Pi}$ is the stress tensor at the wall, $\mathbb{1}$ is the identity tensor, and $\vec{Q}$ is the heat flux vector at the wall.

If the Navier-Stokes constitutive relations for stress and heat flux are substituted into Eq. (1), expressions for velocity slip in terms of flow gradients can be obtained. In his original paper, Maxwell used a one-dimensional expression for the shear stress (appropriate for the typical case he was interested in) which made his final result generally applicable only to nonrotating planar walls (i.e., where the streamwise variation in wall-normal velocity is negligible). In scalar form, Maxwell gave

$$u_{\text{s}} = \frac{(2-\sigma)}{\sigma}\lambda\frac{\partial u_x}{\partial n} + \frac{3}{4}\frac{\mu}{\rho T}\frac{\partial T}{\partial x}, \qquad (2)$$

where n is the coordinate normal to the wall, x is the coordinate tangential to the wall, u_x is the x component of the gas velocity, u_{s} is the x component of the slip velocity, and ρ and T are the density and temperature of the gas at the wall, respectively.

It is because of its relative simplicity, compared to Eq. (1), that Eq. (2) is remembered as Maxwell's main theoretical result. However, for most surface geometries of practical interest, having curvature and/or rotational motion, it is inapplicable because it neglects that the velocity normal to the wall can vary in the streamwise direction. Therefore a more complete expression for the tangential shear stress is required in Eq. (1). Calculations straightforwardly using Eq. (2) are likely to miss important features of the rarefied flow behavior.

In this paper we reassess Maxwell's general equation (1) to examine the effect of implementing the full form of the tangential shear stress expression on the velocity slip. We then propose a form of higher-order condition which is more accurate at greater degrees of gas rarefaction and is able to capture certain microflow phenomena.

II. WALL CURVATURE AND MOTION

If the full Navier-Stokes stress tensor is adopted, for a wall in two dimensions, Eq. (1) reduces to

$$u_s = \frac{(2-\sigma)}{\sigma}\lambda\left(\frac{\partial u_x}{\partial n} + \frac{\partial u_n}{\partial x}\right) + \frac{3}{4}\frac{\mu}{\rho T}\frac{\partial T}{\partial x}, \tag{3}$$

where u_s is the slip component tangential to the wall, and u_n and u_x are the gas velocities normal and tangential to the wall, respectively. The additional term that features in Eq. (3) but not in Eq. (2) can have a significant influence on the overall velocity slip. For example, when there is rotational wall motion (i.e., wall motion in a direction normal to the surface with a velocity that varies in the tangential direction), then even for flat surfaces (e.g., a deflecting flap) there will be a finite tangential velocity slip. For stationary walls, surface curvature will also give rise to a contribution from the additional term.

Although the misapplication of Eq. (2) to general geometries is widespread, it is not universal, and there are instances where curved boundaries have been treated appropriately [3,4]. Einzel, Panzer, and Liu [5] derived a boundary condition similar to Eq. (3) for surfaces with curvature. However, their boundary condition was formulated such that slip due to surface normal motion could not be accommodated. Also, it did not include the contribution of thermal creep to velocity slip and nor was the relationship to Maxwell's general equation realized.

Two examples will show the importance of implementing the complete form of Maxwell's general formulation.

A. Cylindrical Couette flow

Recent analytical and molecular dynamics studies [3,5,6] suggest that the velocity profile in a rarefied cylindrical Couette flow can become inverted. In the case of a stationary outer cylinder and rotating inner cylinder, "inverted" means that the radial velocity of the gas becomes greater farther away from the moving center.

We have performed a simple isothermal calculation using a finite-difference discretization of the Navier-Stokes equations to examine the influence of various boundary conditions on the velocity profile. The inner and outer cylinders have radii of 3λ and 5λ, respectively, and the former has a tangential velocity approximately a third of the speed of sound. The gas is argon at STP conditions and the accommodation coefficient σ is 0.1. Figure 1 shows a comparison of the velocity profiles (nondimensionalized by the tangential velocity of the inner cylinder) predicted using the standard no-slip condition, the conventional slip condition [Eq. (2)], Maxwell's general slip condition [Eq. (1)], direct simulation Monte Carlo (DSMC) molecular dynamics [6], and the analytical method of Einzel, Panzer, and Liu [5].

The DSMC method (being a statistical molecular dynamics simulation) is often used as an independent numerical test in the absence of experimental data [7]. That the DSMC method predicts an inverted velocity profile is strong corroborative evidence that the phenomenon is real. The conventional slip condition, Eq. (2), evidently cannot predict this behavior; however, Maxwell's general slip condition, Eq. (1), produces just such a velocity. Close quantitative agreement between the DSMC method and simulation is not expected here, as the degree of gas rarefaction in this problem means that continuum fluid models are at the limit of their applicability.

