ANALYSIS OF COUETTE FLOW AND HEAT TRANSFER BETWEEN PARALLEL PLATES ENCLOSING RAREFIED GAS BY MONTE CARLO

by Morris Perlmutter
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TECHNICAL PAPER proposed for presentation at Fifth International Symposium on Rarefied Gas Dynamics
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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
RAREFIED GAS DYNAMICS

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Abstract

Couette flow and heat transfer through a hard-sphere rarefied gas enclosed between parallel walls are analyzed by a Monte Carlo procedure. In one case, both walls are stationary and at different temperatures. In the other case, the upper wall is moving, and both walls are at the same temperature. The molecules are assumed to have hard sphere collision and a wall accommodation factor of unity. The wall temperature ratio and wall velocity are taken large so that linearized solutions are not applicable. Sample molecule histories are followed across the channel, which has been divided into zones. The target molecules in each zone are assumed to have a different two-sided half-Maxwellian velocity distribution. By scoring the properties of the sample molecules as they pass scoring positions, the macroscopic quantities of interest, such as temperature, density, shear, and heat transfer, are obtained. Also, the average thermal velocity and number density in each zone are found and compared with the values assumed in the target molecule distribution. The problem is iterated until these values agree.

Symbols

\[ C = \text{average thermal velocity } (2RgT)^{1/2} \]
\[ D = \text{channel width} \]
\[ f = \text{probability distribution function} \]
\[ Kn = \text{Knudsen number } l_M/D = m/\sqrt{2} \rho_A D^2 \]
\[ M = \text{dimensionless velocity } u/C_w \]

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\( m \) = mass of molecule

\( N \) = number of sample molecules emitted from surface 0 in Monte Carlo run, proportional to flux of molecules leaving surface 0

\( P \) = pressure; \( \frac{P_{ij}}{3} \)

\( P_i, j \) = shear stress \((-\rho \langle v_i v_j \rangle)\)

\( \rho \) = zone or scoring-position number

\( P_f \) = last scoring-position number

\( Q \) = property of sample molecule

\( \langle Q \rangle \) = averaged quantity \( \int Q_f \ d^3V \)

\( \langle Q \rangle_+ \) = averaged quantity \( \int Q_{f+} \ d^3V \)

\( q \) = heat transfer

\( q_T \) = total energy transfer

\( R \) = random number between 0 and 1

\( R_g \) = gas constant

\( S \) = mutual collision cross section \( \pi \sigma^2 \)

\( S_{+}, S_{-} \) = number of sample molecules through scoring position in positive, negative \( x_2 \) direction

\( T \) = absolute temperature

\( t \) = dimensionless temperatures \( T/T_w, 0 \)

\( u \) = mean velocity

\( x \) = coordinate

\( V \) = molecular velocity

\( V' \) = thermal velocity; \( v = u \)

\( V'_{\star} \) = velocity after collision

\( \gamma \) = defined by equations (B5) and (B6)

\( \epsilon \) = defined by equations (B5) and (B6)

\( \eta \) = viscosity coefficient

\( \kappa \) = thermal conductivity

\( \theta \) = collision rate of sample molecule with target molecules

\( \lambda \) = path length to collision

\( \lambda_M \) = mean free path length through a Maxwellian gas with density \( \rho \) and thermal velocity \( C \)

\( \lambda_s \) = mean free path length

\( \mu \) = dimensionless velocity, \( V'/C \)

\( \mu_{R, A} \) = defined by equation (All)

\( \rho \) = density

\( \sigma \) = diameter of hard sphere molecule

\( \phi \) = angle between sample molecule and target molecule velocities

Subscripts:

\( \Lambda \) = averaged across channel
Introduction

The present analysis treats a rarefied gas enclosed between two walls. Two cases are treated: in one, both walls are stationary and at different temperatures, while in the other, both walls are at the same temperature but one wall is moving. The molecule are assumed to have hard-sphere collisions and a wall accommodation of 1. The problem is analyzed by a Monte Carlo technique, that is, a model sampling procedure. Sample molecule histories are generated by making choices at points of decision from the appropriate probability distributions. These sample molecules are followed through the model and, by averaging certain molecular properties at various positions, the macroscopic quantities of interest can be obtained. This method reduces the complexity of the analysis since the relations for a single sample molecule history are relatively simple. Thus, simplifying assumptions made in the more usual analytical procedures are also avoided. However, the Monte Carlo method requires extensive calculations on a high-speed computer for the many sample histories needed.

Gross and Ziering (ref. 1) treated the couette flow problem for the case of low relative plate velocities with both plates at the same temperature. They also treated the case where both walls were stationary but at different temperatures (ref. 2). Because small differences in relative wall velocities and wall temperature were assumed in these analyses, the linearized form of the Boltzmann equation was used. The local distribution function was approximated by half-range polynomials in velocity space. The space-dependent coefficients in this distribution were found by
forming half-range moment equations.

Lui and Lees (ref. 3) have analyzed the case of rarefied couette flow with heat transfer assuming Maxwellian molecule collision. They assumed a local two-sided half-Maxwellian velocity distribution. This is substituted into the moment equations, which are then solved for the parameters of the distribution. From this, the macroscopic flow parameters can be found.

This same approach was used by Lavin and Haviland (ref. 4) for the case of stationary walls at different temperatures assuming hard sphere molecule collisions.

