NASA TECHNICAL NOTE

NASA TN D-4579
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RAREFIED-GAS COUETTE FLOW AND HEAT TRANSFER BETWEEN PARALLEL PLATES BY MODEL SAMPLING

by Morris Perlmutter

Lewis Research Center

Cleveland, Ohio

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION • WASHINGTON, D. C. • MAY 1968

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ABSTRACT

A rarefied gas with hard-sphere molecules enclosed between parallel walls is analyzed for the case of couette flow and heat transfer by a model sampling procedure. In one case, both walls are stationary and at different temperatures. In the other case, the upper wall is moving in a direction parallel to the lower wall and both walls are at the same temperature. The wall accommodation factor is taken as unity. The target molecule velocity distribution is presumed to be the sum of two different half-Maxwellians. The parameters describing the half-Maxwellians are assumed constant over a given zone. By scoring the properties of sample molecules as they pass scoring positions, the macroscopic quantities, of interest are obtained. The problem is iterated until these values agree with the assumed distribution values.

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SUMMARY

A rarefied gas with hard-sphere molecules enclosed between parallel walls is analyzed for the case of couette flow and heat transfer by a model sampling procedure. In one case, both walls are stationary and at different temperatures. In the other case, the upper wall is moving in a direction parallel to the lower wall and both walls are at the same temperature. The wall accommodation factor is taken as unity. The wall temperature ratio and wall velocity are taken large so that linearized solutions are not applicable. The channel between the walls has been divided into zones with boundary surfaces parallel to the walls. The target molecule velocity distribution in each zone is presumed to be the sum of two different half-Maxwellians. The parameters describing the half-Maxwellians are assumed constant over a given zone. By scoring the properties of 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 for the target molecule distribution in that zone. The problem is iterated until these values agree.

INTRODUCTION

In rarefied gas transport problems the usual macroscopic approach using Newton's law of friction or Fourier's equation for conduction is no longer applicable because these equations are derived assuming small changes of fluid properties over the mean free path lengths of the molecules. Therefore, a microscopic approach based on the kinetic theory of gases must be used.

The present analysis treats a system consisting of 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. In the present model, the molecules are assumed to have hard-sphere collisions and a wall accommodation coefficient of 1. The problem is analyzed by a Monte Carlo technique, that is, a model sampling procedure. The Monte Carlo method has been extensively used in the field of neutron transport theory. Reference 1 discusses the Monte Carlo method and its various techniques and applications.

Several analytical treatments of the couette flow problem have been carried out (refs. 2 to 5). In general, these consisted of setting up systems of moment equations which are solved to obtain the space dependence of the parameters occurring in the velocity distribution functions. Gross and Ziering used the linearized form of the Boltzmann equation to consider the case where the wall velocities were relatively low and both walls were at the same temperature (ref. 2), and the case where both walls were stationary but at different temperatures (ref. 3). The local molecular velocity distribution was taken as two-sided, each side being approximated by a different polynomial, and then half-range moments were formed from the linearized form of the Boltzmann equations. Liu and Lees (ref. 4) assumed a two-sided Maxwellian velocity distribution and Maxwellian molecule collisions, that is, the repulsive force between the molecules varied inversely as the fifth power of the distance between molecule centers. The moment equations led to the determination of macroscopic quantities of interest such as temperature and heat transfer. This same approach was used by Lavin and Haviland (ref. 5) for the case of stationary walls at different temperatures assuming hard-sphere interaction potentials for the molecular collisions.

In the method of solution based on the Monte Carlo method, sample molecule histories are generated by randomly picking choices at points of decision in the history of the sample molecule from the appropriate probability distributions. The sample molecules are followed through the mathematical model of the system, and by averaging molecular properties at various positions the macroscopic quantities describing the system can be obtained. This method reduces the complexity of the analysis since the relations involved the setting up a single sample molecule history are relatively simple; thus, simplifying approximations made in the analytical procedures are avoided. However, the Monte Carlo method requires extensive calculations on a high-speed computer to obtain the many sample histories needed to obtain necessary accuracy.

