N 66 29682

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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
Oxford, England, July 4-8, 1966

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION · WASHINGTON, D.C. · 1966

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RAREFIED GAS DYNAMICS

E-3361

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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 = average thermal velocity $(2R_gT)^{1/2}$
D = channel width
f = probability distribution function
Kn = Knudsen number $\lambda_M/D = m/\sqrt{2}\,\rho_A D\pi\sigma^2$
M = dimensionless velocity $u/C_{W,0}$

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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; $P_{ii}/3$

$P_{i,j}$ = shear stress $(-\rho\langle V_i'V_j'\rangle)$

p = zone or scoring-position number

p_f = last scoring-position number

Q = property of sample molecule

$\langle Q\rangle$ = averaged quantity $\int Qf\, d^3V$

$\langle Q\rangle_+$ = averaged quantity $\int Qf_+\, d^3V$

q = heat transfer

q_T = total energy transfer

R = random number between 0 and

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^* = velocity after collision

γ = defined by equations (B5) and (B6)

ϵ = defined by equations (B5) and (B6)

η = viscosity coefficient

κ = thermal conductivity

Θ = collision rate of sample molecule with target molecules

λ = path length to collision

λ_M = mean free path length through a Maxwellian gas with density ρ and thermal velocity C

λ_s = mean free path length

μ = dimensionless velocity, V'/C

$\mu_{R,A}$ = defined by equation (A11)

ρ = density

σ = diameter of hard sphere molecule

φ = angle between sample molecule and target molecule velocities

Subscripts:

A = averaged across channel

M = Maxwellian
M=0 = refers to case with both walls stationary
p = increment number
p_f = last increment
R = relative velocity
r = radial coordinate in cylindrical system
s = sample molecule
t = target molecule
w,0;w,1 = at wall 0,1
0,1 = evaluated next to 0,1
1,2,3 = coordinate directions
+,- = positive or negative x_2 direction

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 te peratures 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 wal 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 $u_{w,1}$ 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

$$\rho f_t = \rho_+ f_+ + \rho_- f_- = \frac{2\rho_+}{\pi^{3/2} C_+^3} \left[\exp\left(-\frac{V_+'^2}{C_+^2} \right) \right] \Bigg|_{V_2>0} + \frac{2\rho_-}{\pi^{3/2} C_-^3} \left[\exp\left(-\frac{V_-'^2}{C_-^2} \right) \right] \Bigg|_{V_2<0} \tag{1}$$

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

$$V_2 = (-C_w^2 \ln R_{V_2})^{1/2} \tag{2a}$$

$$V_1 = (-C_w^2 \ln R_{V_r})^{1/2} \cos 2\pi R_\theta + u_{1w} \tag{2b}$$

$$V_3 = (-C_w^2 \ln R_{V_r})^{1/2} \sin 2\pi R_\theta \tag{2c}$$

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 λ to $\lambda + d\lambda$ is given (refs. 8 and 9) as

$$f_\lambda = \frac{\exp(-\lambda/\lambda_s)}{\lambda_s} \tag{3}$$

where λ_s is the mean free path to collision of the sample 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:

$$\lambda = -\lambda_s \ln R_\lambda \tag{4}$$

To pick from this distribution, the mean free path λ_s for the sample molecule in the zone must be known. If the undirected velocities of the target molecules are in a Maxwellian distribution with an average thermal velocity C and density ρ, the mean free path for the sample molecule λ_M, as shown in appendix A, is given by

$$\frac{\lambda_M}{D} = \frac{\sqrt{2\pi}\ \mathrm{Kn} V_s}{C \frac{\rho}{\rho_A}\left[\exp\left(-\frac{V_s'^2}{C^2}\right) + \sqrt{\pi}\left(\operatorname{erf} \frac{V_s'}{C}\right)\left(\frac{V_s'}{C} + \frac{C}{2V_s'}\right)\right]} \tag{5}$$

where 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

$$f_t = f_{M+} + f_{M-} \tag{6}$$

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

$$\frac{1}{\lambda_s} = \frac{1}{\lambda_{M+}} + \frac{1}{\lambda_{M-}} \tag{7}$$

where λ_{M+} or λ_{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 λ is greater than this distance, the sample molecule is started at the beginning of the next zone with its velocity 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 λ_s/λ_{M+}. Then, for a picked random number, if $R < \lambda_s/\lambda_{M+}$, 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

$$\left.\begin{aligned} V_{1s}^* &= \frac{1}{2}(V_{1s} + V_{1t}) + V_R(1 - b^2)^{1/2} H \quad &(8a)\\ V_{2s}^* &= \frac{1}{2}(V_{2s} + V_{2t}) + V_R(1 - 2b^2) \quad &(8b)\\ V_{3s}^* &= \frac{1}{2}(V_{3s} + V_{3t}) + V_R(1 - b^2)^{1/2} \Xi \quad &(8c)\end{aligned}\right\}$$

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

$$H = 2R_H - 1,\ \Xi = 2R_\Xi - 1,\ \text{and}\ b^2 = H^2 + \Xi^2 \qquad (9)$$

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

The sample molecule history is then continued from the point of collision with its new velocity components. The 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

$$\rho\langle V_2Q\rangle_p = (\rho_+\langle V_2Q\rangle_+)_p + (\rho_-\langle V_2Q\rangle_-)_p$$

$$= \frac{\rho_{+,0}C_{w,0}}{N\pi^{1/2}}\left[\left(\sum^{S_+} Q\right)_p - \left(\sum^{S_-} Q\right)_p\right] \qquad (10)$$