The Monte Carlo method has been used previously in rarefied gas problems by Perlmutter (ref. 5) to treat a collisionless plasma flowing through a channel with an imposed magnetic field. Haviland (ref. 6) used Monte Carlo to treat a rarefied gas with hard-sphere collision contained between stationary parallel plates at different wall temperatures. In that analysis, sample molecule histories are followed through collision with target molecules as they travel through the model. From the histories of the sample molecules, tables of the distribution of the velocity components can be obtained in the various zones into which the channel has been divided. These tables can then be used for the target molecule velocity distribution in the next iteration of the sample molecule histories. After the converged distribution of velocities are obtained, the macroscopic quantities of interest, such as temperature, density, and heat transfer, can be obtained by finding the moments of the distribution in each zone.

The present analysis also follows a sample molecule traveling through the model. However, in the present case, the target molecule velocities in each zone are assumed to have a two-sided half-Maxwellian distribution of the form assumed by Lui and Lees in reference 3. By scoring properties of the sample molecules at scoring position across the channel, the parameters of the distribution as well as the macroscopic flow properties such as temperature, velocity profile, heat transfer, and shear stress can be found. This method was used by Perlmutter (refs. 7 and 8) for heat transfer between parallel plates with the walls stationary but at different temperatures. In that solution, it was assumed that the local distribution of target molecules was Maxwellian instead of two-sided half-Maxwellian.
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Sample History

The model analyzed is shown in figure 1. The wall at $x_2$ of 0 is stationary and at temperature $T_W_0$. The other wall at $x_2$ of 1 is moving at velocity $u_{W1}$ and is at temperature $T_W_1$. The distance across the channel is divided into zones. In each zone, the target molecule thermal velocity distribution is assumed to be a two-sided half-Maxwellian distribution given by

$$\rho f = \rho_p f_+ + \rho_n f_- = \frac{2\rho_p}{\pi^{3/2} C^3} \exp\left(-\frac{V_2^2}{2C^2}\right) + \frac{2\rho_n}{\pi^{3/2} C^3} \exp\left(-\frac{V_2^2}{2C^2}\right)$$

for $V_2 > 0$ and $V_2 < 0$. (1)

where $f_+$ refers to the molecules moving in the positive $V_2$ direction and $f_-$ refers to molecules moving in the negative $V_2$ direction.

It is assumed that the molecules reflected are perfectly accommodated, that is, in a Maxwellian distribution at the wall based on the wall temperature. The velocity of the sample molecule leaving the wall as derived in refs. 6 and 8 is given by

$$V_2 = (-C_2 \ln R_{V_2})^{1/2}$$

$$V_1 = (-C_2 \ln R_{V_1})^{1/2} \cos 2\pi R_0 + u_{1W}$$

$$V_3 = (-C_2 \ln R_{V_3})^{1/2} \sin 2\pi R_0$$

where $R$ is a random number between 0 and 1 chosen for each sample molecule leaving the surface.

Path length to collision. - After the sample molecule leaves the wall, its path length to collision must be calculated to find if it has a collision before passing through the first zone. The probability that a sample molecule will collide in the incremental path length $\lambda$ to $\lambda + d\lambda$ is given (refs. 8 and 9) as

$$f_\lambda = \frac{\exp(-\lambda/\lambda_s)}{\lambda_s}$$

where $\lambda_s$ is the mean free path to collision of the sample
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molecule moving at velocity \( V_s \) in that zone. A path length to collision for the sample molecule can be chosen from this distribution by the same procedure of picking a random number used earlier for the sample molecules leaving the surface:

\[
\lambda = -\lambda_s \ln R_\lambda
\]  

(4)

To pick from this distribution, the mean free path \( \lambda_s \) for the sample molecule in the zone must be known. If the un-directed velocities of the target molecules are in a Maxwellian distribution with an average thermal velocity \( C \) and density \( \rho \), the mean free path for the sample molecule \( \lambda_M \), as shown in appendix A, is given by

\[
\frac{\lambda_M}{\lambda_s} = \frac{\sqrt{2\pi} \, \text{Kn} \, \sqrt{V_s}}{C \, \rho \, \left[ \exp\left(-\frac{V_s^2}{2\sigma^2}\right) + \sqrt{\pi} \left( \text{erf}\left(\frac{V_s}{\sigma}\right) \frac{V_s}{C} + \frac{C}{2\sqrt{\pi} \, \sigma}\right) \right]}
\]  

(5)

where \( \text{Kn} \) is the usual definition of Knudsen number for a gas in a Maxwellian distribution with hard-sphere molecule collisions. Since the target molecule velocity distribution has been assumed to be a two-sided half-Maxwellian distribution (eq. (1)), the mean free path is obtained by assuming the distribution of target molecules to consist of two full Maxwellian distributions in each increment

\[
f_t = f_{M+} + f_{M-}
\]  

(6)

where \( f_{M+} \) and \( f_{M-} \) are Maxwellian distributions with densities \( 2\rho_+ \) and \( 2\rho_- \) and thermal velocities of \( C_+ \) and \( C_- \), respectively. However, the molecules of \( f_{M+} \) with \(-V_2 < 0\) and the molecules of \( f_{M-} \) with \( V_2 > 0\) are considered nonexistent. This permits the calculation of the mean free path using the Maxwellian distribution relations. Thus, the mean free path for a sample molecule moving through two Maxwellian gases, as shown in appendix A, is given by

\[
\frac{1}{\lambda_s} = \frac{1}{\lambda_{M+}} + \frac{1}{\lambda_{M-}}
\]  

(7)

where \( \lambda_{M+} \) or \( \lambda_{M-} \) is evaluated, as in equation (5).

After a path length to collision is picked for the sample molecule from equation (4), it is compared with the distance the sample molecule must travel to cross the zone. If \( \lambda \) is greater than this distance, the sample molecule is started at the beginning of the next zone with its velocity
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components unchanged and the procedure is as before. If it is not, there is a collision in the zone and new velocity components must be calculated for the sample molecule after collision.