The Monte Carlo method was used by Perlmutter (ref. 6) to treat a collisionless plasma flowing through a channel with an imposed magnetic field; by Haviland (ref. 7) to treat a rarefied gas enclosed between stationary parallel plates at different temperatures; and by Perlmutter (refs. 8 and 9) to determine the heat transfer through a gas between stationary walls at different temperatures. In the analysis by Haviland (ref. 7), the amounts of time the sample molecule spent in the zone into which the channel had been divided were noted, and from these values a numerical table could be made up for

the molecular velocity distribution in each zone. This distribution constituted the target molecule distribution in the next iteration. After three or four iterations, although full convergence was not obtained, no evidence of the results being nonconvergent was found. The moments of the distribution for each zone corresponding to the macroscopic quantity of interest was then found by integration of the last obtained velocity distribution. In the analysis by Perlmutter (refs. 8 and 9) a full Maxwellian was assumed for the form of the target molecule velocity distribution with assumed initial values of the parameters under investigation. Then by summing properties of the sample molecules as they cross the zone boundaries, the macroscopic local conditions could be found. These new parameters of the target molecule distribution served as the basis for the next iteration of the target molecule distribution as in Haviland's case. Three or four iterations were needed to obtain the required agreement.

The present analysis also follows a sample molecule traveling through the model. However, in the present case, the target molecule velocity distribution in each zone within the channel is assumed to be two half-Maxwellian distributions of the form assumed by Liu and Lees in reference 4. By averaging 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.

SYMBOLS

C   average thermal velocity $(2R_gT)^{1/2}$

c_p specific heat at constant pressure

D   channel width

erf(x)   error function $(2/\sqrt{\pi}) \int_0^x e^{-u^2} du$

f   probability density function

g   quantity obtained by Monte Carlo procedure (appendix F)

K   Boltzmann's constant

Kn   Knudsen number, $\lambda_M/D = m/\sqrt{2} \, \rho_A D\pi\sigma^2$

k   number of values of g obtained (appendix F)

M   dimensionless velocity, u/C_{w0}

m   mass of molecule

N	number of sample molecules emitted from surface $w0$ in Monte Carlo run, proportional to flux of molecules leaving surface $w0$
P	pressure, $P_{ii}/3$
P_{ij}	shear stress, $-\rho \langle V_i' V_j' \rangle$
Pr	Prandtl number, $\mu c_p / K$
p	zone or scoring-position number
p_f	last scoring-position situated at surface $w1$
Q	property of sample molecule
$\langle Q \rangle$	average quantity $\int Q f \, d^3 V$
$\langle Q \rangle_+$	average quantity $\int Q f_+ \, d^3 V$
q	heat-transfer rate
q_T	total energy transfer rate
R	random number between 0 and 1
R_g	gas constant, K/m
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_{w0}
u_i	mean velocity, i^{th} component
u_{i+}, u_{i-}	i^{th} mean velocity of molecules in positive, negative x_2-direction
u_{w0}, u_{w1}	velocity of walls 0 and 1
V_i	molecular velocity, i^{th} component
V_i'	thermal velocity, $V_i - u_i$
V_i''	transformed i^{th} component of thermal velocity
V_i^*	velocity after collision
V_R	relative velocity
X_i	i^{th} coordinate
x_i	dimensionless i^{th} coordinate, x_i/D
γ	defined by eqs. (C6) and (C7)

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ϵ	defined by eqs. (C6) and (C7)
η	viscosity coefficient
κ	thermal conductivity
Θ	collision rate of sample molecule with target molecules
θ	angle
λ	path length to collision
λ_M	mean free path length through Maxwellian gas with density ρ and thermal velocity C
λ_s	mean free path length
μ	dimensionless velocity, V'/C
μ_R	relative dimensionless velocity, V'_R/C
$\mu_{R,A}$	defined by eq. (B10)
ρ	mass density
σ	diameter of hard sphere molecule
φ	angle