If Q is taken as $1/V_2$,

$$\frac{\rho}{\rho_{+,0}} = \frac{\rho_+}{\rho_{+,0}} + \frac{\rho_-}{\rho_{+,0}} = \frac{C_{w,0}}{N\pi^{1/2}}\left[\left(\sum^{S_+}\frac{1}{V_2}\right)_p - \left(\sum^{S_-}\frac{1}{V_2}\right)_p\right] \qquad (11)$$

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, ρ_+, ρ_-, can be obtained as well as the local density ρ. 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

$$\frac{\rho u}{\rho_{+,0}C_{+,0}} = \frac{\rho_{+,p}u_{+,p}}{\rho_{+,0}C_{+,0}} + \frac{\rho_{-,p}u_{-,p}}{\rho_{+,0}C_{+,0}} = \frac{1}{N\pi^{1/2}}\left[\sum^{S+}\left(\frac{V_1}{V_2}\right) - \sum^{S-}\left(\frac{V_1}{V_2}\right)\right] \qquad (12)$$

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 $(1/2)R_gT$. This can be written as

$$\left(\frac{3}{2}\right)R_gT = \frac{1}{2}\langle V'^2\rangle = \frac{1}{2}\langle V^2\rangle - \frac{1}{2}u_1^2 \qquad (13)$$

Then from equation (10) is obtained

$$\frac{T}{T_{w,0}} = \frac{2}{3N\pi^{1/2}C_{w,0}}\left(\frac{\rho}{\rho_{+,0}}\right)^{-1}\left[\sum^{S_+}\left(\frac{V^2}{V_2}\right) - \sum^{S_-}\left(\frac{V^2}{V_2}\right)\right] - \frac{2u_1^2}{3C_{w,0}^2} \tag{14}$$

The thermal velocity of the molecules with $V_2 > 0$ is given by

$$\frac{C_+^2}{C_{w,0}^2} = \frac{2}{3C_{w,0}N\pi^{1/2}}\left(\frac{\rho_+}{\rho_{+,0}}\right)^{-1}\left[\sum^{S_+}\left(\frac{V^2}{V_2}\right)\right] - \frac{2}{3}\,\frac{u_{1,+}^2}{C_{w,0}^2} \tag{15}$$

and similarly for the molecules with $V_2 < 0$

$$\frac{C_-^2}{C_{w,0}^2} = -\frac{2}{3C_{w,0}N\pi^{1/2}}\left(\frac{\rho_-}{\rho_{+,0}}\right)^{-1}\left[\sum^{S_-}\left(\frac{V^2}{V_2}\right)\right] - \frac{2}{3}\,\frac{u_{1-}^2}{C_{w,0}^2} \tag{16}$$

The shear stress across the channel is given by $P_{12} = \rho\langle V_1'V_2'\rangle$. This can be shown to be equal to

$$P_{12} = \rho\langle V_1V_2\rangle = \frac{\rho_{+,0}C_{+,0}}{N\pi^{1/2}}\left(\sum^{S_+} V_1 - \sum^{S_-} V_1\right) \tag{17}$$

The total energy being transferred across the channel is given by

$$q_T = \frac{1}{2}\,\rho\langle V_2(V^2)\rangle = \frac{\rho_{+,0}C_{w,0}}{2N\pi^{1/2}}\left[\sum^{S_+}(V^2) - \sum^{S_-}(V^2)\right] \tag{18}$$

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

$$q = q_T - u_1P_{12} \tag{19}$$

By using these equations, the macroscopic quantities of interest are found. The values of ρ_+, ρ_-, C_+, C_- 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 carreid out 20 times with 2500 sample molecules each time for $Kn = 0.5$. The temperature and density had a value of δ, the 95 percent confidence interval, of close to 1 percent of their value, while the value of δ for the heat transfer across the channel was about 2 percent of its value. The derivations and equation used in obtaining δ 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 $M_w = u_{w1}/C_{w1}$ 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 in figure 10 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 became 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

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^3 for hard sphere molecules is given (ref. 8) as

$$d\Theta = \rho f_t V_R S \, dV_t^3$$

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

$$V_R = \left[(V_{1t} - V_{1s})^2 + (V_{2t} - V_{2s})^2 + (V_{3t} - V_{3s})^2\right]^{1/2} \qquad \text{(A2)}$$

If we subtract the local mean velocity u_1 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

$$d\Theta_M = \frac{\rho S}{m\pi^{3/2}c^3}\left(\exp - \frac{V_t'^2}{c^2}\right)V_R \, dV_{1t}' \quad dV_{2t} \, dV_{3t} \qquad \text{(A3)}$$

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

$$V_{it}' = A_{ij}^{-1}V_{jt}'' \qquad \text{(A4a)}$$

where

$$A_{ij}^{-1} = \begin{vmatrix} \frac{V_{2s}}{V_{rs}} & \frac{V_{1s}'}{V_s'} & \frac{-V_{3s}V_{1s}'}{V_{rs}V_s'} \\ \frac{-V_{1s}'}{V_{rs}} & \frac{V_{2s}}{V_s'} & \frac{-V_{3s}V_{2s}}{V_{rs}V_s'} \\ & \frac{V_{3s}}{V_s'} & \frac{V_{rs}}{V_s'} \end{vmatrix} \qquad \text{(A4b)}$$

