Velocity Inversion In Cylindrical Couette Gas Flows

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Abstract. We investigate a power-law probability distribution function to describe the mean free path of rarefied gas molecules in non-planar geometries. A new curvature-dependent model is derived by taking into account the boundary-limiting effects on the molecular mean free path for surfaces with both convex and concave curvatures. In comparison to a planar wall, we find that the mean free path for a convex surface is higher at the wall and exhibits a sharper gradient within the Knudsen layer. In contrast, a concave wall exhibits a lower mean free path near the surface and the gradients in the Knudsen layer are shallower. The Navier-Stokes constitutive relations and velocity-slip boundary conditions are modified based on a power-law scaling to describe the mean free path, in accordance with the kinetic theory of gases, i.e. transport properties can be described in terms of the mean free path.

Velocity profiles for isothermal cylindrical Couette flow are obtained using the power-law model. We demonstrate that our model is more accurate than the classical slip solution, especially in the transition regime, and we are able to capture important non-linear trends associated with the non-equilibrium physics of the Knudsen layer. In addition, we establish a new criterion for the critical accommodation coefficient that leads to the non-intuitive phenomena of velocity-inversion. Our results are compared with conventional hydrodynamic models and direct simulation Monte Carlo data. The power-law model predicts that the critical accommodation coefficient is significantly lower than that calculated using the classical slip solution and is in good agreement with available DSMC data. Our proposed constitutive scaling for non-planar surfaces is based on simple physical arguments and can be readily implemented in conventional fluid dynamics codes for arbitrary geometric configurations.

1. Introduction

In rarefied/micro gas flows, the behavior of the gas near a solid boundary is dominated by surface and near-wall interactions and will lead to the formation of a Knudsen layer. This is a local thermodynamically non-equilibrium region of thickness $O(\lambda)$ from the surface, where $\lambda$ is the mean free path (MFP) of the gas. In this Knudsen layer, molecular collisions are considerably modified due to the presence of the solid boundary with a corresponding reduction in the mean time between collisions, i.e. the MFP of the gas will effectively be reduced and will also vary non-linearly in this thin layer [1]. Linear constitutive relations for shear stress and heat flux are also no longer valid in the Knudsen layer [2, 3, 4].

The behavior of a rarefied gas can accurately be described by the Boltzmann equation [5, 6]. However, directly solving the Boltzmann equation for practical applications remains
computationally challenging due to the complicated structure of the molecular collision term. The direct simulation Monte Carlo (DSMC) method [7] provides an excellent alternative approach for solving high-speed rarefied flows. Unfortunately, the computational cost of the DSMC method for low-speed flows in the slip- and transition-flow regimes is still also formidable. Many researchers developing engineering applications have instead proposed modifications to the velocity-slip boundary condition originally proposed by Maxwell [8]. This has generally led to first- and second-order treatments of the velocity gradient at the wall (see Beskok [9], Barber et al. [10] for a review), but with limited success because this approach fails to reproduce the non-linear stress/strain-rate relationship observed in the Knudsen layer.

An alternative strategy is to introduce a slip coefficient that depends on the Knudsen number or to introduce an effective viscosity term. The latter approach has met with some engineering success but has relied on fitting data to solutions from the Boltzmann equation. Cercignani [5] used kinetic theory to propose a “wall-function” that scaled with the mean free path. This introduces a function that complements the constitutive relations, effectively modifying the viscosity, and is able to capture some non-equilibrium behavior of the Knudsen layer. This idea has been adopted and extended [11, 12, 13] with some success.

Recently, Dongari et al. [14] carried out molecular dynamics (MD) studies of gases and the results indicate that molecules perform Levy-type flights under rarefied conditions, i.e. the free paths of gas molecules follow a power-law (PL) distribution. Consequently, they hypothesized that the probability distribution function for the molecular free paths of a rarefied gas followed a PL form, and this was validated against the MD data under various rarefied conditions. Using a PL distribution to describe free paths, Dongari et al. [15] derived an effective MFP model for flows confined by planar surfaces by taking into account the solid boundary effects and they obtained good agreement with the MD data up to the early transition regime. Further, they modified the Navier-Stokes constitutive relations using this PL-based MFP scaling and were then able to accurately capture the non-equilibrium effects in the Knudsen layer for isothermal pressure-driven gas flows between planar parallel walls.

A fundamental non-planar test case concerns the flow between two concentric cylinders. This is a classical no-slip fluid dynamics problem that is treated in many well-known textbooks [16]. However, under certain conditions, the flow between the cylinders can exhibit highly non-intuitive behavior. For example, if the outer cylinder is stationary and the inner cylinder is rotating, it is possible for the velocity profile to become inverted i.e. the velocity will increase from the inner to the outer cylinder wall. This unusual phenomenon was first predicted by Einzel et al. [17] for the case of liquid helium. Tibbs et al. [18] extended the analysis to the case of a rarefied gas and, using DSMC, demonstrated that velocity inversion could occur provided the tangential momentum accommodation coefficient (TMAC) for the surfaces was small. This early work has led to a number of important curvature studies for rotating Couette flow [10, 19, 20]. These confirmed the existence of velocity inversion for small values of the TMAC and also showed that the phenomenon could be related to a critical accommodation coefficient. Indeed, Yuhong et al. [20] derived an analytical criterion for the critical accommodation coefficient and also showed that velocity inversion was solely dependent on the value of the TMAC associated with the outer cylinder.