Sample Molecule Velocity After Collision

To find the new sample molecule velocity components after collision, the velocity components of the target molecule collision partner must first be found. Since there are two distributions of target molecules locally, \( f_{M^+} \) and \( f_{M^-} \), the distribution the target molecule collision partner is to be picked from must first be decided. The fraction of all the collision partners that come from the \( f_{M^+} \) distribution is given by \( \lambda_2 / \lambda_{M^+} \). Then, for a picked random number, if \( R < \lambda_2 / \lambda_{M^+} \), the collision partner velocity components are picked from the \( f_{M^+} \) distribution. Otherwise, they are picked from the \( f_{M^-} \) distribution. The equations for obtaining the velocity components of the target molecule collision partner are given in appendix B.

If \( V_{2t} \) picked from the \( f_{M^+} \) distribution is negative or, if picked from \( f_{M^-} \), if \( V_{2t} \) is positive, the collision partner is considered nonexistent. This is because half the molecules in the \( f_{M^+} \) and \( f_{M^-} \) distribution are nonexistent, as discussed before. In this case, the sample molecule continues its history from the point of collision with its original velocity.

After collision of the sample molecule with the chosen collision partner, the new components of velocity \( V_s^* \) of the sample molecule are given (ref. 8) by

\[
\begin{align*}
V_{1s}^* &= \frac{1}{2} (V_{1s} + V_{1t}) + V_R (1 - b^2)^{1/2} H \\
V_{2s}^* &= \frac{1}{2} (V_{2s} + V_{2t}) + V_R (1 - 2b^2) \\
V_{3s}^* &= \frac{1}{2} (V_{3s} + V_{3t}) + V_R (1 - b^2)^{1/2} \Xi
\end{align*}
\]

where \( V_R \) is given by equation (A2). The values of \( H \) and \( \Xi \) are obtained by picking two random numbers which are used in the following equations:

\[
H = 2R_H - 1, \quad \Xi = 2R_\Xi - 1, \quad \text{and} \quad b^2 = H^2 + \Xi^2
\]

where \( b^2 \) must be less than 1, or a new set of random numbers must be chosen to find \( H \) and \( \Xi \).

The sample molecule history is then continued from the point of collision with its new velocity components. The
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Sample histories are completed when the sample molecule returns to the surface from which it has been emitted.

Scoring to Find Macroscopic Flow Properties

The macroscopic fluid characteristics needed are density, temperature, velocity, and heat transfer across the channel. These properties are obtained at scoring positions located at various distances across the channel, as shown in figure 1. The average quantity of \( Q \) transported across the scoring cross-section \( p \), as shown in ref. 8, is

\[
\rho \langle V_2 Q \rangle_p = \left( \rho_+ \langle V_2 Q \rangle_+ + \rho_- \langle V_2 Q \rangle_- \right)_p
\]

\[
= \rho_+ C_{w_1} \left[ \left( \sum Q^+ \right)_p \left( \sum Q^- \right)_p \right]
\]

If \( Q \) is taken as \( 1/V_2 \),

\[
\frac{P}{\rho P+ P_0} = \frac{C_{w_1} C_{w_0}}{N_{x^2}} \left[ \left( \sum \frac{1}{V_2^+} \right)_p \left( \sum \frac{1}{V_2^-} \right)_p \right]
\]

Thus, by summing the inverse \( V_2 \) velocity of the sample molecules as they cross the scoring position the local density of the molecule with a positive, negative component of \( V_2 \), \( \rho_+, \rho_- \), can be obtained as well as the local density \( \rho \). The average density across the channel is then obtained by averaging the density of all the scoring cross sections.

If \( Q \) is taken as \( V_1/V_2 \), eq. 10 becomes

\[
\frac{\rho u}{\rho_+ C_{w_1} C_{w_0} + \rho_- C_{w_1} C_{w_0}} = \frac{1}{N_{x^2}} \left[ \sum \frac{V_1}{V_2^+} - \sum \frac{V_1}{V_2^-} \right]
\]

Dividing by the appropriate densities obtained previously gives the local mean velocity for the molecules with \( V_2 > 0 \), \( u_+ \), and \( V_2 < 0 \), \( u_- \), and also the local mean velocity, \( u \).

The undirected kinetic energy per unit mass of a monatomic gas is equal to the degrees of freedom times \((1/2)R_g T\). This can be written as

\[
\left( \frac{3}{2} \right) R_g T = \frac{1}{2} \langle V_1^2 \rangle = \frac{1}{2} \langle V_2^2 \rangle - \frac{1}{2} u_1^2
\]

Then from equation (10) is obtained
The thermal velocity of the molecules with \( V_2 > 0 \) is given by

\[
\frac{c^2}{c_{w,0}^2} = \frac{2}{3c_{w,0} \pi^{1/2}} \left( \frac{\rho}{\rho_{+0}} \right)^{-1} \left[ \sum_{v_2^+} (v_2^2) - \sum_{v_2^-} (v_2^2) \right] - \frac{2u_{1+}^2}{3c_{w,0}^2} \tag{15}
\]

and similarly for the molecules with \( V_2 < 0 \)

\[
\frac{c_{2}^2}{c_{w,0}^2} = -\frac{2}{3c_{w,0} \pi^{1/2}} \left( \frac{\rho}{\rho_{+0}} \right)^{-1} \left[ \sum_{v_2^+} (v_2^2) - \sum_{v_2^-} (v_2^2) \right] - \frac{2u_{1-}^2}{3c_{w,0}^2} \tag{16}
\]

The shear stress across the channel is given by

\[ P_{12} = \rho(V_1V_2) \]. This can be shown to be equal to

\[ P_{12} = \rho(V_1V_2) = \rho_{+0} c_{+0} \pi^{1/2} \left( \sum_{v_1^+} v_1 - \sum_{v_1^-} v_1 \right) \tag{17} \]

