2008

A slip model for rarefied gas flows at arbitrary Knudsen number

Lin Wu
University of Nebraska-Lincoln, linwu@unlserve.unl.edu

A slip model for rarefied gas flows at arbitrary Knudsen number

Lin Wu[a)]
Department of Mechanical Engineering, University of Nebraska, Lincoln, Nebraska 68588, USA

(Received 16 October 2008; accepted 20 November 2008; published online 22 December 2008)

A slip model for wall bounded rarefied gas flows is derived from kinetic theory. A corresponding modified Reynolds lubrication equation is obtained from the slip velocity boundary conditions at walls for high Knudsen number gas flows. The slip model in a simplest form has predictions very close to the numerical solutions of linearized Boltzmann equation in the whole Knudsen number range, and is preferable to the widely applied 1st order (Maxwell slip model), 2nd order, and 1.5 order slip models. © *2008 American Institute of Physics*. [DOI: 10.1063/1.3052923]

At a length scale close to or below the mean free path of gas molecules, the nonslip boundary condition, which requires the average velocity of gas molecules directly adjacent to wall to be equal to wall velocity, is no longer valid. Instead, gas molecules slip at the solid wall. The slip boundary condition is critical for the accurate prediction of rarefied gas flows at micro-/nanoscale.

Widely applied slip models are the 1st order slip model (Maxwell slip model),[1,2] 2nd order slip model,[3] 1.5 order slip model,[4] and Fukui–Kaneko (FK) model.[5] The 1st order, 2nd order, and 1.5 order slip models are derived from kinetic theory by considering the momentum transfer rate of gas molecules impinging on the wall. The FK model is a database of direct numerical solutions of linearized Boltzmann equation.

The FK model is believed to be the most accurate available model due to its closer to first principles nature than other slip models. But the FK model database strongly depends on geometry and flow parameters, and consequently is not convenient to apply in practice. On the other hand, predictions of 1st order, 2nd order, and 1.5 order slip models are close to the FK model when the Knudsen number is small (for example, less than 1). The Knudsen number $K_n=\lambda/h$ is the ratio of molecular mean free path λ to a length scale h. As a result, the simplest 1st order, 2nd order, and 1.5 order slip models are still widely used in the study of diverse engineering applications.

Nevertheless, with the advance of micro-/nanotechnologies, the dimension of micro-/nanoscale devices is frequently pushed to the limit of significantly smaller than the mean free path of gas molecules, i.e., high Knudsen number gas flows. Typical examples are gas flows inside nanotubes, and air lubrication of head-disk interface of disk drives to mention just a few.

When the Knudsen number becomes greater than 1, the prediction of 1st order, 2nd order, and 1.5 order slip models starts to quickly deviate from the linearized Boltzmann solution. As a result, improved slip model that is not only convenient to apply but also offers reliable predictions at high Knudsen numbers is highly desirable. In this paper, we derive a much improved slip model from kinetic theory by incorporating more in-depth consideration of interaction physics between gas molecules and walls.

In the original derivations of the first order and second order slip models,[1–3] a length scale equal to the mean free path of gas molecules was used in a Taylor series expansion of the tangential bulk velocity $u(z)$ in a direction normal to the wall for all wall collision molecules. The slip velocity boundary condition at wall is obtained by substituting the bulk velocity expansion into the tangential momentum transfer rate of wall collision molecules, which is then matched to the local wall shear stress to yield

$$u_{\text{slip}}=\left(\frac{2-\alpha}{\alpha}\right)\lambda\frac{\partial u}{\partial z}-\frac{\lambda^2}{2}\frac{\partial^2 u}{\partial z^2}. \tag{1}$$

The accommodation coefficient α represents the portion of total wall-colliding molecules that are diffusively reflected back by wall and have a bulk velocity equal to the wall velocity U after collision. Rest molecules are reflected back specularly. Equation (1) is the second order slip model in literature.[3] The first order slip model (Maxwell slip model)[1,2] is obtained by dropping the second order derivative term on the right-hand side (RHS) of Eq. (1). The 1.5 order slip model has a factor of 2/9 instead of 1/2 in front of the second order derivative term.[4]

The coefficients of correction terms on the RHS of Eq. (1) depend on the length scale used to do Taylor series expansion of $u(z)$ in the normal direction z. The choice of expansion length scale to be the mean free path λ for all wall collision molecules is inaccurate to some extent.[1–3] This is especially true when the separation between two walls is smaller than the mean free path, i.e., when the Knudsen number is greater than 1.