Subscripts:

A	averaged across channel
M	Maxwellian
M=0	both walls stationary
p	zone or scoring position number
p_f	last zone or scoring position number, situated at surface w1
R	relative velocity
r	radial coordinate in cylindrical system
s	sample molecule
t	target molecule
w0	wall 0
w1	wall 1
α, β	subscripts used in appendix B
0;1	evaluated in gas adjacent to wall 0 or 1
1, 2, 3	coordinate directions

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+, −   positive or negative x_2-direction

∞   collisionless solution

ANALYSIS

The problem under consideration is the determination of the properties of a rarefied gas contained between two parallel walls, each infinite in area. As can be seen from figure 1, which illustrates the geometry involved, the normal to the walls is in the x_2-direction. One wall is located at $x_2 = 0$, the other at $x_2 = 1$. The wall at $x_2 = 0$ is stationary and at temperature T_{w0}; the other wall at $x_2 = 1$ is moving with a velocity u_{w1} in the x_1-direction and its temperature is T_{w1}.

The channel width is divided into zones, with boundary surfaces parallel to the walls. The zones act to break up the distance between walls into subintervals. Sample molecule histories are generated by starting out from the wall a molecule picked from a Maxwellian velocity distribution corresponding to the wall temperature and following the molecule through the various zones where it can collide with target molecules distributed throughout the space between the walls. In each zone, the velocity distribution of the target molecules is taken as uniform over the zone and consists of two half-Maxwellians, each half corresponding to a different temperature, density, and velocity. Thus the velocity distribution of target molecules per unit velocity space is given by

$$\rho f_t = \begin{cases} \rho_+ f_+ = \dfrac{2\rho_+}{\pi^{3/2} C_+^3}\left[\exp\left(-\dfrac{V_+'^2}{C_+^2}\right)\right] & \text{for } V_2 > 0 \\[2em] \rho_- f_- = \dfrac{2\rho_-}{\pi^{3/2} C_-^3}\left[\exp\left(-\dfrac{V_-'^2}{C_-^2}\right)\right] & \text{for } V_2 < 0 \end{cases} \tag{1}$$

where the subscript + refers to molecules moving in the positive V_2 direction, that is, toward the wall w1 at $x_2 = 1$ and the subscript − refers to molecules moving toward w0 at $x_2 = 0$. It is assumed that the molecules reflected from the walls are perfectly accommodated, that is, the reflected molecules are assumed to have been emitted from a Maxwellian distribution corresponding to the wall temperature. The velocity of the sam-