The total energy being transferred across the channel is given by

\[ q_t = \frac{1}{2} \rho(V_2^2) = \frac{\rho_{+0} c_{w,0}^{1/2}}{2N^{1/2}} \left[ \sum_{v_2^+} (v_2^2) - \sum_{v_2^-} (v_2^2) \right] \tag{18} \]

The transfer of the undirected kinetic energy across the channel is \( q = (1/2)\rho(V_1^2(V_2^2)) \), so that equation (18) becomes

\[ q = q_t - u_{1+} P_{12} \tag{19} \]

By using these equations, the macroscopic quantities of interest are found. The values of \( \rho_{+}, \rho_{-}, \rho_{+}, \rho_{-} \) are then compared with the assumed values used in the target molecule distribution, and the problem is iterated until they are in agreement. Also obtained at the same time from the above equations are the local temperature, density, shear, and energy transfer.
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Results and Conclusions

Stationary walls with a temperature ratio $t_{w,1}$ of 0.25 was treated first. The local gas temperature divided by the temperature of the hot wall is shown in figure 2. The local density divided by the average density across the channel is given in figure 3. In figure 4, the heat flux transferred divided by the heat flux for the collisionless case, as given in appendix C, are shown.

The present results can be seen to be in good agreement with the results of another Monte Carlo solution by Haviland (ref. 6). The linearized solution of Gross and Ziering (ref. 2) gives very good agreement with the present results except for the temperature profile. In the linearized solution of ref. 2, the centerline temperature is taken midway between the wall temperatures. The present results have their centerline temperature significantly below this value for the Knudsen number of 2; hence, the large disagreement in the results.

The nonlinear results of Liu and Lees (ref. 3) of the temperature and density are of the correct magnitude but of a somewhat different gradient. The nonlinear heat transfer results fall somewhat above the other solutions.

Also shown in the figures are the slip continuum results. These results are obtained by using the fluid temperature in the continuum equations (appendix D). By using the slip wall temperatures that gave the best fit both to the temperature and density results of the present solution, the results shown were obtained. However, when the heat transfer was calculated using these same slip wall temperatures and the continuum thermal conductivity, the heat transfer was found to be considerable above the other solutions. Since the slip solutions with the continuum conductivity are only expected to apply close to continuum conditions, this result is to be expected.

The heat transfer at various positions across the channel is shown in figure 6. Theoretically, this should be constant at each point across the channel (appendix D), although the present method does not impose this condition in its method of solution. This condition, however, is satisfied in the present results, as can be seen from this figure.

To check the confidence limits of the present results, the solution was carried out 20 times with 2500 sample molecules each time for $Kn = 0.5$. The temperature and density had a value of 8, the 95 percent confidence inter-
val, of close to 1 percent of their value, while the value of $\delta$ for the heat transfer across the channel was about 2 percent of its value. The derivations and equation used in obtaining $\delta$ are given in appendix E.

The second case treated is when both walls are at the same temperature, but one wall is moving at a wall Mach number $M_w = u_{wl}/C_{wl}$ of 4. The velocity profile is shown in figure 6. The linearized solution (ref. 1) is in poor agreement with the present result, as would be expected for the nonlinear large wall Mach number case.

The temperature profile across the channel is shown in figure 7. There is a substantial rise in temperature for smaller Knudsen numbers because, as the strongly directed stream of molecules leaves the moving wall, it encounters the undirected stream. This gives a lower value for the average directed motion of the fluid. This decrease in directed kinetic energy is now included in the thermal motion which gives the higher temperature.

The shear stress for the channel, shown in figure 8, has been nondimensionalized by the shear stress for the collisionless case (eq. (C5)). The results fall above the linearized solution of reference 1. The total energy transfer across the channel nondimensionalized by the total energy transfer for the collisionless case (eq. (C6)) gives the same values as the dimensionless shear stress for the cases studied. This is also shown in figure 8, where shear stress and total heat transfer across the channel are plotted. Again, from the microscopic laws of conservation and the moment equations, it can be shown that the shear stress and total heat transfer at various positions across the channel should be constant. Although this condition is not imposed by the present method of solution, the results indicate that the shear stress and total energy transfer are nearly constant at different positions across the channel.

In conclusion, the Monte Carlo method gives reasonable results for the present problem without the necessity of extreme assumptions. The major drawback to the method is the increasing amount of computer time necessary to carry out the calculations as the Knudsen number becomes smaller.

Some typical running times for 10,000 sample molecules on an IBM 7094 were: $Kn = 30$, 8 minutes; $Kn = 2$, 10 minutes; $Kn = 0.5$, 15 minutes. These running times would make results difficult to obtain for small Knudsen numbers with the present procedure. Generally, three iterations of
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50,000 samples were used.

The present method is very flexible and can readily be used in other transport problems not readily solved by the more usual procedures.