In this paper, we build on the approach of Dongari et al. [15] and derive a PL-based effective MFP model for non-planar surfaces by incorporating the effects of curvature. We develop a curvature-dependent MFP solution for both convex and concave surfaces, and extend this analysis to deduce the effective MFP solution for a gas confined between two concentric cylinders. Further, constitutive relations and velocity-slip boundary conditions are modified in accordance with the kinetic theory of gases, and tested for the classical case of isothermal rarefied Couette flow between two concentric rotating cylinders. Modified governing equations are solved for low-speed gas flows, and semi-analytical solutions are derived for velocity profiles and the critical
accommodation coefficient for velocity inversion. Our PL model results are compared with an existing slip model [20], the linearized BGK solution [19], and DSMC simulation data [18, 21]. We show that our PL model captures important non-linear trends associated with the physics of transition regime cylindrical Couette gas flows.

2. Geometry-Dependent Molecular Mean Free Path

We consider a homogeneous gas, where molecules moving at an average speed $\bar{v}$ and experiencing an inter-molecular collision rate of $\dot{\theta}_v$ have a molecular mean free path $\lambda = \bar{v}/\dot{\theta}_v$. Kinetic theory-based classical expressions for the probability distribution of the free paths and the mean free path ($\lambda$) are, respectively [22]:

$$\psi(r) = \frac{1}{\lambda} \exp\left(-\frac{|r|}{\lambda}\right),$$  

$$\lambda = \frac{m}{\pi \rho \delta^2 \sqrt{2}},$$

where $|r|$ is the length of free path, given by $\bar{v}t$, that has been traveled by a molecule at time $t$; $N_{Av} = 6.0221415 \times 10^{23}$ is Avogadro’s number; $m$ is the mass of a molecule; $\rho$ is the gas density, and $\delta$ is the hard-sphere diameter of the gas molecules.

MD results [14] show that the exponential distribution function for free paths (Eq. 1) is only valid when the gas is under thermodynamic equilibrium conditions. Under non-equilibrium conditions, the MD data exhibit long-tail behavior (i.e., molecules perform Lévy-type flights) whereas the exponential distribution has a faster decay. Montroll and Scher [23] pointed out that a finite moment of the probability distribution function implies an exponential character of the randomness. So results obtained using exponential forms of the distribution functions applicable only to homogeneous media at equilibrium. A distribution function with diverging higher-order moments (such as the standard deviation) is essential to describe non-equilibrium transport [23]. Instead of the classical exponential form of distribution function, Dongari et al. [14, 15] have recently hypothesized the following power-law form for the free path distribution function for non-equilibrium gas MFP, which satisfies the requirements for diverging higher-order moments:

$$\psi(r) = C(a + r)^{-n},$$

where $a$ and $C$ are constants with positive values that are determined through the zero and first moments. The range of values for the exponent $n$ can be obtained by making one of the higher-order moments divergent. Zero and first moments are given as follows:

$$1 = \int_0^\infty C(a + r)^{-n} dr,$$

$$\lambda = \int_0^\infty Br(a + r)^{-n} dr.$$  

Equation 4 requires the probability to range only from zero to one. Equation 5 defines the unconfined, conventional MFP value, $\lambda$. It then follows that

$$B = (n - 1)a^{n-1},$$

$$a = \lambda(n - 2).$$

To develop an expression for the effective mean free path, we use the approach of Dongari et al. [15], based on an integrated form of the probability distribution function, i.e.

$$p(r) = \int_0^r \psi(r) dr = \left[1 - \left(1 + \frac{r}{a}\right)^{1-n}\right].$$
where $p(r)$ describes the probability a molecule travels a distance $r$ with experiencing a collision.

The probability distribution function has to be real and positive and thus $a > 0$ and $n > 2$. As $n \to \infty$, the distribution function will have finite moments, which is the condition required of an equilibrium distribution function. For a finite $n$, the distribution function describes a system deviating from equilibrium. So $n$ acts as a decisive parameter to define the extent of the deviation from equilibrium. If one wishes to make the $i^{th}$ moment diverging, then $n_{\text{max}} = i + 1$.

In the current paper, all our power-law (PL) model based results have been obtained for $n = 3$, unless otherwise explicitly stated. Dongari et al. [14] validated the PL free path distribution function (Eq. 3) with MD simulations under various rarefied conditions.

Following a similar approach to that adopted by Dongari et al. [15], here, we derive an effective mean free path model for non-planar surfaces based on the PL form of free path distribution. Our model is derived for two generalized non-planar cases: (i) gas placed over a cylinder of radius $R_1$, i.e. a surface with convex curvature, and (ii) gas inside a cylinder of radius $R_2$, i.e a surface with concave curvature. Both convex and concave curvature models are then used to deduce an effective MFP model for gas confined between concentric cylinders.

Note that in the following discussion we use the notation $R^-$ if a test molecule is placed over a cylinder/surface with convex curvature, and $R^+$ if the molecule is placed inside the cylinder/surface with concave curvature. We also use the notations $\theta^-$ and $\theta^+$ for the equally probable zenith angle traveling direction of the molecule, towards convex and concave surfaces, respectively.