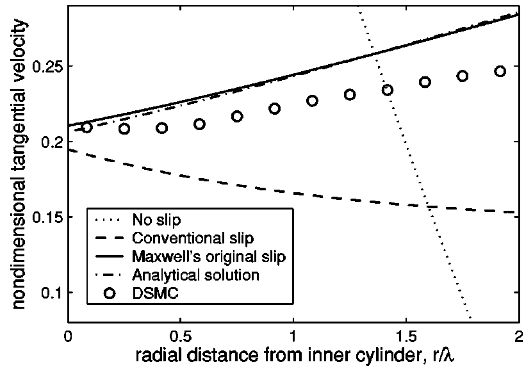

FIG. 1. Nondimensional velocity profiles in cylindrical Couette flow. Comparison of no slip (···), conventional slip (- -), Maxwell's general slip (—) solutions, an analytical solution [5] (· - ·), and DSMC data [6] (○).

B. Drag on an unconfined sphere

Isothermal slip flow past an unconfined sphere at very low Reynolds and Mach numbers was first analyzed by Basset [4] using Stokes' creeping flow approximation. The effect of slip was incorporated into the analysis using a velocity boundary condition for isothermal flows of an equivalent form to Maxwell's general boundary condition, Eq. (1). Basset's analysis showed that the skin friction drag D_s on an unconfined sphere of radius a, in a flow stream of velocity U, can be written as

$$D_s = 4\pi\mu U a^2\left(\frac{\sigma}{\sigma(a-3\lambda)+6\lambda}\right). \tag{4}$$

However, if the conventional form of Maxwell's boundary condition, Eq. (2), is used in the derivation, a different expression for the skin friction drag is obtained:

$$D_s = 4\pi\mu U a\left(\frac{\sigma(a+\lambda)-2\lambda}{\sigma(a-2\lambda)+4\lambda}\right). \tag{5}$$

The disparity between the two drag predictions is due to the exclusion of curvature effects from the conventional boundary condition. In the limiting case of a perfectly smooth sphere, such that all incident molecules are reflected specularly (σ=0), there is no means by which the wall can transfer tangential momentum to or from the gas. Therefore, the drag due to skin friction should be zero and, indeed, we find that Basset's drag equation predicts no skin friction. However, Eq. (5) predicts a finite value of *negative* skin friction drag (i.e., a thrust). This nonphysical prediction demonstrates the importance of employing the general, as opposed to the conventional, form of Maxwell's boundary condition for curved surfaces.

III. HIGHER-ORDER BOUNDARY CONDITIONS

In wall-dominated flows, such as those typical of microfluidics, the accuracy of the overall numerical solution is highly dependent on the accuracy of the boundary conditions. This sensitivity is such that several attempts have been made to derive boundary conditions of second or higher spatial order [8–13]. However, even for simple flows, there has been no general consensus as to the exact form these should take.

While there is no commitment made to the form of the shear stress tensor or heat flux vector in Maxwell's general condition, Eq. (1), normally the Navier-Stokes constitutive relations are assumed. This leads us to propose in this paper that, instead, higher-order constitutive relations (appropriate for high Knudsen number flows) are employed. These yield higher-order boundary conditions that will also be applicable to flows over three-dimensional nonstationary surfaces, unlike previous higher-order slip boundary conditions.

One such higher-order set of constitutive relations is the set of Burnett equations, derived from terms up to second order in a series solution in Knudsen number to the Boltzmann equation [14]. Although their complexity and nonlinearity makes them difficult to solve numerically [15], their assumed applicability to rarefied, high Knudsen number flows can be exploited within Maxwell's boundary condition without having to solve the tensor expressions over the entire flow field. In flows dominated by gas-surface interactions, there is also justification in adopting a more accurate model at the boundaries (Burnett) than the flow itself (Navier-Stokes).

The complete two-dimensional form of this equation is lengthy, so attention is restricted here to the linear higher-order terms only, which makes our present analysis applicable only to weak variations in flow variables (the full nonlinear forms of the Burnett stress tensor and heat flux vector are given in Ref. [14]). Substituting the Burnett constitutive relations into Eq. (1), linearizing, and again examining flows over general two-dimensional surfaces, we propose the "linearized Maxwell-Burnett boundary condition"