Appendix A

Evaluation of Mean Free Path

The number of collisions per unit time $d\theta$ of a sample molecule moving at velocity $V_s$ through target molecules in velocity-volume space $dV_T$ for hard sphere molecules is given (ref. 8) as

$$d\theta = \rho t V_R dV_T$$

where $V_R$ is the velocity of the target molecules relative to the sample molecule velocity before collision and can be written as

$$V_R = \sqrt{(V_{1t} - V_{1s})^2 + (V_{2t} - V_{2s})^2 + (V_{3t} - V_{3s})^2}^{1/2} \quad (A2)$$

If we subtract the local mean velocity $\bar{u}$ from both the velocity of the sample molecules and the target molecules we can then write the collision rate for a Maxwellian distribution of target molecules as

$$d\theta_M = \frac{\rho s}{3/2} \left( \exp \frac{-V_{1t}^2}{c^2} \right) V_R dV_{1t} dV_{2t} dV_{3t} \quad (A3)$$

Then transforming variables by a rotation using Eulerian angles (refs. 8 and 10) yields

$$V''_{it} = A^{-1}_{ij} V''_{jt} \quad (A4a)$$

where

$$A^{-1}_{ij} = \begin{vmatrix} V_{2s} & V_{1s} & V_{3s} \ V_{2s} & V_{1s} & V_{3s} \ \frac{V_{rs}}{V_s} & \frac{V_{rs}}{V_s} & \frac{V_{rs}}{V_s} \ \end{vmatrix} \quad (A4b)$$

The inverse transformation is given by

$$V_{it}'' = A_{ij} V_{jt}$$

$$V_{3s} \ V_{3s} \ \ V_{3s}$$

$$\begin{vmatrix} V_{2s} & V_{1s} & V_{3s} \ V_{2s} & V_{1s} & V_{3s} \ \frac{V_{rs}}{V_s} & \frac{V_{rs}}{V_s} & \frac{V_{rs}}{V_s} \ \end{vmatrix}$$
where

\[ A_{ij} = \begin{bmatrix}
V_{2s} & -V_{1s} & 0 \\
V_{1s} & V_{2s} & V_{3s} \\
-V_{3s}V_{1s} & -V_{2s}V_{3s} & V_{rs}
\end{bmatrix} \] (A5b)

Then, equation (A3) becomes

\[ \text{d} \theta_M = \frac{\rho S}{m \tau^{3/2} \sqrt{\pi}} \left( \exp \left( \frac{t_i^2}{C^2} \right) \right) \left[ \frac{\rho S}{m \tau^{3/2} \sqrt{\pi}} \right] \text{d} \nu_t (A6a) \]

Transforming into spherical coordinates

\[ V_{1t} = V_t \cos \theta \sin \phi, \quad V_{2t} = V_t \cos \phi, \quad V_{3t} = V_t \sin \theta \sin \phi \] (A6b)

yields

\[ d \theta_M = \frac{C \rho S}{m \tau^{3/2} \sqrt{\pi}} \left[ \exp \left( -\frac{\mu_t^2}{C^2} \right) \right] \mu_t^2 \mu_R \sin \phi \, d\phi \, d\theta \, d\mu_t \] (A7)

where \( \mu \) is the nondimensionalized velocity \( \nu_t / C \) and

\[ \mu_R = (\mu_t^2 + \mu_s^2 - 2 \mu_t \mu_s \cos \phi)^{1/2} \] (A8)

To obtain the total collision rate for the target molecules over all velocities, equation (A7) must be integrated over \( \phi, \theta, \) and \( \mu_t \). Integrating over \( \theta \) from 0 to \( \pi \) gives

\[ d \theta_M(\mu_t) = \frac{4 \rho S}{m \tau^{1/2} \sqrt{\pi}} \left[ \exp \left( -\mu_t^2 \right) \right] \mu_t^2 \mu_R, A \, d\mu_t \] (A9)

\[ \mu_R, A = \begin{cases} 
\mu_s + \mu_t^2 / 3 \mu_s & \text{if } \mu_s > \mu_t \\
\mu_t + \mu_s^2 / 3 \mu_t & \text{if } \mu_t > \mu_s
\end{cases} \] (A10)

Integrating equation (A9) over \( \mu_t \) from 0 to \( \infty \), the total collision frequency \( \theta_M \) is obtained for a sample molecule moving at velocity \( \mu_s \) through a Maxwellian gas:
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\[ \theta_M = \frac{\rho SC}{m} \left[ \frac{\exp(-\mu_s^2)}{\pi^{1/2}} + (\text{erf}_\mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right) \right] \]  (A11)

The nondimensional mean free path is then found, as discussed in ref. 6, by dividing the sample molecule velocity by the total collision rate, which gives

\[ \frac{\lambda_M}{\bar{D}} = \frac{V_s}{\theta_M} = \frac{\sqrt{2} KnV_s}{C \frac{\rho}{\rho_A}} \left( \frac{1}{\sqrt{\pi}} \left[ \exp\left(-\frac{\mu_s^2}{2}\right) \right] + (\text{erf}_\mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right) \right) \]  (A12)

If there were two different Maxwellian gases in the increment \( f_{M+} \) and \( f_{M-} \), the total collision rate would be given by \( \theta = \theta_{M+} + \theta_{M-} \), where \( \theta_{M+} \) and \( \theta_{M-} \) are given as in equation (A12) but with different densities and mean thermal velocities. Since \( \lambda_s/\bar{D} \) is given by \( V_s/\theta \),

\[ \frac{\lambda_s}{\bar{D}} = \frac{\theta_{M+}}{V_s} + \frac{\theta_{M-}}{V_s} = \frac{1}{\theta_{M+}} + \frac{1}{\theta_{M-}} \]  (A13)

Appendix B

The Target-Molecule Collision Partner

The velocity distribution of target-molecule collision partners for a sample molecule passing through target molecules in a Maxwellian distribution (ref. 6) is

\[ \frac{d\theta_M}{\theta_M} = \frac{\mu_t^2 uR \sin \phi \, d\phi \, du_t}{\pi \left[ \exp(-\mu_s^2) \right] + \pi^{3/2}(\text{erf}_\mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right)} \]  (B1)

The distribution in \( \theta \) for the target-molecule collision partners is

\[ f_\theta d\theta = \frac{d\theta}{2\pi} \quad \text{or} \quad \theta = 2\pi B_\theta \]  (B2)