2.1. Gas placed outside a cylinder

Figure 1a presents the situation of a gas molecule placed outside a solid cylinder at a distance $r$ from the centre of the cylinder. The traveling distance limit for a molecule traveling towards the cylinder is denoted $R_u^-$, and this is associated with a critical limit for $\theta^-$ defined as $\theta_u^-$, above which the molecule passes the cylinder and travels into the bulk. This angle can be calculated by using the geometry of a formed right-angled triangle, with its right angle at the point connecting the radius of the cylinder, and $R_u^-$ which is tangential to the cylinder. The following relation can then be found:

$$ r^2 = R_1^2 + (R_u^-)^2. \quad (9) $$

By using the relation $R_1 = r \sin(\theta_u^-)$, the value of $\theta_u^-$ is obtained as:

$$ \theta_u^- = \arcsin \left( \frac{R_1}{r} \right). \quad (10) $$

The distance of the molecule away from the cylinder surface, $R^-$, as a function of $\theta^-$, can be determined in terms of $r$ and $R_1$ by using the cosine law:

$$ R_1^2 = r^2 + (R^-)^2 - 2rR^- \cos(\theta^-), \quad (11) $$

which results in:

$$ R^-(r, \theta^-) = r \cos(\theta^-) - \sqrt{\left( r \cos(\theta^-) \right)^2 + R_1^2 - r^2}. \quad (12) $$

The average distance a molecule travels to the cylinder’s surface, with respect to the angle $\theta^-$, is achieved by the following integral mean value theorem:

$$ \langle R^- \rangle = \frac{1}{\Omega} \int_0^\Omega R^-(r, \theta^-) d\theta^-, \quad (13) $$
Figure 1. (a) A gas molecule placed outside a solid cylinder and situated at a radial distance $r$ from the centre of the cylinder of radius $R_1$. $R^-$ is the travelling distance limit for a molecule moving towards the cylinder surface, for a given zenith angle $\theta^-$. The largest travelling distance $R_u^-$ is achieved for the zenith angle direction $\theta_u^-$, above which the molecule by-passes the cylinder surface and travels into the bulk. (b) A gas molecule inside a cylindrical cavity of radius $R_2$, at a wall normal distance of $R_2 - r$, where $r$ is the radial distance of the molecule from the centre of the cylinder. The molecule has a traveling distance of $R^+$ to the wall for a traveling direction of $\theta^+$, where $\theta^+$ is varied from 0 to $\pi$.

where $\Omega$ is the solid angle subtended by the cylinder at a point in the base plane, at a distance $r$ ($> R_1$) from the axis of the cylinder of length $L$, and which can be expressed as [24]:

$$\Omega = \theta_u^- - \frac{1}{2} \left[ \left( \frac{r}{R_1} \right)^2 - 1 \right]^{\frac{1}{2}} + \theta_u^- - \frac{\pi}{2} \right] L^{-2} + O \left( L^{-4} \right). \tag{14}$$

If we consider the length of the cylinder $L$ tending to infinity, $\Omega$ then can be simplified to:

$$\Omega = \theta_u^-.$$ \tag{15}

Using Eq. 8, the mean free path of the molecules traveling in the direction of the cylinder (a surface with convex curvature) is then,

$$\lambda_{\text{eff(\text{conv})}} = \lambda \left[ 1 - \frac{1}{\theta_u^-} \int_0^{\theta_u^-} \left( 1 + \frac{R^-(r, \theta^-)}{a} \right)^{\frac{1-n}{n}} d\theta^- \right]. \tag{16}$$
Figure 2. Variation of the effective mean free path of gas molecules outside a solid cylinder (surface with a convex curvature) as a function of normalized wall normal distance \([r − R_1]/\lambda\). Here \(r \geq R_1\), as the gas is placed outside a cylinder and on the x-axis, \(r\) is varied by fixing \(R_1\) and \(\lambda\), for a given value of \(b_1\). The MFP profiles for various values of \(b_1\) \((R_1/\lambda)\) are illustrated to show the effect of the convex curvature and their comparison with the planar one-wall solution [15].

The general mean free path expression is obtained by considering all possible molecular traveling directions. This is achieved in a similar manner to the analysis for a gas confined between planar parallel walls presented in Dongari et al. [15]. In the case of planar parallel walls, it is equally probable that a molecule travels towards one surface or the other. In the present case, solid angle theory is used to determine the likelihood of a molecule traveling in the direction of the cylinder, as opposed to traveling towards the bulk; the probabilities being expressed as \(\theta_u/\pi\) and \([1 − (\theta_u/\pi)]\), respectively. From this weighting, the general expression for the effective mean free path of a gas placed outside a cylinder is:

\[
\lambda_{\text{eff}(o)} = \lambda_{\text{eff( conv)}} \left(\frac{\theta_u}{\pi}\right) + \lambda \left[1 − \left(\frac{\theta_u}{\pi}\right)\right],
\]

(17)

where \(\lambda\) is the unconfined gas mean free path. This equation can also be written as \(\lambda_{\text{eff}(o)} = \lambda \beta_{(o)}(r, R_1/\lambda)\), where

\[
\beta_{(o)} = \left(\frac{\theta_u}{\pi}\right) \left[1 − \frac{1}{\theta_u} \int_{\theta_u}^{\theta_u} \left(1 + \frac{R^−(r, \theta_−)}{a}\right)^{(1−n)} d\theta_−\right] + \left[1 − \left(\frac{\theta_u}{\pi}\right)\right],
\]