$$u_s = \frac{(2-\sigma)}{\sigma}\lambda\left(\frac{\partial u_x}{\partial n} + \frac{\partial u_n}{\partial x}\right) + \frac{3}{4}\frac{\mu}{\rho T}\frac{\partial T}{\partial x} + \frac{(2-\sigma)}{\sigma} \times\lambda\left(2\frac{\mu}{\rho^2}\frac{\partial^2 \rho}{\partial x \partial n} - \frac{\mu}{\rho T}\frac{\partial^2 T}{\partial x \partial n}\right) + \frac{3}{16\pi}\frac{N_{\mathrm{Pr}}(\gamma-1)}{\gamma} \times\lambda^2\left[(45\gamma-61)\frac{\partial^2 u_x}{\partial x^2} + (45\gamma-49)\frac{\partial^2 u_n}{\partial x \partial n} - 12\frac{\partial^2 u_x}{\partial n^2}\right], \tag{6}$$

which is formally second order in space. We now show the effect this form of the boundary condition has in two fundamental configurations.

A. Plane Poiseuille flow

For plane Poiseuille flow, second-order slip boundary conditions have the general form

$$u_s = A_1\lambda\frac{\partial u_x}{\partial n} - A_2\lambda^2\frac{\partial^2 u_x}{\partial n^2}. \tag{7}$$

As yet, no consensus has been reached on the correct value of the coefficient A_2 since, on the whole, theoretical predictions have compared poorly to experimental observations. It is, in any case, likely that both A_1 and A_2 are geometry dependent. In our proposed Maxwell-Burnett boundary condition, Eq. (6), the value of the coefficient in the $\lambda^2\partial^2 u_x/\partial n^2$ term is in the range 0.145–0.19, depending on the Prandtl number of the gas. Other theoretical predictions for this coefficient A_2 range from -0.5 to 1.43 [9–13]. Recent experimental work by Maurer *et al.* [16] indicates values of 0.26 ± 0.1 for nitrogen and 0.23 ± 0.1 for helium, although older work by Sreekanth [17] indicated 0.14 for nitrogen (from cylindrical Poiseuille flow experiments). Caution is required in interpreting these experimental data, as the values of A_2 are derived from measurements of mass flow rates. It is possible that the effect of near-wall Knudsen layers has resulted in a significant underestimation of the experimental value of A_2—from the calculations of Hadjiconstantinou, by as much as 0.3 [9].

B. Thermal-stress slip flow

Thermal-stress slip flow is a rarefaction phenomenon that was originally predicted by Sone [18]. Using an asymptotic analysis of the Boltzmann equation, he showed that a tangential variation in the wall-normal temperature gradient could induce velocity slip. This is distinct from thermal creep and cannot be captured by either the conventional slip equation, Eq. (2), or Maxwell's general boundary conditions using the Navier-Stokes expressions for the shear stress and heat flux terms.

Sone's configuration is a gas (initially stationary) between two stationary noncoaxial cylinders of different uniform temperature T_1 and T_2. In the absence of thermal creep (i.e., the boundary temperature jump is not considered) no conventional boundary condition has the mechanism to predict a slip flow. Sone, however, calculated the slip-flow field as shown by the streamlines and directional arrows in Fig. 2(a). The outer cylinder is held at a higher temperature and this generates a steady clockwise circulation in the gas (and anticlockwise when $T_1 > T_2$).

For a similar cylindrical configuration and using a finite-volume code to solve the Navier-Stokes equations with the linearized Maxwell-Burnett boundary condition, Eq. (6) (nonlinear effects are negligible as the temperature difference is small), we obtain the steady flow pattern shown in Fig. 2(b). It is clear that the phenomenon predicted by Sone is captured in our simulation due to the inclusion of our form of the boundary condition. Independent experimental verification is now needed.

For a stationary gas, Eq. (6) reduces to a single term

$$u_s = -\frac{(2-\sigma)}{\sigma}\lambda\left(\frac{\mu}{\rho T}\frac{\partial^2 T}{\partial x \partial n}\right). \tag{8}$$

It is this term that is responsible for initiating the thermal-stress slip flow in Fig. 2. Interestingly, Maxwell also pre-