The inverse transformation is given by

$$V_{it}'' = A_{ij}V_{jt}' \qquad \text{(A5a)}$$

where

$$A_{ij} = \begin{vmatrix} \dfrac{V_{2s}}{V_{rs}} & \dfrac{-V'_{1s}}{V_{rs}} & 0 \\ \dfrac{V'_{1s}}{V'_s} & \dfrac{V_{2s}}{V'_s} & \dfrac{V_{3s}}{V'_s} \\ \dfrac{-V_{3s}V'_{1s}}{V_{rs}V'_s} & \dfrac{-V_{2s}V_{3s}}{V_{rs}V'_s} & \dfrac{V_{rs}}{V'_s} \end{vmatrix} \qquad \text{(A5b)}$$

where $V_r = (V_1'^2 + V_2^2)^{1/2}$ and $V' = (V_r^2 + V_3^2)^{1/2}$ Then, equation (A3) becomes

$$d\Theta_M = \frac{\rho S}{m\pi^{3/2}C^3}\left(\exp - \frac{V_t''^2}{C^2}\right)\left[V''^2_{1t} + (V''_{2t} - V'_s)^2 + V''^2_{3t}\right]^{1/2} dV''^3_t \qquad \text{(A6a)}$$

Transforming into spherical coordinates

$$V''_{1t} = V'_t \cos\theta \sin\phi, \ V''_{2t} = V'_t \cos\varphi, \ V''_{3t} = V'_t \sin\theta \sin\varphi \qquad \text{(A6b)}$$

yields

$$d\Theta_M = \frac{C\rho S}{m\pi^{3/2}}\left[\exp(-\mu_t^2)\right]\mu_t^2\mu_R \sin\varphi \, d\varphi \, d\theta \, d\mu_t \qquad \text{(A7)}$$

where μ is the nondimensionalized velocity V'/C and where

$$\mu_R = (\mu_t^2 + \mu_s^2 - 2\mu_t\mu_s \cos\varphi)^{1/2} \qquad \text{(A8)}$$

To obtain the total collision rate for the target molecules over all velocities, equation (A7) must be integrated over φ, θ, and μ_t. Integrating over θ from 0 to π gives

$$d\Theta_M(\mu_t) = \frac{4\rho CS}{m\pi^{1/2}}\left[\exp(-\mu_t^2)\right]\mu_t^2\mu_{R,A} \, d\mu_t \qquad \text{(A9)}$$

$$\mu_{R,A} = \begin{cases} \mu_s + \mu_t^2/3\mu_s & \text{if } \mu_s > \mu_t \\ \mu_t + \mu_s^2/3\mu_t & \text{if } \mu_t > \mu_s \end{cases} \qquad \text{(A10)}$$

Integrating equation (A9) over μ_t from 0 to ∞, the total collision frequency Θ_M is obtained for a sample molecule moving at velocity μ_s through a Maxwellian gas:

$$\Theta_M = \frac{\rho S C}{m}\left[\frac{\exp(-\mu_s^2)}{\pi^{1/2}} + (\mathrm{erf}\,\mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right)\right] \qquad \text{(A11)}$$

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

$$\frac{\lambda_M}{D} = \frac{V_s}{\Theta_M} = \frac{\sqrt{2}\,\mathrm{Kn}V_s}{C\,\frac{\rho}{\rho_A}\left\{\frac{1}{\pi^{1/2}}\left[\exp(-\mu_s^2)\right] + (\mathrm{erf}\,\mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right)\right\}} \qquad \text{(A12)}$$

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 Θ_{M+} and Θ_{M-} are given as in equation (A12) but with different densities and mean thermal velocities. Since λ_s/D is given by V_s/Θ,

$$\lambda_s = \frac{D}{\frac{\Theta_{M+}}{V_s} + \frac{\Theta_{M-}}{V_s}} = \frac{1}{\frac{1}{\lambda_{M+}} + \frac{1}{\lambda_{M-}}} \qquad \text{(A13)}$$

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

$$\frac{d\Theta_M}{\Theta_M} = \frac{\left[\exp(-\mu_t^2)\right]\mu_t^2\mu_R \sin\varphi\, d\varphi\, d\mu_t}{\pi\left[\exp(-\mu_s^2)\right] + \pi^{3/2}(\mathrm{erf}\,\mu_s)\left(\mu_s \quad \frac{1}{2\mu_s}\right)} \qquad \text{(B1)}$$

The distribution in θ for the target-molecule collision partners is

$$f_\theta d_\theta = \frac{d\theta}{2\pi} \quad \text{or} \quad \theta = 2\pi R_\theta \qquad \text{(B2)}$$

The distribution of μ_t for the target-molecule collision partners is obtained from the marginal distribution

$$f_{\mu_t} d_{\mu_t} = \frac{4\left[\exp(-\mu_t^2)\right]\mu_t^2\mu_{RA} d\mu_t}{\left[\exp(-\mu_s^2)\right] + \pi^{1/2}(\text{erf } \mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right)} \qquad \text{(B3)}$$

Then μ_t can be picked from this distribution, using

$$R_{\mu_t} = \frac{\gamma(\mu_s,\mu_t) + \epsilon(\mu_s,\mu_t)}{\left[\exp(-\mu_s^2)\right] + \pi^{1/2}(\text{erf } \mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right)} \qquad \text{(B4)}$$

where, when $\mu_s > \mu_t$, $\epsilon = 0$ and

$$\gamma(\mu_s,\mu_t) = -2\mu_s\mu_t\left[\exp(-\mu_t^2)\right] + \mu_s\sqrt{\pi}(\text{erf } \mu_t) - \frac{2}{3}\frac{\mu_t^3}{\mu_s}\left[\exp(-\mu_t^2)\right] - \frac{\mu_t}{\mu_s}\left[\exp(-\mu_t^2)\right] + \frac{\sqrt{\pi}}{2\mu_s}(\text{erf } \mu_t) \qquad \text{(B5)}$$