In this paper, an improved slip model is derived using a somewhat more physical approach, in which the requirement that the expansion length scale be the mean free path for all wall collision molecules is relaxed. In this approach, we divide wall collision molecules into two separate groups (see Fig. 1). One group of molecules impinge on the wall at an

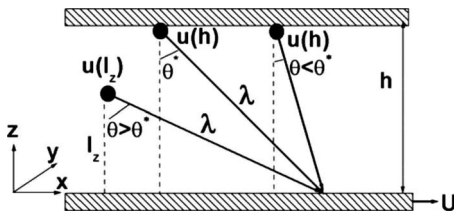

FIG. 1. Diagram of the gas flow system.

[a)]Electronic mail: linwu@unlserve.unl.edu.

angle θ to the surface normal greater than a critical angle $\theta^*=\cos^{-1}(\min[h/\lambda,1])$. The function $\min[a,b]$ yields the smaller value of the two variables a and b. The separation between two walls is denoted h. The rest molecules form the second group, which impinges on the wall at an angle θ less than θ^*.

From kinetic theory, gas molecules are expected to be incident on a wall from all directions. The impinging rate at an angle θ relative to the wall normal in a solid angle element $d\omega$ (see Fig. 1) is $n\bar{v}\cos\theta d\omega/4\pi$, where n is the number density of the molecules, and $\bar{v}$ is the mean molecular speed.[1] The solid angle element is $d\omega=\sin\theta d\theta d\varphi$, in which φ is the azimuthal angle.

For a shear flow, the bulk gas velocity $u(z)$ of molecules can only be changed through collisions with other molecules or wall. Consequently, the first group of molecules brings with them a bulk velocity $u(l_z)$ before wall collision when $\theta>\theta^*$. According to the definition of mean free path λ of collisions between molecules, we have $l_z=\lambda\cos\theta$. Due to the upper wall confinement, the second group of molecules with $\theta\leq\theta^*$ brings with them a bulk velocity $u(h)$ before wall collision (see Fig. 1).

Only the diffusively reflected back molecules contribute to a net tangential momentum transfer rate at wall. The total tangential momentum transfer rate at the wall is obtained by summing up the contributions from the two groups of impinging gas molecules and the reflected back molecules over the whole solid angle of a half plane

$$\begin{aligned}\tau &= \frac{1}{4\pi}\alpha mn\bar{v}\int_0^{2\pi}\int_{\theta^*}^{\pi/2} u(\lambda\cos\theta)\cos\theta\sin\theta d\theta d\varphi \\ &+ \frac{1}{4\pi}\alpha mn\bar{v}\int_0^{2\pi}\int_0^{\theta^*} u(h)\cos\theta\sin\theta d\theta d\varphi \\ &- \frac{1}{4\pi}\alpha mn\bar{v}\int_0^{2\pi}\int_0^{\pi/2} U\cos\theta\sin\theta d\theta d\varphi \\ &= \frac{1}{4}\alpha mn\bar{v}\left\{u(0)-U+\left[\frac{2}{3}\lambda\cos^3\theta^* + h(1-\cos^2\theta^*)\right]\right. \\ &\times\left.\frac{\partial u}{\partial z}\right|_{z=0} + \frac{1}{4}[\lambda^2\cos^4\theta^* + 2h^2(1-\cos^2\theta^*)] \\ &\times \left.\frac{\partial^2 u}{\partial z^2}\right|_{z=0}. \end{aligned} \quad (2)$$

The molecular mass is denoted m. The velocities $u(\lambda\cos\theta)$ and $u(h)$ can be obtained from a second order Taylor series expansion of velocity at wall $z=0$. The difference between bulk gas velocity at wall $u(0)$ and wall velocity U in Eq. (2) is the slip velocity $u_{\text{slip}}=u(0)-U$. Equation (2) is also valid when $h>\lambda$, which corresponds to $\theta^*=0$.