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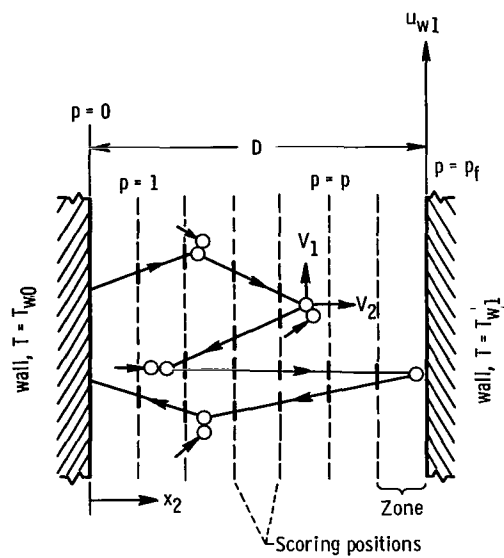
(a) Constant property zones.
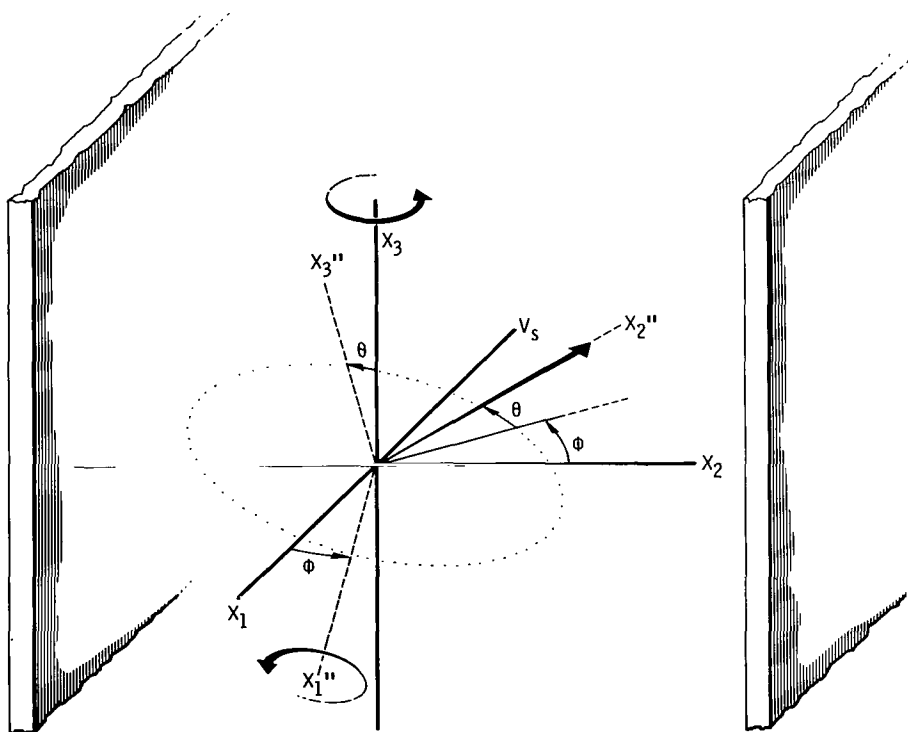
(b) Rotation of coordinate axis for sample molecule.

Figure 1. – Analytical model of channel.

ple molecule leaving the wall (computer flow chart position 1, see fig. 2) as derived in appendix A is given by

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

$$V_{1w} = \left(-C_w^2 \ln R_{V_r}\right)^{1/2} \cos 2\pi R_\theta + u_w \tag{2b}$$

$$V_{3w} = \left(-C_w^2 \ln R_{V_r}\right)^{1/2} \sin 2\pi R_\theta \tag{2c}$$

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 it is necessary to calculate its path length to first collision (flow chart position 2) to find if it has undergone a collision before passing through the first zone. The probability density function that a sample molecule will collide in the incremental path length λ to $\lambda + d\lambda$ is given (refs. 9 and 10) as

$$f_\lambda = \frac{\exp\left(-\dfrac{\lambda}{\lambda_s}\right)}{\lambda_s} \tag{3}$$

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 first collision for the sample molecule can be chosen from this distribution by the same procedure used previously, that is, employing the random number R_λ with range between 0 and 1 and relating it to mean free path λ by the equation

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

In order 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 were in a

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Figure 2. - Monte Carlo flow chart. (Blocks designated positions 1 to 5 are discussed in text.)

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 B (eq. (12)), would be given by

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

where Kn is the usual definition of Knudsen number for a gas in a Maxwellian distribution with hard-sphere molecule collisions.

However, the target molecule velocity distribution has been assumed to be two half-Maxwellians (eq. (1)). The direct calculation for a collision for a sample molecule with a target molecule picked from this distribution would be very complex. One method of treating the collision that introduces no additional assumptions and allows the calculations to be greatly simplified, although at the expense of additional calculations, is to resort to the following artifice.