(18)

which is the normalized effective MFP based on a power-law distribution function, where the subscript \((o)\) denotes our considerations of gas molecules outside a solid cylindrical surface. Eq. 18 is dependent on \(r\), \(R_1\) and \(\lambda\), and evaluated as a function of normalized wall normal distance \([(r − R_1)/\lambda]\), using the parameter \(b_1 = R_1/\lambda\). It should be noted that \(a\) is dependent on the mean free path (see Eq. 4) and \(r \geq R_1\), as the gas is placed outside a cylinder. The parameter \(b_1\) denotes the inverse of the normalized curvature and as \(b_1 → \infty\), the solution of Eq. 18 should reduce to the planar case. Eq. 18 can be computed numerically using Simpson’s rule, here we use 16 subintervals.

The solution of the effective mean free path for a convex surface must reduce to that for a planar one-wall case when the radius of the cylinder tends to infinity. To verify this limiting case, the normalized effective MFP solutions (i.e. \(\beta_{(o)}\)) based on Eq. 18, are plotted in Fig. 2 for
various values of $b_1$ and are compared with the planar one-wall solution derived by Dongari et al. [15]. For a value of $b_1 = 3$, the non-planar solution predicts a higher $\beta$ value at the surface and also exhibits sharper gradient compared to the planar one-wall case. Fig. 2, shows that as the radius $R_1$ of the cylinder increases, our non-planar solution tends to the planar one.

2.2. Gas inside a hollow cylinder

Using a similar approach, it is possible to obtain the effective mean free path for gas molecules inside a hollow cylinder of radius $R_2$, i.e. for a surface with a concave curvature. As illustrated in Fig. (1b), $r$ is a target molecule’s radial distance from the centre of the cylinder and $R^+$ is the molecule’s distance to the wall if the molecule has a traveling trajectory of $\theta^+$. To calculate the effective mean free path, the wall distance of the molecule has first to be calculated using the cosine law:

$$R_2^2 = r^2 + (R^+)^2 - 2rrR^+\cos(\theta^+), \quad (19)$$

where the molecule’s traveling trajectory $\theta^+$ can vary from 0 to $\pi$. The molecular traveling distance to the wall $R^+$, dependent on $r$ and $\theta^+$, can then be expressed as:

$$R^+(r, \theta^+) = -r\cos(\theta^+) + \sqrt{(r\cos(\theta^+))^2 + R_2^2 - r^2}. \quad (20)$$

The solid angle subtended by the cylinder at a point lying inside the cylinder is $2\pi$. Based on the quarter symmetry, it is sufficient to integrate $\theta^+$ from 0 to $\pi/2$. Using our PL distribution to describe the molecular free paths (Eq. 8), the expression for the effective mean free path of a gas molecule inside a cylinder (i.e. interacting with a surface with concave curvature) is:

$$\lambda_{\text{eff(conc)}} = \lambda \left[ 1 - \frac{2}{\pi} \int_0^{\pi/2} \left( 1 + \frac{R^+(r, \theta^+)}{a} \right)^{(1-n)} d\theta^+ \right], \quad (21)$$

or the normalized expression is:

$$\beta(i) = \frac{\lambda_{\text{eff(conc)}}}{\lambda}, \quad (22)$$

where the subscript $(i)$ denotes that the gas molecules are located inside the cylinder. Eq. 22 is dependent on $r$, $R_2$ and $\lambda$, and evaluated as a function of normalized wall normal distance $[(R_2 - r)/\lambda]$, using the parameter $b_2 = R_2/\lambda$. Here $r \leq R_2$, as the gas is inside the cylinder.

In a similar manner to the convex case, the effective MFP solution for a concave surface must also reduce to the planar one-wall case when the radius of the cylinder tends to infinity. Fig. 3 shows the variation of the normalized effective mean free path $\beta(i)$, for various $b_2$ values and a comparison with the planar one-wall solution [15]. For a value of $b_2 = 5$, the non-planar solution predicts a lower $\beta$ value at the surface and exhibits a shallower gradient compared to the planar case. For higher values of $b_2$, the non-planar concave solution approaches the planar case. However, at the surface, even for $b_2 = 30$, the non-planar solution predicts a lower value of $\beta(i) \sim 0.4691$ compared to the corresponding planar wall value of 0.5. This is due to the concave nature of the surface, where a molecule will encounter more frequent collisions with the wall before it escapes from the concave well.
Figure 3. Variation of the effective mean free path of a gas molecule inside a cylinder (i.e., a bounding surface with concave curvature) as a function of normalized wall normal distance \([(R_2 - r)/\lambda]\). Here \(r \leq R_2\), as the gas is placed outside a cylinder and on the \(x\)-axis, \(r\) is varied by fixing \(R_2\) and \(\lambda\), for a given value of \(b_2\). The MFP profiles for various values of \(b_2\) \((R_2/\lambda)\) are illustrated to show the effect of the concave curvature and their comparison with the planar one-wall solution [15].