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

$$\epsilon = -2\left[\exp(\mu_t^2)\right]\left(\frac{\mu_s^2}{3} + 1 + \mu_t^2\right) + \left[2\exp(-\mu_s^2)\right]\left(\frac{4\mu_s^2}{3} + 1\right) \qquad \text{(B6)}$$

To find φ for the target molecule, the distribution of target molecules can be written as a product of a marginal times a conditional distribution

$$\frac{d\Theta(\mu_t,\varphi)}{\Theta} = f(\mu_t)f(\varphi|\mu_t) \qquad \text{(B7)}$$

Then it is necessary to pick φ from the conditional distribution:

$$f(\varphi|\mu_t) = \frac{\mu_R \sin\varphi \, d\varphi}{2\mu_{R,A}} \qquad \text{(B8)}$$

Picking φ for a given μ_t is found as before from

$$R_\varphi = \frac{\mu_R^3 - |\mu_t - \mu_s|^3}{(\mu_t^2 + \mu_s^2 + 2\mu_t\mu_s)^{3/2} - |\mu_t - \mu_s|^3} \qquad \text{(B9)}$$

After picking φ, μ_t, and θ, it is necessary to find the velocity components V''_{it}, using equation (A6b). Then, from equation (A4),

$$V_{1t} = V''_{1t}\left(\frac{V_{2s}}{V_{rs}}\right) + V''_{2t}\left(\frac{V'_{1s}}{V'_s}\right) - V''_{3t}\left(\frac{V_{3s}V'_{1s}}{V_{rs}V'_s}\right) + u_1 \qquad \text{(B10a)}$$

$$V_{2t} = - V''_{1t}\left(\frac{V'_{1s}}{V_{rs}}\right) + V''_{2t}\left(\frac{V_{2s}}{V'_s}\right) - V''_{3t}\left(\frac{V_{2s}V_{3s}}{V'_{rs}V'_s}\right) \qquad \text{(B10b)}$$

$$V_{3t} = 0 + V''_{2t}\left(\frac{V_{3s}}{V'_s}\right) + V''_{3t}\left(\frac{V_{rs}}{V'_s}\right) \qquad \text{(B10c)}$$

APPENDIX C

Collisionless Solution

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

$$\rho f_\infty = \frac{2\rho_{w,0}}{\pi^{3/2}C^3_{w,0}}\left[\exp -\left(\frac{V'^2_{w,0}}{C^2_{w,0}}\right)\right]\Bigg|_{V_2>0} + \frac{2\rho_{-1}}{\pi^{3/2}C^3_{w,1}}\left[\exp - \left(\frac{V'^2_{w,1}}{C^2_{w,1}}\right)\right]\Bigg|_{V_2<0} \qquad \text{(C1)}$$

The local density is then given by $\rho\langle 1\rangle = \rho = \rho_{+0} + \rho_{-1}$. Since there is no net flow across the channel, one can write $\rho\langle V_2\rangle = \frac{1}{\pi^{1/2}}\left[\rho_{+,0}C_{w,0} - \rho_{-1}C_{w,1}\right] = 0$. Combining gives

$$\left(\frac{\rho_{+,0}}{\rho}\right)_\infty = \frac{1}{1 + t_{w,1}^{-1/2}}\ ; \ \left(\frac{\rho_{-1}}{\rho}\right)_\infty = 1 - \frac{\rho_{+,0}}{\rho} \qquad \text{C2)}$$

The flow parallel to the channel wall is given by

$$u_1 = \langle V_1 \rangle = \frac{\rho_{+,0}}{\rho} u_{1,w,0} + \frac{\rho_{-1}}{\rho} u_{1,w,1} \qquad \text{(C3)}$$

The local temperature is given by $\frac{T}{T_{w,0}} = \frac{2}{3C_{w,0}^2} \langle V_1^2 + V_2^2 + V_3^2 \rangle - \frac{1}{2} M^2$ which, when integrated gives

$$t = \frac{2}{3}\left(\frac{\rho_{+,0}}{\rho} M_{w,0}^2 + \frac{\rho_-}{\rho} M_{w,1}^2 - M^2\right) + \frac{\rho_+}{\rho}\left(1 + t_{w,1}^{1/2}\right) \qquad \text{(C4)}$$

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

$$\frac{\pi^{1/2} P_{12}}{\rho 2R_g T_{w,0}} = \frac{\rho_+}{\rho}(M_{w,0} - M_{w,1}) \qquad \text{(C5)}$$

The total energy transferred given by $q_T = \frac{\rho}{2}\langle V'^2 V_2 \rangle + u_1 P_{12}$ is

$$\frac{\pi^{1/2} q_T}{\rho(2R_g T_{w,0})^{3/2}} = \frac{\rho_{+,0}}{\rho} - \frac{\rho_{-1}}{\rho} t_{w,1}^{3/2} + \frac{\rho_{+,0}}{\rho} \frac{M_{w,0}^2}{2} - \frac{\rho_{-1}}{\rho} \frac{M_{w,1}^2}{2t_{w,1}^{1/2}} \qquad \text{(C6)}$$