The net tangential momentum transfer rate of gas molecules at wall is equal to the wall shear stress $\tau=\mu\partial u/\partial z$. From kinetic theory, we have the dynamic viscosity $\mu=nm\bar{v}\lambda/2$.[1] Substitute the wall shear stress to the left-hand side of Eq. (2), we obtain a slip velocity boundary condition at wall $z=0$ as follows:

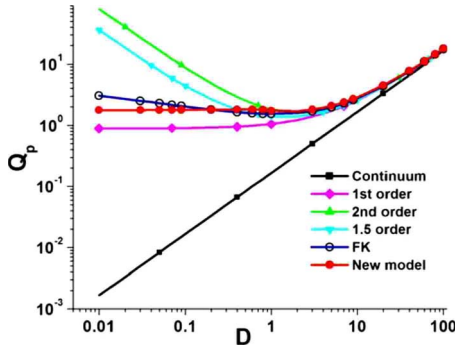

FIG. 2. (Color online) Comparison of the dimensionless flow rate.

$$\begin{aligned}u_{\text{slip}} &= \frac{2}{3}\left[\frac{(3-\alpha f^3)}{\alpha} - \frac{3}{2}\frac{(1-f^2)}{K_n}\right]\lambda\frac{\partial u}{\partial z} \\ &- \frac{1}{4}\left[f^4 + \frac{2}{K_n^2}(1-f^2)\right]\lambda^2\frac{\partial^2 u}{\partial z^2}, \end{aligned} \quad (3)$$

where $f=\min[1/K_n,1]$. Equation (3) is a slip velocity boundary condition suitable for gas flows at arbitrary Knudsen number.

For a two-dimensional lubrication geometry consisting of a stationary inclined top wall and a moving horizontal bottom wall, we can obtain a steady state modified Reynolds equation using slip boundary condition (3) for an isothermal layer of ideal gas

$$\Lambda_x\frac{\partial}{\partial X}(PH) = \frac{\partial}{\partial X}\left[\left(PH^3 + \beta K_{n0}H^2 + \gamma K_{n0}^2\frac{H}{P}\right)\frac{\partial P}{\partial X}\right], \quad (4)$$

where P and H are the dimensionless pressure and spacing normalized by the ambient pressure p_a and the smallest spacing h_0, respectively. The Knudsen number under ambient condition is denoted $K_{n0}=\lambda_0/h_0$, while λ_0 is the ambient mean free path. The bearing number in the x direction is $\Lambda_x=6\mu UL/(p_a h_0^2)$. The horizontal length scale is L. The dimensionless horizontal coordinate normalized by L is X. For the current model, the two model coefficients are $\beta=4[(3-\alpha f^3)/\alpha-3(1-f^2)P/(2K_{n0})]$ and $\gamma=3[f^4+2(1-f^2)P^2/K_{n0}]$ with $f=\min[P/K_{n0},1]$. The values of β and γ for other slip models are available in literature.[2–4,6]

To compare the performance of the newly derived slip model with other models, we first plot in Fig. 2 the dimensionless mass flow rates $Q_p=-\int_0^h\rho u dz\sqrt{2RT_0}/(h^2\partial p/\partial x)$ of the different models against the modified inverse Knudsen

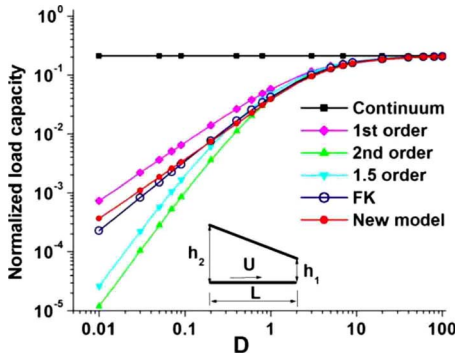

FIG. 3. (Color online) Comparison of the normalized load capacity of a two-dimensional gas lubrication geometry.