The distribution of \( \mu_t \) for the target-molecule collision partners is obtained from the marginal distribution.
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\[ f(\mu_t, d\mu_t) = \frac{4 \exp(-\mu_t^2) \mu_t^2 \mu_{RA} d\mu_t}{\exp(\omega \mu_s^2) + \pi^{\frac{1}{2}}/2(\text{erf} \mu_s) \left( \mu_s + \frac{1}{2\mu_s} \right)} \]  

(B3)

Then \( \mu_t \) can be picked from this distribution, using

\[ R_{\mu_t} = \frac{\gamma(\mu_s, \mu_t) + \epsilon(\mu_s, \mu_t)}{\exp(-\mu_t^2) + \pi^{\frac{1}{2}}/2(\text{erf} \mu_s) \left( \mu_s + \frac{1}{2\mu_s} \right)} \]  

(B4)

where, when \( \mu_s > \mu_t \), \( \epsilon = 0 \) and

\[ \gamma(\mu_s, \mu_t) = -2\mu_s \mu_t \left[ \exp(-\mu_t^2) + \mu_s \sqrt{\pi}(\text{erf} \mu_t) \right] - \frac{\mu_t}{\mu_s} \left[ \exp(-\mu_t^2) + \frac{\sqrt{\pi}}{2\mu_s} (\text{erf} \mu_t) \right] \]  

(B5)

and, when \( \mu_s < \mu_t \), \( \gamma(\mu_s, \mu_t) = \gamma(\mu_t, \mu_s) \) and

\[ \epsilon = -2 \left[ \exp(\mu_s^2) \left( \frac{\mu_s^2}{2} + 1 + \mu_t^2 \right) + \left[ 2 \exp(-\mu_s^2) \right] \left( \frac{4\mu_s^2}{5} + 1 \right) \right] \]  

(B6)

To find \( \phi \) for the target molecule, the distribution of target molecules can be written as a product of a marginal times a conditional distribution

\[ \frac{d\theta(\mu_t, \phi)}{\theta} = f(\mu_t)f(\phi|\mu_t) \]  

(B7)

Then it is necessary to pick \( \phi \) from the conditional distribution:

\[ f(\phi|\mu_t) = \frac{\mu_R \sin \phi \ d\phi}{2\mu_{RA}} \]  

(B8)

Picking \( \phi \) for a given \( \mu_t \) is found as before from
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\[
\Psi = \frac{\left(\mu^3 - |\mu_t - \mu_s|^3 \right)}{\left(\mu_t^2 + \mu_s^2 + 2\mu_t \mu_s \right)^{3/2} - |\mu_t - \mu_s|^3}
\]  

(B9)

After picking \( \varphi, \mu_t, \) and \( \theta, \) it is necessary to find the velocity components \( V''_t, \) using equation (A6b). Then, from equation (A4),

\[
V_{1t} = V''_t \left(\frac{V_{2s}}{V_{rs}}\right) + V''_t \left(\frac{V_{1s}}{V_{rs}}\right) \quad V''_t \left(\frac{V_{3s}}{V_{rs}}\right) + u_l
\]

(B10a)

\[
V_{2t} = -V''_t \left(\frac{V_{1s}}{V_{rs}}\right) + V''_t \left(\frac{V_{2s}}{V_{rs}}\right) \quad -V''_t \left(\frac{V_{3s}}{V_{rs}}\right) \quad V_{3t} = 0 + V''_t \left(\frac{V_{3s}}{V_{rs}}\right) + V''_t \left(\frac{V_{rs}}{V_{rs}}\right)
\]

(B10b)

APPENDIX C

Collisionless Solution

For negligible molecular collisions, the local distribution in the channel is given by

\[
\rho_{\infty}^{V} = \frac{2\rho_{w,0}}{\pi^{3/2}C_{w,0}^3} \left[ \exp \left( -\frac{V_{w,0}^2}{2C_{w,0}^2} \right) \right] + \frac{2\rho_{-1}}{\pi^{3/2}C_{w,1}^3} \left[ \exp \left( -\frac{V_{w,1}^2}{2C_{w,1}^2} \right) \right] \quad V_{2} > 0
\]

(C1)

\[
\left[ \exp \left( -\frac{V_{w,1}^2}{2C_{w,1}^2} \right) \right]_{V_{2} < 0}
\]

The local density is then given by \( \rho(1) = \rho = \rho_{+0} + \rho_{-1}. \) Since there is no net flow across the channel, one can write

\[
\rho(V_2) = \frac{1}{\pi} \left[ \rho_{+0} C_{w,0} - \rho_{-1} C_{w,1} \right] = 0. \quad \text{Combining gives}
\]

\[
\left( \frac{\rho_{+0}}{\rho} \right)_{\infty} = \frac{1}{1 + \frac{1}{C_{w,1}}} ; \quad \left( \frac{\rho_{-1}}{\rho} \right)_{\infty} = 1 - \frac{\rho_{+0}}{\rho}
\]

(C2)

The flow parallel to the channel wall is given by
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\[ u_1 = \langle V_1 \rangle = \frac{\rho_{+}^{0}}{\rho} u_{1,w,0} + \frac{\rho_{-}^{-1}}{\rho} u_{1,w,1} \]  \hspace{1cm} (C3)

The local temperature is given by

\[ \frac{T}{T_{w,0}} = \frac{2}{3c_{w,0}^2} \left( \langle V_1^2 \rangle + \langle V_2^2 \rangle + \langle V_3^2 \rangle \right) - \frac{1}{2} M^2 \]  \hspace{1cm} \text{which, when integrated gives}

\[ t = \frac{2}{3} \left( \frac{\rho_{+}^{0}}{\rho} M_{w,0}^2 + \frac{\rho_{-}^{-1}}{\rho} M_{w,1}^2 - M^2 \right) + \frac{\rho_{+}^{0}}{\rho} \left( 1 + t_{w,1}^{1/2} \right) \]  \hspace{1cm} (C4)