2.3. Gas confined between concentric cylinders

We now consider a gas between two concentric cylinders, with \(R_1\) and \(R_2\) being the radii of the inner and outer cylinders, respectively. Let us consider a molecule situated at a distance \(r\) from the coincident centres of the two cylinders. The inner cylinder presents a surface with convex curvature (Fig. 1a) to the molecule and the outer cylinder presents a surface with a concave curvature (Fig. 1b). The probability of a molecule traveling towards the inner and outer cylinder directions can be evaluated as \(\theta^-_u/\pi\) and \([1 - (\theta^-_u/\pi)]\), respectively. Using Eqs. 16 and 21 and accounting for this weighting, the complete expression for the effective mean free path of a gas confined between two concentric cylinders is:

\[
\lambda_{\text{eff}} = \lambda_{\text{eff(\text{conv})}} \left(\frac{\theta^-_u}{\pi}\right) + \lambda_{\text{eff(\text{conc})}} \left[1 - \left(\frac{\theta^-_u}{\pi}\right)\right],
\]

where \(\lambda_{\text{eff}} = \lambda \beta\), and so

\[
\beta = \left(\frac{\theta^-_u}{\pi}\right) \left[1 - \frac{1}{\theta^-_u} \int_{\theta^-_u}^{\pi/2} \left(1 + \frac{R^-(r, \theta^-)}{a}\right)^{(1-n)} d\theta^- \right] + \left[1 - \left(\frac{\theta^-_u}{\pi}\right)\right] \left[1 - \frac{1}{\theta^+_u} \int_{0}^{\theta^+_u} \left(1 + \frac{R^+(r, \theta^+)}{a}\right)^{(1-n)} d\theta^+ \right],
\]

with

\[
\theta^+_u = \pi - \theta^-_u.
\]

Here, \(\beta\) is the normalized geometry-dependent MFP based on a power-law distribution function, and is dependent on the Knudsen number \(Kn\) through the mean free path, \(\lambda\) and a geometry constraint \(R_2/R_1\), defining \(Kn\) as:

\[
Kn = \frac{\lambda}{R_2 - R_1}.
\]
Figure 4. (a) Variation of $\beta$ with normalized radial distance $(r - R_1)/(R_2 - R_1)$ between the inner and outer cylinders for various Knudsen numbers in the slip and transition regimes, for the case of $R_2/R_1 = 5/3$. (b) Illustration of the curvature effects through the ratio of the normalized MFP values of gas confined between non-planar (NP) and planar (P) surfaces. The non-planar solution is obtained from Eq. 24 and the planar-surface values are computed using Equation 12 in Dongari et al. [15].

Figure (4a) shows the variation of $\beta$ between inner and outer cylinders (with $R_2/R_1 = 5/3$) for various Knudsen numbers in the slip and early transition regimes. The MFP profiles are sharper at the inner cylinder and shallower at the outer cylinder and they are not symmetric about the midpoint of the gap between the cylinders. This finding is in contrast to the solution for the planar parallel wall case, where the MFP profile is symmetric about the midpoint of the gap between the surfaces [15]. The anti-symmetric effect increases with Knudsen number. The values of $\beta$ are relatively high at the inner cylinder surface compared to the outer cylinder, due to the convex and concave curvature effects, respectively. The difference in the values of $\beta$ at the inner and outer cylinders is also dependent on the Knudsen number.

To illustrate further the curvature effects, Fig. (4b) presents the ratio of the normalized effective MFPs non-planar to planar. Non-planar $\beta_{NP}$ values are obtained from Eq. (24) for $R_2/R_1 = 5/3$ and $\beta_P$ for the case of planar parallel walls is evaluated using Equation 12 in Dongari et al. [15]. For $Kn = 0.01$, the curvature effects are negligible, except in a thin layer close to the outer cylinder surface. As the Knudsen number increases, both the curvature and
anti-symmetric effects become more pronounced, whereas the difference in the values of \( \beta \) at the inner and outer cylinders decreased. The ratio \( \beta_{NP}/\beta_{P} \) has its minimum at the outer cylinder for all \( Kn \) and its maximum at a position close to the surface of the inner-cylinder. However, this point moves away from the inner cylinder with increase in \( Kn \), as the thickness of the Knudsen-layer increases.

3. Cylindrical Couette Flow

3.1. Problem description, governing equations and results

To test the merits of our PL-based effective MFP scaling for non-planar cases, we consider a rarefied gas confined between two concentric rotating cylinders. The flow is assumed to be fully developed, two-dimensional, isothermal, laminar and steady, with a low Reynolds number (\( Re \)) so that inertial effects may be neglected.

With these assumptions, the governing flow equation in polar coordinates is

\[
\frac{1}{r^2} \frac{d}{dr} \left( r^2 \tau_{r\phi} \right) = 0,
\]

where \( r \) is the radial coordinate, \( \phi \) the tangential coordinate and \( \tau_{r\phi} \) the stress, which is defined as:

\[
\tau_{r\phi} = \mu \left( \frac{du_\phi}{dr} - \frac{u_\phi}{r} \right),
\]

where \( \mu \) is the fluid dynamic viscosity and \( u_\phi \) is the velocity of the fluid in the tangential direction.