The assumption is made that the distribution of target molecules consists of two full Maxwellian distributions:

$$\rho f_t = 2\rho_+ f_{M+} + 2\rho_- f_{M-} \tag{6}$$

where f_{M+} and f_{M-} are Maxwellian distributions with densities $2\rho_+$ and $2\rho_-$ and thermal velocities of C_+ and C_-, respectively. (It is realized that the molecules corresponding to f_{M+} with $V_2 < 0$ and the molecules corresponding to f_{M-} with $V_2 > 0$ are in actuality not present in the present model.) This assumption permits the calculation of the mean free path using the Maxwellian distribution relations (eq. (B13) of appendix B). Thus, the mean free path for a sample molecule moving through the two full Maxwellian gases is given by

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

where λ_{M+} and λ_{M-} are determined by equation (5), appropriately modified by $+$ and $-$ subscripts, respectively.

The mean free path λ_s calculated in this manner will be shorter than for the case for the assumed two half-Maxwellian target distributions (eq. (1)), since collisions with the nonexistent target molecules are now included. These collisions with nonexistent

target molecules are made to have no effect on the sample molecule, by taking the path and velocity of the sample molecule as unchanged after a collision with a nonexistent target molecule. In essence, then, the nonexistent target molecules do not interact with the sample molecule.

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 (flow chart position 3). 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 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 from which the target molecule collision partner is to be picked 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 C.

If the V_{2t} picked from the f_{M+} distribution is negative or, if the V_{2t} picked from f_{M-} is positive, a collision does not occur because these target molecules are nonexistent, as discussed previously. In these cases, the sample molecule continues on from the point of no collision with its original velocity.

After collision of the sample molecule with the chosen collision partner, the new components of velocity V_{is}^*, i = 1, 2, 3, of the sample molecule (flow chart position 4) are given (ref. 7) by

$$V_{1s}^* = \frac{1}{2}(V_{1s} + V_{1t}) + V_R(1 - b^2)^{1/2} H \tag{8a}$$

$$V_{2s}^* = \frac{1}{2}(V_{2s} + V_{2t}) + \frac{V_R}{2}(1 - 2b^2) \tag{8b}$$

$$V_{3s}^* = \frac{1}{2}(V_{3s} + V_{3t}) + V_R(1 - b^2)^{1/2} \Xi \tag{8c}$$

where V_R is given by equation (B2). The values of H and Ξ are obtained by picking two random numbers which are used in the following equations:

$$\left.\begin{array}{c} H = 2R_H - 1 \\[2mm] \Xi = 2R_\Xi - 1 \\[2mm] b^2 = H^2 + \Xi^2 \end{array}\right\} \tag{9}$$

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 history is completed when the sample molecule is returned to the surface from which it had been emitted. The numbers of sample molecule histories originating at the two walls were taken equal.

The reason for emitting sample molecules from both walls was to improve the accuracy of the results. Especially for the cases involving small mean free paths, not enough of the sample molecules emitted from one wall reach the other wall to give sufficiently large sample sizes. This problem was avoided by emitting sample molecules from both walls.

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 (flow chart position 5). If some property of the molecule is designated by Q, the average quantity of Q transported per sample molecule across the scoring cross section p in the positive x_2 direction can be written as

$$\frac{\left(\displaystyle\sum_{}^{S_+} Q\right)_p}{S_{+,p}} \approx \frac{\left(\rho_+ \displaystyle\int QV_{2_+} f_+ \, d^3v\right)_p}{\left(\rho_+ \displaystyle\int V_{2_+} f_+ \, d^3v\right)_p} \equiv \frac{\left(\rho_+ \langle QV_2\rangle_+\right)_p}{\left(\rho_+ \langle V_2\rangle_+\right)_p} \tag{10}$$

where $S_{+,p}$ is the number of sample molecules passing across the scoring cross section p in the positive x_2 direction. Similarly, the average quantity Q transported per sample molecule in the negative x_2 direction is

$$\frac{\left(\overset{S_-}{\underset{}{\sum}} Q\right)_p}{S_{-,p}} \approx \frac{\left(\rho_- \langle QV_2 \rangle_-\right)_p}{\left(\rho_- \langle V_2 \rangle_-\right)_p} \tag{11}$$