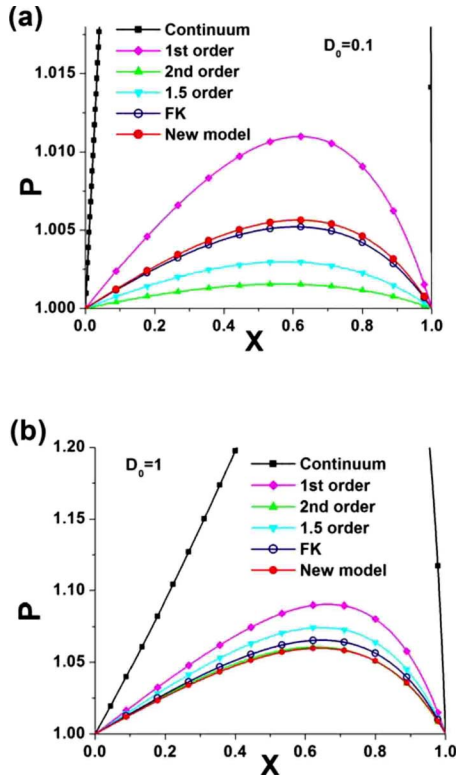

FIG. 4. (Color online) Comparison of the dimensionless pressure distributions of a two-dimensional gas lubrication geometry: (a) $D_0=0.1$ and (b) $D_0=1$.

number, while ρ is density, T_0 is temperature, and R is the gas constant. For the current model, we have

$$Q_p=\frac{D}{6}+\left[\frac{3-\alpha f^3}{\alpha}-\frac{3D}{\sqrt{\pi}}(1-f^2)\right]\frac{\sqrt{\pi}}{3}+\left[f^4+\frac{8D^2}{\pi}(1-f^2)\right]\frac{\pi}{8}\frac{1}{D}, \tag{5}$$

where $D=\sqrt{\pi}/(2K_n)$ is the modified inverse Knudsen number, and $f=\min[2D/\sqrt{\pi},1]$, respectively. The mass flow rates for other models are available from the listed references.[2–5] The figure shows that the current slip model predicts a mass flow rate very close to the FK model and in this sense outperforms other slip models in the whole modified inversed Knudsen number range. Slight divergence between the current model and the FK model is observed when the modified inversed Knudsen number is reduced below 0.02. It is previously known that the FK model does not have a correct asymptotic prediction when the modified inverse Knudsen number is reduced to zero, i.e., the FK model predicts an unphysical contact pressure singularity.[6] The current model has a higher than first order correction and it does not predict unphysical contact pressure singularity.

Figure 3 shows the normalized load capacity of a two-dimensional lubrication geometry as a function of the ambient modified inverse Knudsen number $D_0=\sqrt{\pi}h_1/(2\lambda_0)$. The system has a fixed gap ratio $h_2/h_1=2$ from the leading edge to the trailing edge, and has a fixed bearing number $\Lambda_x=10$. Figure 3 shows that the current slip model predicts a load capacity much more closer to the FK model than all other slip models in pretty much the whole Knudsen number range except at locations while other model curves intersect the FK model curve. The 1st order slip model (2nd order and 1.5 order slip models) significantly overpredicts (underpredicts) the load capacity when D_0 is below 1.

Figure 4 compares the predicted bearing pressures of the lubrication system shown in Fig. 3. Again, the current model predicts a pressure profile very close to the FK model at $D_0=0.1$ and $D_0=1$. The 1st order slip model (2nd order and 1.5 order slip models) overpredicts (underpredicts) the pressure with a difference small at $D_0=1$ and significant at $D_0=0.1$.

In conclusion, we derived an improved slip model from kinetic theory. The derived slip model in a simplest form has predictions very close to the numerical solutions of linearized Boltzmann equation in the whole Knudsen number range, and is preferable to the widely applied 1st order (Maxwell slip model), 2nd order, and 1.5 order slip models. The improved slip model does not suffer from the pressure singularity of the FK model at contact.

[1] E. H. Kennard, *Kinetic Theory of Gases* (McGraw-Hill, New York, 1938).
[2] A. Burgdorfer, ASME J. Basic Eng. **81**, 94 (1959).
[3] Y. T. Hsia and G. A. Domoto, ASME J. Lubr. Technol. **105**, 120 (1983).
[4] Y. Mitsuya, ASME J. Tribol. **115**, 289 (1993).
[5] S. Fukui and R. Kaneko, ASME J. Tribol. **112**, 78 (1990).
[6] L. Wu and D. B. Bogy, Phys. Fluids **13**, 2237 (2001).