From the kinetic theory of gases, the fluid viscosity can be explained in terms of the collisions between gas molecules, and of the free paths which the molecules describe between collisions. The unconfined MFP is then related to the shear viscosity [5]:

\[
\mu = \rho \frac{\lambda}{\sqrt{\pi/2RT}},
\]

where \( \rho \) is the gas density, \( R \) the specific gas constant and \( T \) the gas temperature.

Equation (29) is assumed to be valid only for flows that are quasi-equilibrium. Within the Knudsen layer the flight paths of gas molecules are affected by the presence of a solid wall. If we wish to use Eq. (29), we need to take into account the MFP affected by gas molecular collisions with surfaces. If the unconfined expression for the MFP, \( \lambda \), is replaced by our effective and geometry-dependent mean free path, \( \lambda_{eff} \) (Eqs. 23 and 24), we obtain a non-constant, geometry-dependent, effective viscosity, \( \mu_{eff}(PL) \), that can then be used to deduce a non-linear stress/strain-rate relation:

\[
\tau_{r\phi} = \mu_{eff} \left( \frac{du_\phi}{dr} - \frac{u_\phi}{r} \right).
\]

Substituting Eq. (30) into Eq. (27) results in the modified governing equation:

\[
\frac{\mu}{r^2} \frac{d}{dr} \left[ r^2 \beta \left( \frac{du_\phi}{dr} - \frac{u_\phi}{r} \right) \right] = 0.
\]

This needs to be solved in conjunction with the following slip boundary conditions at the inner and outer cylinder surfaces, respectively:
\begin{align}
  u_\phi |_{r=R_1} &= \omega_1 R_1 + \frac{2 - \sigma_1}{\sigma_1} \lambda \left[ \beta \left( \frac{du_\phi}{dr} - \frac{u_\phi}{r} \right) \right] |_{r=R_1}, \\
  u_\phi |_{r=R_2} &= \omega_2 R_2 - \frac{2 - \sigma_2}{\sigma_2} \lambda \left[ \beta \left( \frac{du_\phi}{dr} - \frac{u_\phi}{r} \right) \right] |_{r=R_2},
\end{align}

where \( \omega_1 \) and \( \omega_2 \) are the angular velocities and \( \sigma_1 \) and \( \sigma_2 \) are the tangential moment accommodation coefficients of inner and outer cylinders, respectively.

The solution for the velocity profile can then be obtained as:

\[ u_\phi(r) = r \left[ \omega_1 + \frac{\alpha_1 \lambda C}{R_1^3} + G(r)C \right], \tag{34} \]

where

\[
G(r) = \int_{R_1}^{r} \frac{dr}{r^3 \beta_{PL}},
\]

\[
C = \frac{\omega_2 - \omega_1}{H + \frac{\alpha_1 \lambda}{R_1^3} + \frac{\alpha_2 \lambda}{R_2^3}},
\]

\[
H = \int_{R_1}^{R_2} \frac{dr}{r^3 \beta_{PL}}.
\]

When the effects of the Knudsen layer are neglected, i.e. the mean free path has no geometry dependence, then Eq. (34) simply reduces to the velocity profile based on the classical slip solution, as presented in Equation (6) of Yuhong et al. [20]. Normalized velocity profiles \( U^* = u_\phi/\omega_1 R_1 \) are presented in Fig. 5) for the case of \( Kn = 0.5 \), a stationary outer cylinder \( (\omega_2 = 0) \), \( R_2/R_1 = 5/3 \), and various combinations of accommodation coefficients.

To illustrate the phenomenon of velocity profile inversion, the outer cylinder is stationary \( (\omega_2 = 0) \) and the inner cylinder is rotating. The radii of the inner and outer cylinders are chosen to be \( 3\lambda \) and \( 5\lambda \), respectively, and the accommodation coefficients are assumed to be equal at the inner and outer cylinder surfaces \( (\sigma_1 = \sigma_2 = \sigma) \). Figure. (5a) presents a comparison between our solution based on the PL effective MFP (Eq. 34) and the DSMC data reported by Tibbs et al. [18]. The PL model is in very good quantitative agreement with the DSMC results for the \( \sigma = 1.0 \) and 0.7 cases. The results show that the DSMC data and PL formulation follow the same basic trends and predict an inverted velocity profile when the accommodation coefficient is 0.1. However, slight deviations are discernible at the surface of the outer cylinder for the \( \sigma = 0.4 \) and 0.1 cases.

It is interesting to note that, for the specific case of the accommodation coefficients of the inner and outer cylinders having the same value, the family of velocity profiles all pass through a common point that is independent of the value of the accommodation coefficient. This intersection point in the PL profiles is fairly close to the point predicted by DSMC data, whereas the classical slip solution predicts this point closer to the outer cylinder, see Fig. 5b. This figure presents the results based on the classical governing equation together with the conventional slip boundary conditions, i.e. without considering any Knudsen layer effects (see Equation 6 in Yuhong et al. [20]), alongside the PL model results. It is evident that the classical slip solution fails to capture non-linear effects associated within the Knudsen layers at the inner and outer cylinders. The discrepancies are greatest at \( \sigma = 1.0 \), although at lower values of \( \sigma \) the discrepancies are smaller. At smaller values of \( \sigma \), the PL and classical slip solution are identical and yield the same solid body rotation solution when \( \sigma = 0 \).
3.2. Critical accommodation coefficients

In this section, we identify limiting analytical criterion for critical accommodation coefficients that produce (i) normal, (ii) fully-inverted, and (iii) partially-inverted velocity profiles. A normal (non-inverted) velocity profile occurs when the tangential velocity decreases monotonically from the inner to the outer cylinder. In contrast, a fully-inverted case occurs when the velocity monotonically increases. Finally, a partially-inverted profile occurs when there is a decrease and increase at multiple locations between the inner and outer cylinders.