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

$$\frac{\partial}{\partial x_i}(\rho\langle V_i Q \rangle) = \frac{1}{m} \Delta Q \qquad \text{(D1)}$$

where ΔQ 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:

$$\frac{\partial}{\partial x_i}(\rho u_i) = 0 \qquad \text{(D2)}$$

$$\rho u_i \frac{\partial u_j}{\partial x_i} = - \frac{\partial}{\partial x_i} \rho \langle V_i' V_j' \rangle = - \frac{\partial}{\partial x_i} P_{ij} \qquad \text{(D3)}$$

$$\frac{\partial}{\partial x_i}(\rho u_i u_j^2) + \frac{\partial}{\partial x_i}(u_i P_{jj}) \quad \frac{\partial}{\partial x_i}(\rho \langle V_i' V_j'^2 \rangle) + \frac{\partial}{\partial x_i}(2u_j P_{ij}) = 0 \qquad \text{(D4)}$$

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

$$\frac{1}{2} \rho \langle V_i' V'^2 \rangle = q_i = - \kappa \frac{\partial T}{\partial x_i} \qquad \text{(D5)}$$

$$P_{ij} = \delta_{ij} P - 2\mu \left(\frac{1}{2} \frac{\partial u_i}{\partial x_j} + \frac{1}{2} \frac{\partial u_j}{\partial x_i} - \frac{1}{3} \delta_{ij} \frac{\partial u_\kappa}{\partial x_\kappa} \right) \qquad \text{(D6)}$$

Since, in the present model, there is no x_1 or x_3 dependence, these results simplify to give $u_1 = g(x_2)$, p = 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

$$\kappa = \kappa_0 t^{1/2} \qquad \kappa_0 = \frac{75m}{64\sigma^2} \frac{R_g C_0}{(2\pi)^{1/2}} \qquad \text{(D7)}$$

$$\mu = \mu_0 t^{1/2} \qquad \mu_0 = \frac{5mC_0}{16\sigma^2 (2\pi)^{1/2}} \qquad \text{(D8)}$$

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

Since the pressure across the channel is constant using the ideal gas law,

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

The heat transfer across the channel can be found equal to

$$\left(\frac{q}{\rho_A C_0^3}\right)_{M=0} = \frac{25}{64} \pi^{1/2} \left(1 - t_{w,1}^{3/2}\right) Kn \qquad \text{(D1C}$$

When the upper wall is moving, the energy equation can be written as

$$\frac{\partial}{\partial x_2}\left(C_pT + \frac{u_1^2}{2}\right) = -\frac{C_p}{\kappa}\,q_T \tag{D11}$$

This can be rewritten using $(\mu C_p/\kappa) = 2/3$; $C_p = (5/2)R_g$, as

$$\frac{\partial}{\partial x_2}\left(t + \frac{4}{15}M^2 - \frac{8}{15}\,\frac{q_t}{P_{12}C_0}\,M\right) = 0 \tag{D12}$$

When the upper wall is moving at a velocity $u_{w,1}$ 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

$$P_{12} = -\mu_0 t^{1/2}\frac{\partial u_1}{\partial x_2} \tag{D14}$$

This can be integrated to give

$$x_2 = \left\{\left(\frac{15}{4} + M_{w,1}M - M^2\right)^{1/2}\left(\frac{2M - M_{w,1}}{4}\right) + \left(\frac{15}{4}\right)^{1/2}\frac{M_{w,1}}{4} - \left(\frac{M_{w,1}^2 + 15}{8}\right)\left[\sin^{-1}\left(\frac{M_{w,1} - 2M}{(15 + M_{w,1}^2)^{1/2}}\right) - \sin^{-1}\left(\frac{M_{w,1}}{(15 + M_{w,1}^2)^{1/2}}\right)\right]\right\} \Bigg/ \left\{(15)^{1/2}\frac{M_{w,1}}{4} + \frac{(M_{w,1}^2 + 15)}{4}\left[\sin^{-1}\left(\frac{M_{w,1}}{(15 + M_{w,1}^2)^{1/2}}\right)\right]\right\} \tag{D15}$$

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:

$$\frac{-\pi^{1/2}P_{12}}{\rho C_0^2} = \frac{5\pi Kn}{16}\left\{\frac{M_{w,1}}{2} + \frac{(M_{w,1}^2 + 15)}{2-\sqrt{15}}\left[\sin^{-1}\left(\frac{M_{w,1}}{(M_{w,1} + 15)^{1/2}}\right)\right]\right\} \tag{D16}$$

To obtain the total heat transfer equation (D11) is integrated:

$$\left(\pi^{1/2}\,\frac{q_t}{\rho C_0^3}\right) = \left(\frac{\pi^{1/2}P_{12}}{\rho C_0^2}\right)\frac{M_{w,1}}{2} \qquad \text{(D17)}$$

Appendix E

Confidence Limits of Results

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

$$S^2 = \frac{(\overline{Q^2} - \bar{Q}^2)\kappa}{\kappa - 1} \qquad \text{(E1)}$$

This gives the 95 percent confidence interval δ as

$$|\langle Q\rangle - \bar{Q}| \overline{<} \delta = 2\left(\frac{\overline{Q^2} - \bar{Q}^2}{\kappa - 1}\right)^{1/2} \qquad \text{(E2)}$$