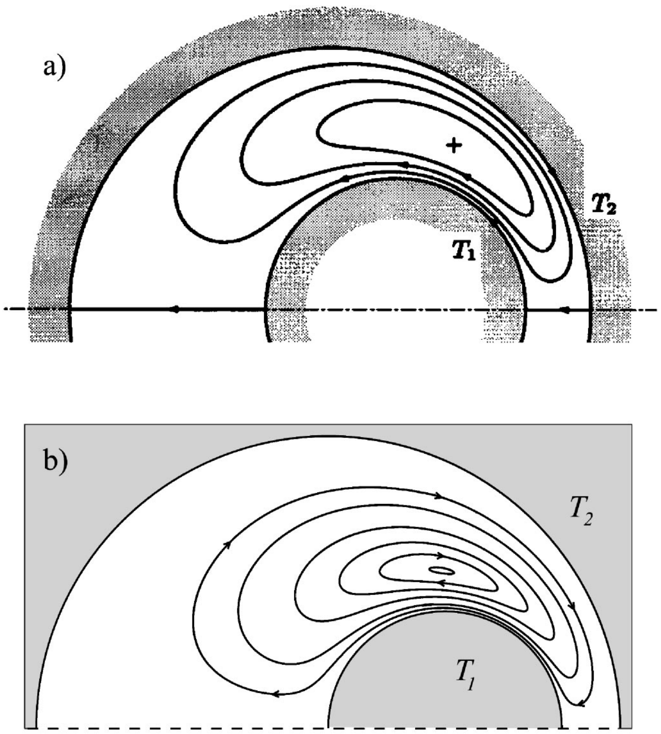

FIG. 2. Streamlines of thermal-stress slip flow between noncoaxial cylinders (uniform temperatures $T_2 > T_1$): (a) solution of the Boltzmann equation reproduced from [19], (b) finite-volume solution using the Maxwell-Burnett boundary condition.

dicted a second-order thermal shear stress in the main part of his paper [1] and a term of this form originally featured as part of the conventional boundary condition, Eq. (2). However, its presence has been forgotten over time, perhaps believed to be of negligible importance compared to first-order slip effects.

IV. DISCUSSION

The conventional form of Maxwell's slip boundary condition that has been passed down through successive research generations is not generally applicable to the boundaries typical of rarefied gas flows in complex geometries. If Maxwell's boundary condition is to be used, then care should be taken in adopting the full form of Maxwell's general equation (1), which relates tangential velocity slip to tangential shear stress and heat flux.

Compared to other higher-order boundary conditions derived from kinetic theory, the Maxwell-Burnett boundary condition we propose has the advantage of simplicity but also shows reasonable agreement with the limited experimental Poiseuille flow data available and can predict the phenomenon of thermal-stress slip flow. This boundary condition is straightforwardly applicable to three-dimensional moving surfaces and can also be used for diatomic gas molecules if appropriate changes are made to the Burnett coefficients.

ACKNOWLEDGMENTS

The authors are grateful to the U.K.'s Leverhulme Trust (Research Project Grant No. F/07040/G) and the Medical Research Council (MicroFAST programme, Grant. No. 57719) for supporting this research financially.

[1] J. C. Maxwell, Philos. Trans. R. Soc. London **170**, 231 (1879).
[2] M. Gad-el-Hak, ASME J. Fluids Eng. **121**, 5 (1999).
[3] K. Aoki, H. Yoshida, T. Nakanishi, and A. L. Garcia, Phys. Rev. E **68**, 016302 (2003).
[4] A. B. Basset, *A Treatise on Hydrodynamics* (Deighton, Bell and Co., Cambridge, England, 1888).
[5] D. Einzel, P. Panzer, and M. Liu, Phys. Rev. Lett. **64**, 2269 (1990).
[6] K. W. Tibbs, F. Baras, and A. L. Garcia, Phys. Rev. E **56**, 2282 (1997).
[7] J. M. Reese, M. Gallis, and D. A. Lockerby, Philos. Trans. R. Soc. London, Ser. A **361**, 2967 (2003).
[8] C. Cercignani, *Mathematical Methods in Kinetic Theory* (Plenum, New York, 1969).
[9] N. G. Hadjiconstantinou, Phys. Fluids **15**, 2352 (2003).
[10] G. E. Karniadakis and A. Beskok, *Micro Flows: Fundamentals and Simulation* (Springer, Berlin, 2002).
[11] H. Lang, Phys. Fluids **19**, 366 (1976).
[12] R. Deissler, Int. J. Heat Mass Transfer **7**, 681 (1964).
[13] R. Schamberg, Ph.D. thesis, California Institute of Technology, 1947.
[14] S. Chapman and T. G. Cowling, *The Mathematical Theory of Non-Uniform Gases*, 2nd ed. (Cambridge University Press, Cambridge, England, 1970).
[15] X. L. Zhong, R. W. MacCormack, and D. R. Chapman, AIAA J. **31**, 1036 (1993).
[16] J. Maurer, P. Tabeling, P. Joseph, and H. Willaime, Phys. Fluids **15**, 2613 (2003).
[17] A. Sreekanth, in *Proceedings of the Sixth International Symposium on Rarefied Gas Dynamics*, edited by L. Trilling and H. Y. Wachman (Academic Press, New York, 1969), p. 667.
[18] Y. Sone, Phys. Fluids **15**, 1418 (1972).
[19] Y. Sone, Annu. Rev. Fluid Mech. **32**, 779 (2000).