The shear stress given by \( P_{12} = \rho \langle V_1 V_2 \rangle \) can be integrated to give

\[ \frac{t_{1/2}^{P_{12}}}{2R_c T_{w,0}} = \frac{\rho_{+}^{0}(M_{w,0} - M_{w,1})}{\rho} \]  \hspace{1cm} (C5)

The total energy transferred given by \( q_T = \frac{\rho}{2} \langle V_1^2 \rangle + u_1 P_{12} \)

\[ \frac{t_{1/2}^{P_{12}}}{2R_c T_{w,0}^{3/2}} = \frac{\rho_{+}^{0}}{\rho} - \frac{\rho_{-}^{-1}}{\rho} t_{w,1}^{3/2} + \frac{\rho_{+}^{0}}{\rho} \frac{M_{w,0}^2}{2} - \frac{\rho_{-}^{-1}}{\rho} \frac{M_{w,1}^2}{2t_{w,1}^{1/2}} \]  \hspace{1cm} (C6)

APPENDIX D

Continuum Solutions

Maxwell's equation of transfer, which describes the rates of change of a quantity \( Q \) in a volume element of space, is given by

\[ \frac{\partial}{\partial x_1} (\rho \langle V_1 Q \rangle) = \frac{1}{m} \Delta Q \]  \hspace{1cm} (D1)

where \( \Delta Q \) denotes the rate change in some molecular quantity \( Q \) due to molecular collisions. This term is zero where \( Q \) is conserved during collision. This is the case for \( Q \) equal to \( 1, V, \) or \( V^2 \) because of conservation of mass, momentum, and energy, respectively:

\[ \frac{\partial}{\partial x_1} (\rho u_i) = 0 \]  \hspace{1cm} (D2)
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\[ \rho u_i \frac{\partial u_j}{\partial x_i} = - \frac{\partial}{\partial x_i} \rho \langle v_i v_j \rangle = - \frac{\partial}{\partial x_i} P_{ij} \]  
\[ (D3) \]

\[ \frac{\partial}{\partial x_i} (\rho u_i u_j) + \frac{\partial}{\partial x_i} (u_i P_{ij}) = \frac{\partial}{\partial x_i} (\rho \langle v_i v_j^2 \rangle) + \frac{\partial}{\partial x_i} (2 u_j P_{ij}) = 0 \]
\[ (D4) \]

Introducing the gas conductivity, viscosity and \( P \) as the static pressure gives the well known Navier-Stokes equations:

\[ \frac{1}{2} \rho \langle v_i v_i^2 \rangle = q_i = - \kappa \frac{\partial T}{\partial x_i} \]
\[ (D5) \]

\[ P_{ij} = \delta_{ij} P - 2 \mu \left( \frac{1}{2} \frac{\partial u_i}{\partial x_j} + \frac{1}{2} \frac{\partial u_j}{\partial x_i} - \frac{1}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \]
\[ (D6) \]

Since, in the present model, there is no \( x_1 \) or \( x_3 \) dependence, these results simplify to give \( u_1 = g(x_2) \), \( \dot{\gamma} = \text{constant across the channel} \), and \( P_{12} = - \mu (\partial u_1 / \partial x_2) \) (a constant), and also \( q_2 + u_1 P_{12} = q_T \) (a constant).

For hard-sphere molecules, assuming a small perturbation from equilibrium of the local distribution, the conductivity and viscosity can be written (ref. 6) as

\[ \kappa = \kappa_0 t^{1/2} \quad \kappa_0 = \frac{75 m}{64 \sigma (2\pi)^{1/2}} \frac{R_g C_0}{L^{1/2}} \]  
\[ (D7) \]

\[ \mu = \mu_0 t^{1/2} \quad \mu_0 = \frac{5 m C_0}{16 \sigma^2 (2\pi)^{1/2}} \]  
\[ (D8) \]

With both walls stationary, \( q = - \kappa (\partial T / \partial x_i) \). This can be readily solved to give \( t_{M=0} = \left[ 1 - \left( 1 - t^{3/2} \right)^2 / 3 \right]^{1/2} \).

Since the pressure across the channel is constant using the ideal gas law, \( P \)

\[ \left( \frac{\rho}{\rho_A} \right)_{M=0} = \frac{1 + t_{w,1}^{1/2} + t_{w,1}}{3(t)_{M=0}} \]  
\[ (D9) \]

The heat transfer across the channel can be found equal to

\[ \left( \frac{q}{\rho_A C_0} \right)_{M=0} = \frac{25}{64} \pi^{1/2} \left( 1 - t_{w,1}^{3/2} \right) \text{Kn} \]
\[ (D1C) \]
When the upper wall is moving, the energy equation can be written as
\[
\frac{\partial}{\partial x_2} \left( C_p T + \frac{u_1^2}{2} \right) = - \frac{C_p}{\kappa} q_t \tag{D11}
\]
This can be rewritten using \((\mu C_p /\kappa) = 2/3; C_p = (5/2) R_g\) as
\[
\frac{\partial}{\partial x_2} \left( t + \frac{4}{15} M^2 - \frac{8}{15} \frac{q_t}{P_{12}} M \right) = 0 \tag{D12}
\]
When the upper wall is moving at a velocity \(u_w\) and both walls are at the same temperature, integration can be performed to obtain
\[
t = \frac{4}{15} M (M_{w,1} - M) + 1 \tag{D13}
\]
The equation for \(P_{12}\) can be rewritten as
\[
P_{12} = -u_0 t^{1/2} \frac{3u_1}{2} \nabla_x \frac{d}{d x_2} \tag{D14}
\]
This can be integrated to give
\[
x_2 = \left\{ \left( \frac{15}{4} + M_{w,1} - M^2 \right)^{1/2} \left( \frac{2M - M_{w,1}}{4} \right) + \left( \frac{15}{4} \right) \frac{M_{w,1}}{4} \right\}^{1/2}