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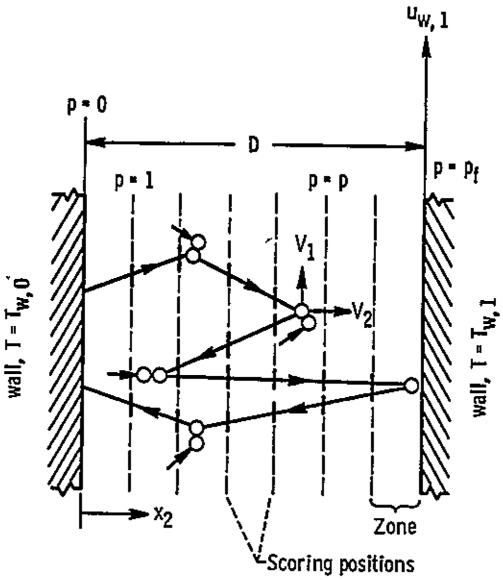

Figure 1. - Model.

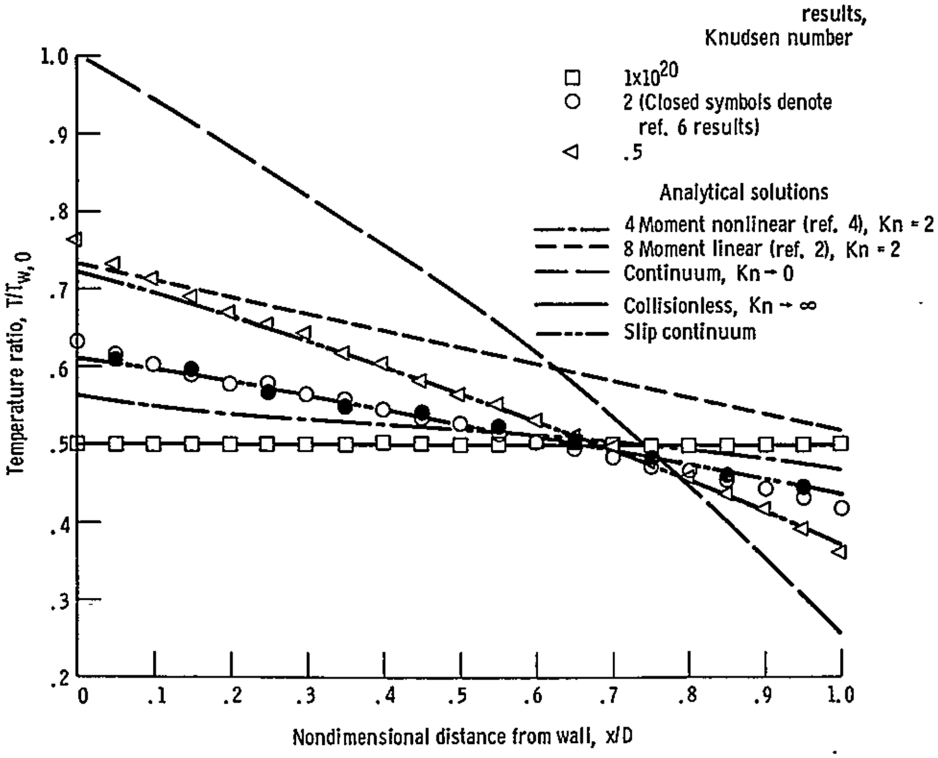

Figure 2. - Temperature distributions; wall-temperature ratio, 0.25; wall Mach number, 0.

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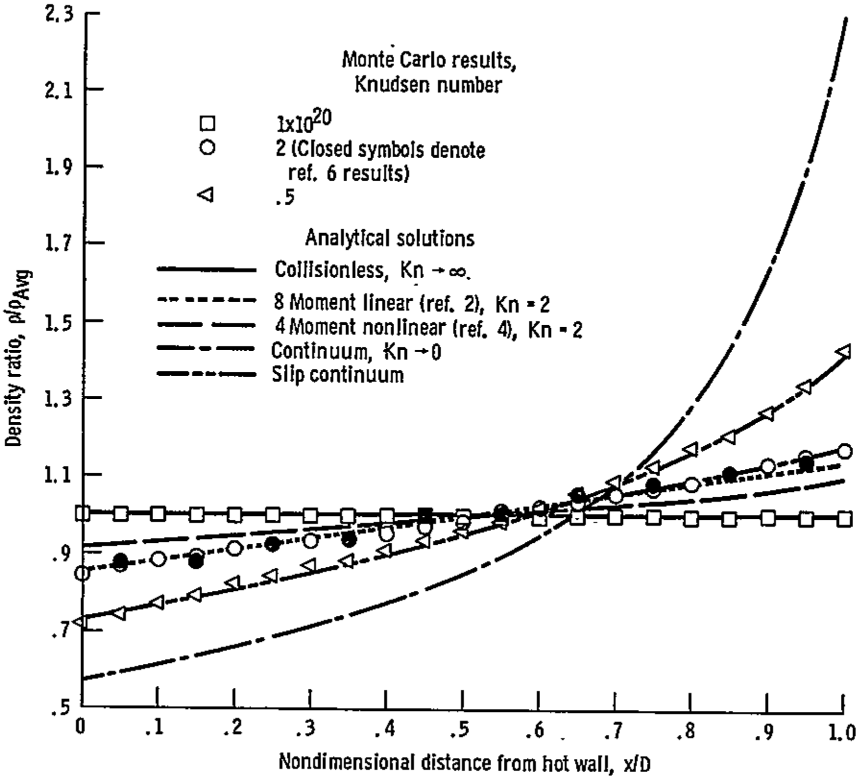

Figure 3. - Density ratio for various Knudsen numbers; wall-temperature ratio, 0.25; wall Mach number, 0.