The velocity profile is given in Eq. (34); the gradient of this can be used as a criterion to judge whether the function is monotonically decreasing or increasing. After some simplifications, the velocity gradient for the case of a rotating inner cylinder and stationary outer cylinder can be expressed as:

$$
\frac{du_\phi}{dr} = \omega_1 \left[ 1 - \frac{1}{H + \frac{\alpha_1 \lambda}{R_1^4} + \frac{\alpha_2 \lambda}{R_2^4}} \left( \frac{\alpha_1 \lambda}{R_1^4} + G(r) + \frac{1}{r^2 \beta_{PL}} \right) \right].
$$

(38)

If $du_\phi/dr > 0$ a fully inverted velocity profile exists, and this is only satisfied when:
\[
\frac{\left(\frac{1}{R_1^2} + G(r) + \frac{1}{r^2 \beta_{PL}}\right)}{H + \frac{1}{R_1^2} + \frac{1}{R_2^2}} < 1, \tag{39}
\]

which can only hold throughout the annular clearance \((R_1 \leq r \leq R_2)\), when \(G(r) + 1/(r^2 \beta_{PL})\) is at its maximum value, which occurs at \(r = R_1\). Using this condition, the criterion for the critical accommodation coefficient for a fully inverted velocity profile (i.e. positive velocity gradient) can be expressed as:

\[
(\sigma_a)_P = 2 \left[ 1 + \frac{R_3^3}{R_1^3 \beta_{PL} \lambda} - \frac{R_3^3}{\lambda} \right]^{-1}. \tag{40}
\]

Equation 40 provides an upper bound, so for \(\sigma_a < (\sigma_a)_P\) a fully inverted velocity will always occur, and this phenomenon is independent of the value of the accommodation coefficient at the inner cylinder. In the absence of any Knudsen layer in the flow, i.e. a constant mean free path between the inner and outer cylinders, Eq. 40 simply reduces to the classical slip solution presented in Equation 17 of Yuhong et al. [20].

From Eq. 38, if \(du/\phi/dr < 0\) the velocity will be a decreasing function of \(r\) and no inverted velocity profile will be observed. This situation can only exist when:

\[
\frac{\left(\frac{1}{R_1^2} + G(r) + \frac{1}{r^2 \beta_{PL}}\right)}{H + \frac{1}{R_1^2} + \frac{1}{R_2^2}} > 1, \tag{41}
\]

which can only hold throughout the annular clearance \((R_1 \leq r \leq R_2)\), when \(G(r) + 1/(r^2 \beta_{PL})\) is at its minimum value, which occurs for \(r = r_c\) \((R_1 < r_c < R_2)\). The value of \(r_c\) can be obtained numerically for a given \(Kn\) and \(R_2/R_1\) and then the critical accommodation coefficient for no velocity inversion (i.e. negative velocity gradient) follows as:

\[
(\sigma_a)_N = 2 \left[ 1 + \frac{R_3^3}{R_2^3 \beta_{PL} (r_c) \lambda} - \frac{R_3^3}{\lambda} (G(r_c) - H) \right]^{-1}. \tag{42}
\]

Equation (42) provides a lower bound, so for \(\sigma_a > (\sigma_a)_N\) no inverted velocity profile will occur and this phenomenon is also independent of the value of the accommodation coefficient at the inner cylinder, as in the case above. When there is no mean free path variation between the inner and outer cylinders, Eq. 42 also reduces to the corresponding classical slip solution, (see Equation 19 of Yuhong et al. [20]).

Considering these two cases of Eqs. 40 and 42, where the velocity is monotonically decreasing or increasing, it is evident that a partially-inverted velocity profile will occur when the accommodation coefficient at the outer cylinder lies within the range:

\[
(\sigma_a)_P < \sigma_a < (\sigma_a)_N. \tag{43}
\]

This also does not depend on the accommodation coefficient of the inner cylinder.

Figure 6a presents the variation of the critical accommodation coefficient \((\sigma_a)_N\) as a function of Knudsen number for the case of no velocity inversion. Our PL model results are compared with DSMC data [21], the classical slip solution (Equation 19 of Yuhong et al. [20]) and the linearized BGK model [19], in the flow regime of \(0 < Kn < 1\). In the continuum regime \((Kn < 0.01)\), all three theoretical models converge to similar values. In the slip flow regime \((0.01 < Kn < 0.1)\), the PL model lies below the classical slip solution and the BGK model. The PL model results show very good quantitative agreement with the DSMC data in the early transition regime \((0.1 < Kn < 0.5)\), whereas the other two models show significant deviations. Although DSMC
Figure 6. Variation of critical accommodation coefficient with Knudsen number for the geometric configuration of $R_2/R_1 = 5/3$: (a) $(\sigma_2)_N$ the lower bound for no velocity inversion, i.e. negative velocity gradient throughout the annular clearance ($R_1 < r < R_2$); (b) $(\sigma_2)_P$ the upper bound for full velocity inversion, i.e. positive velocity gradient throughout the annular clearance.

data is not available beyond $Kn > 0.5$, by extrapolating the trend up to $Kn = 0.5$, the PL model may slightly overpredict $(\sigma_2)_N$ in the later part of the transition regime. In the free-molecular regime, the PL model asymptotically reaches a constant value ($\sim 0.7$) and both the classical slip solution and the BGK model diverge (not shown in Fig. 6a).