\left\{ \left( \frac{M_{w,1}}{15 + M_{w,1}^2} \right)^{1/2} \right\}

\left\{ \sin^{-1} \left( \frac{M_{w,1} - 2M}{(15 + M_{w,1}^2)^{1/2}} \right) - \sin^{-1} \left( \frac{M_{w,1}}{(15 + M_{w,1}^2)^{1/2}} \right) \right\} \tag{D15}
\]
This gives an implicit form of the velocity profile across the channel. This result can be used in conjunction with equation (D13) to obtain the temperature distribution across the channel.

Similarly integrating equation (D14) from \(x = 0\) to \(1\), the following can be obtained:
\[
-\pi^{1/2} \frac{P_{12}}{\rho c_0^2} = \frac{5\pi R_0}{16} \left\{ \frac{M_{w,1}}{2} + \left( \frac{M_{w,1}}{2}, 15 \right) \right\} \sin^{-1} \left( \frac{M_{w,1}}{(M_{w,1} + 15)^{1/2}} \right) \tag{D16}
\]
To obtain the total heat transfer equation (D11) is integrated:
Appendix B

Confidence Limits of Results

For some number of sample molecules, a resulting quantity $Q$ is obtained. Repeating this process $k$ times will give a sample set of $Q$. The average of the $k$ values would give $\bar{Q}$, which is the average value of the sample set. If an infinite number of values of $Q$ were obtained, this would give a population of $Q$ with some average value $\langle Q \rangle$. The problem is finding the value of $\delta$ such that the absolute difference between $\langle Q \rangle$ and $\bar{Q}$ is less than $\delta$ with a 95 percent probability. The central limit theorem states that the distribution of sample means $f(Q)$ approaches a normal distribution with a mean value equal to the population mean and with a variance equal to the population variance divided by $k$, the size of the sample averaged to obtain the sample mean. Since the 95 percent confidence interval is defined as twice the standard deviation, $\delta = 2\sigma/(\kappa)^{1/2}$, where $\sigma^2$ is the approximation to the variance of the population obtained by finding the variance of the sample set

$$s^2 = \frac{(q^2 - \bar{q}^2)\kappa}{k - 1} \tag{E1}$$

This gives the 95 percent confidence interval $\delta$ as

$$|\langle Q \rangle - \bar{Q}| < \delta = 2\sqrt{(q^2 - \bar{q}^2)/\kappa}^{1/2} \tag{E2}$$

References

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Figure 1. - Model.

Figure 2. - Temperature distributions; wall-temperature ratio, 0.25; wall Mach number, 0.
2.3 Monte Carlo results, Knudsen number

Analytical solutions
- Collisionless, Kn → ∞
- 8 Moment linear (ref. 2), Kn = 2
- 4 Moment nonlinear (ref. 4), Kn = 2
- Continuum, Kn → 0
- Slip continuum

Figure 3. Density ratio for various Knudsen numbers; wall-temperature ratio, 0.25; wall Mach number, 0.

Monte Carlo results
- Present
- Ref. 6
Analytical solutions
- Slip continuum

Collisionless, Kn → ∞
- 8 Moment linear (ref. 2)
- 4 Moment nonlinear (ref. 4)
- Continuum, Kn → 0

Figure 4. Dimensionless heat flux; wall-temperature ratio, 0.25; wall Mach number, 0.
Figure 5. - Dimensionless heat flux, wall-temperature ratio, 0.25, wall Mach number, 0

Figure 6. - Velocity ratio distribution for various Knudsen numbers; wall Mach number, 4; wall temperature ratio, -
Monte Carlo results, Knudsen number

Analytical solutions
Collisionless, $Kn = \infty$
Continuum, $Kn \rightarrow 0$

Figure 7. - Temperature distribution for various Knudsen numbers; wall Mach number, 4; wall-temperature ratio, 1.

Analytical solutions
Continuum, $Kn \rightarrow 0$
Linearized (ref. 1)
Collisionless, $Kn = \infty$

Figure 8. - Dimensionless shear stress; wall-temperature ratio, 1; wall Mach number 4.
Monte Carlo results, Knudsen number

\[
\begin{align*}
\square & \quad 1 \times 10^{-20} \\
\triangle & \quad 2 \\
\triangle & \quad 1 \\
\end{align*}
\]

Shear stress:
(Closed symbols)

\[
\text{Shear stress} = \frac{\sqrt{2/\rho_A C_{W,0}^2}}{\sqrt{2/\rho_A C_{W,0}^2}} \left( \frac{\sqrt{2/\rho_A C_{W,0}^2}}{\sqrt{2/\rho_A C_{W,0}^2}} \right)_{Kn = \infty}
\]

Total energy transfer:
(Open symbols)

\[
\text{Total energy transfer} = \frac{\sqrt{2/\rho_A C_{W,0}^3}}{\sqrt{2/\rho_A C_{W,0}^3}} \left( \frac{\sqrt{2/\rho_A C_{W,0}^3}}{\sqrt{2/\rho_A C_{W,0}^3}} \right)_{Kn = \infty}
\]

Figure 9: Dimensionless total energy transfer and shear stress, wall-temperature ratio, 1; wall Mach number, 4.