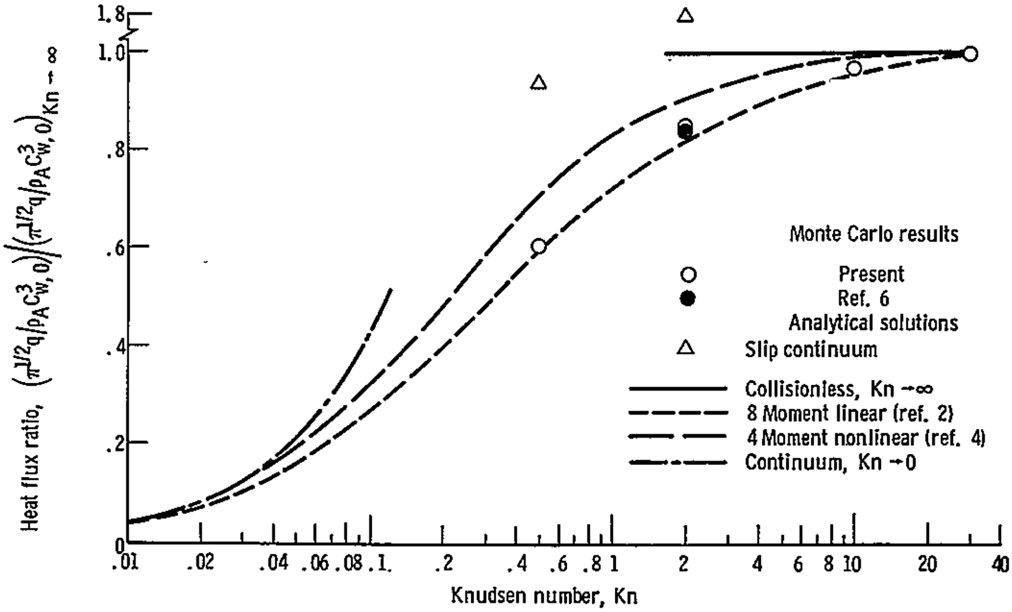

Figure 4. - Dimensionless heat flux; wall-temperature ratio, 0.25; wall Mach number, 0.

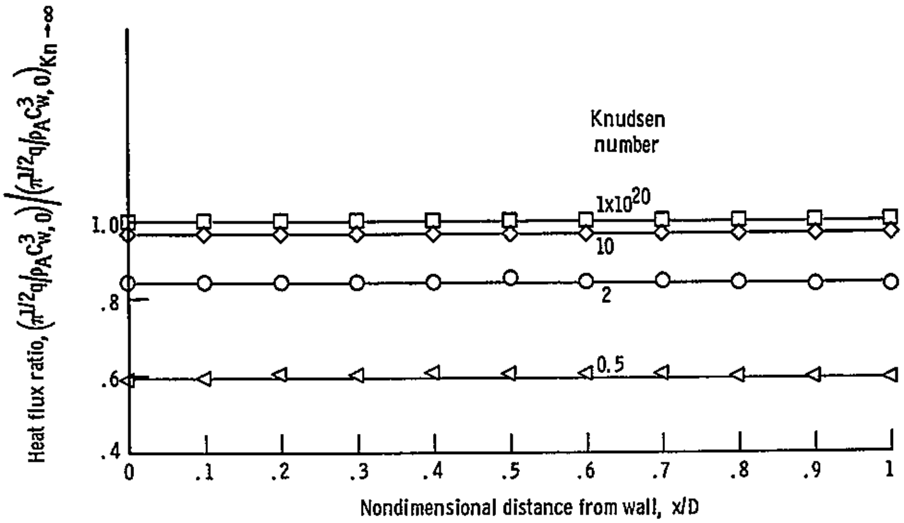

Figure 5. - Dimensionless heat flux; wall-temperature ratio, 0.25; wall Mach number, 0

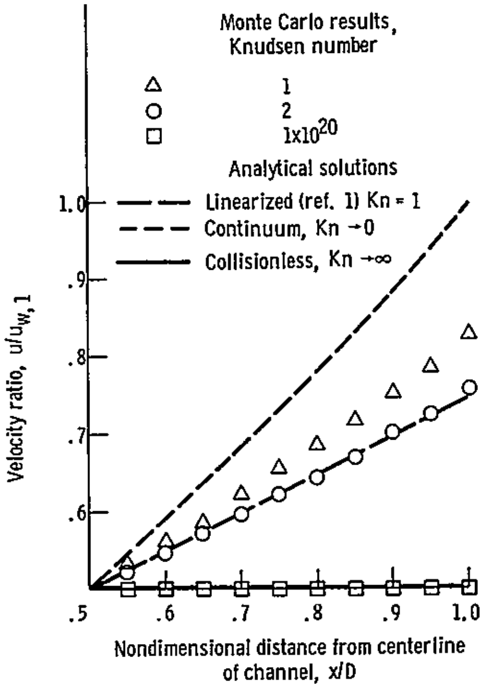

Figure 6. - Velocity ratio distribution for various Knudsen numbers; wall Mach number, 4; wall temperature ratio,