Figure 6b shows the variation of the critical accommodation coefficient of fully inverted velocity $(\sigma_2)_P$, as a function of Knudsen number. Our PL model results are compared with the classical slip solution (Equation 17 of Yuhong et al. [20]) from the slip to the free-molecular regime ($0.01 < Kn < 10$), although the continuum fluid assumptions are highly questionable for $Kn > 1$. The classical slip solution significantly overpredicts the PL model in the transition regime and beyond. For $Kn >> 1$, the slip solution indeed shows a diverging and unphysical behavior with $(\sigma_2)_P$ values greater than unity. Conversely our PL model reaches a constant value for accommodation coefficient of $\sim 0.3$.

4. Conclusions

The non-equilibrium flow physics of rarefied gases interacting with non-planar surfaces has been described using a power-law (PL) probability distribution function for the free-paths of the gas molecules. We have developed new geometry-dependent mean free path solutions for both convex and concave surfaces that take into account the termination of the free paths of gas molecules at the curved surfaces. Subsequently an hypothetical constitutive scaling approach to model the Knudsen layer within a conventional continuum fluid dynamics framework has been proposed, in accordance with the kinetic theory of gases. This has been tested for the case of isothermal rarefied Couette flow between two concentric rotating cylinders.

The gas velocity profiles show good agreement with DSMC simulation data in the transition regime for various values of the accommodation coefficients of the inner and outer cylinder surfaces. When the accommodation coefficients of the inner and outer cylinders have the same value, the family of velocity profiles all pass through a common point. This intersection point for our PL model is very close to the point predicted by the DSMC data, whereas the classical slip solution predicts this point much closer to the outer cylinder. New analytical criteria have been developed for the critical accommodation coefficients for non-inverted, fully inverted and partially inverted velocity profiles. The PL model shows excellent agreement with the DSMC data for these, too.
Our new PL model is more accurate than conventional continuum fluid solutions in capturing the non-linear effects associated with Knudsen layers in the slip and transition flow regimes. With the current approach we can also model the velocity profile at a fixed Knudsen number by modifying the power-law exponent, to provide accurate results in both the Knudsen layer and bulk flow. Whereas using the conventional slip modeling technique we can only modify the slip velocity at the surface by tuning the value of the slip coefficient. This PL mean free path scaling can be readily extended to more complex geometries and straightforwardly incorporated into existing CFD codes to solve for low-speed rarefied gas flows in arbitrary geometries.

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References
[1] Stops D W 1970 J. Phys. D Appl. Phys. 3 685
[2] Burnett D 1935 Proc. Lond. Math. Soc. 40 382
[3] Grad H 1949 Comm. on Pure and App. Math. 2 325
[4] Chapman S and Cowling T G 1970 Mathematical theory of non-uniform gases (Cambridge University press)
[5] Cercignani C 1988 The Boltzmann Equation and its Applications (Springer-Verlag, New York)
[6] Sone Y 2002 Kinetic theory and fluid dynamics (Birkhauser, Boston)
[7] Bird G A 1994 Molecular gas dynamics and the direct simulation of gas flows (Oxford University Press, New York)
[8] Maxwell J C 1879 Philos. Trans. R. Soc. 1 170 231
[9] Beskok A 2001 Numerical Heat Trans. Part B: Fund. 40(6) 451
[10] Barber R W et al. 2004 Vacuum 76 73
[11] Lockerby D A and Reese J M 2008 J. Fluid Mech. 604 235
[12] Lilley C R and Sader J E 2007 Phys. Rev. E. 76 026315
[13] Guo Z L et al. 2007 Euro. Phys. Lett. 80 24001
[14] Dongari N et al. 2011 J. Phys. D. App. Phys. 44 125502
[15] Dongari N et al. 2011 J. Fluid. Engg. 133(7) 071101
[16] Schlichting H 1979 Boundary-layer theory (7th ed. McGraw-Hill, New York)
[17] Einzel D et al. 1990 Phys. Rev. Lett. 64 2269
[18] Tibbs K W et al. 1997 Phys. Rev. E 56 2282
[19] Aoki K et al. 2003 Phys. Rev. E 68 016302
[20] Yuhong S et al. 2005 Phys. Fluids 17 047102
[21] Stefanov S K et al. 2007 Proc. 25th Int. Symp. on Rarefied Gas Dynamics 1146
[22] Kennard, E. H., 1938, Kinetic Theory of Gases with an Introduction to Statistical Mechanics, McGraw-Hill, New York.
[23] Montroll E W and Scher H 1973 J. Stat. Phys. 9 (2) 101
[24] Guest P G 1961 Rev. Sci. Instrum. 32 164