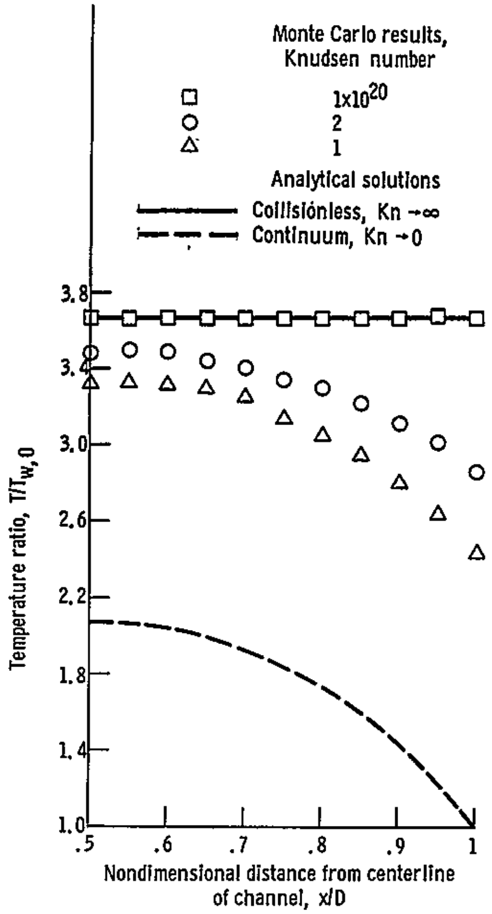

Figure 7. - Temperature distribution for various Knudsen numbers; wall Mach number, 4; wall-temperature ratio, 1.

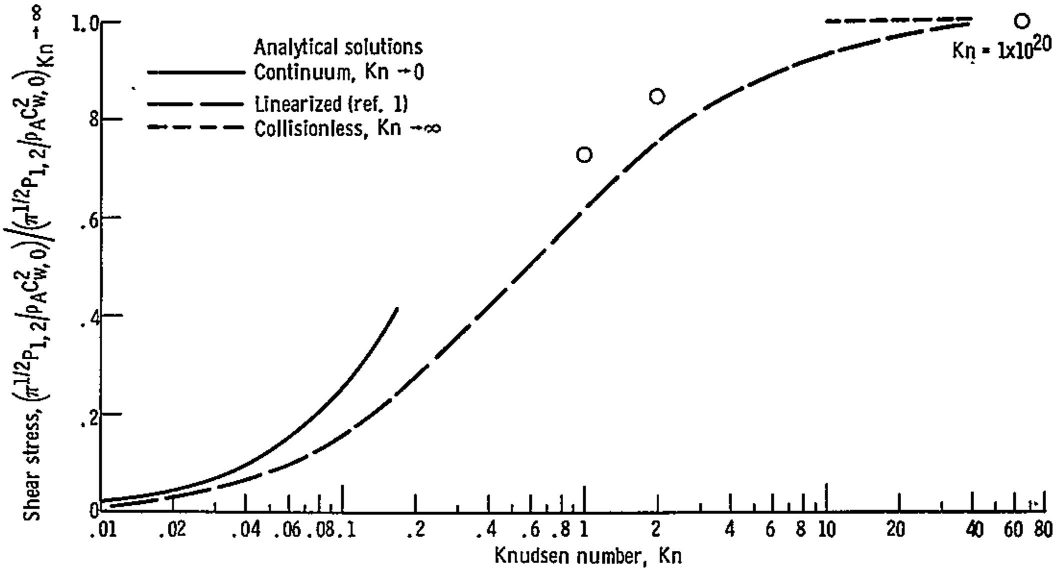

Figure 8. - Dimensionless shear stress; wall-temperature ratio, 1; wall Mach number 4.

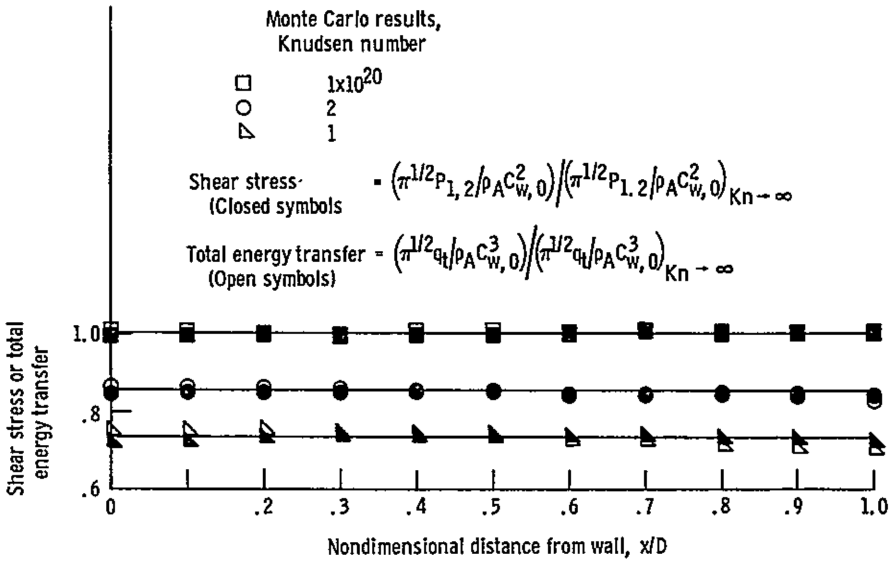

Figure 9. - Dimensionless total energy transfer and shear stress; wall-temperature ratio, 1; wall Mach number, 4.