Since there is no net flow across the channel and all sample histories start and end at the same wall, $S_{+,p} = S_{-,p}$ and

$$\left(\rho_+ \int V_2 f_+ \, d^3 v\right)_p = -\left(\rho_- \int V_2 f_- \, d^3 v\right)_p \tag{12}$$

Then, since $\rho \langle V_2 Q \rangle = \rho_+ \langle V_2 Q \rangle_+ + \rho_- \langle V_2 Q \rangle_-$,

$$\frac{\rho \langle V_2 Q \rangle}{\rho_+ \langle V_2 \rangle_+} = \frac{1}{S_+} \left(\overset{S_+}{\underset{}{\sum}} Q - \overset{S_-}{\underset{}{\sum}} Q\right) \tag{13}$$

can be obtained.

The number of sample molecules S_+ that pass the scoring cross section in the positive X_2 direction at p divided by the total number N of sample molecule histories leaving wall 0, can be related to the mass flux passing in the positive X_2 direction at p by

$$\frac{S_{+,p}}{N} \approx \frac{\left(\rho_+ \langle V_2 \rangle_+\right)_p}{\left(\rho_+ \langle V_2 \rangle_+\right)_{w0}} \tag{14}$$

where $\left(\rho_+ \langle V_2 \rangle_+\right)_{w0}$ the mass flux leaving wall w0, is equal to $\rho_{+,w0} C_{w,0} / \pi^{1/2}$. Combining equations (13) and (14) results in

$$\rho \langle V_2 Q \rangle_p = \left(\rho_+ \langle V_2 Q \rangle_+ \right)_p + \left(\rho_- \langle V_2 Q \rangle_- \right)_p = \frac{\rho_{+0} C_{w0}}{N_\pi^{1/2}} \left(\overset{S_+}{\sum} Q - \overset{S_-}{\sum} Q \right)_p \tag{15}$$

If Q is taken as $1/V_2$, equation (15) gives

$$\left(\frac{\rho}{\rho_{+0}} \right)_p = \left(\frac{\rho_+}{\rho_{+0}} \right)_p + \left(\frac{\rho_-}{\rho_{+0}} \right)_p = \frac{C_{w0}}{N_\pi^{1/2}} \left[\left(\overset{S_+}{\sum} \frac{1}{V_2} \right)_p - \left(\overset{S_-}{\sum} \frac{1}{V_2} \right)_p \right] \tag{16}$$

Thus, summing the inverse V_2 velocity of the sample molecules as they cross the scoring positions yields ρ_+ and ρ_-, the local densities of the molecule with positive and negative components of V_2, respectively, and also the local density, ρ. These values are used in the assumed form of the target molecule velocity distribution in the next iteration. The average density across the channel is then obtained by averaging the density of all the scoring cross sections

$$\frac{\rho_A}{\rho_{+0}} = \frac{1}{p_f} \left[\frac{1}{2} \left(\frac{\rho_0}{\rho_{+0}} + \frac{\rho_{p_f}}{\rho_{+0}} \right) + \sum_{p=1}^{p_f - 1} \frac{\rho_p}{\rho_{+0}} \right] \tag{17}$$

If Q is taken as V_1/V_2, equation (15) becomes

$$\frac{(\rho u_1)_p}{\rho_{+0} C_{w0}} = \frac{\rho_+ u_{+p}}{\rho_{+0} C_{w0}} + \frac{\rho_- u_{-p}}{\rho_{+0} C_{w0}} = \frac{1}{N_\pi^{1/2}} \left[\overset{S_+}{\sum} \left(\frac{V_1}{V_2} \right)_p - \overset{S_-}{\sum} \left(\frac{V_1}{V_2} \right)_p \right] \tag{18}$$

Dividing by the appropriate densities obtained previously gives the local mean velocity for the molecules with $V_2 > 0$, which is u_{1+}, the local mean velocity for the molecules with $V_2 < 0$, which is u_{1-}, and the local mean velocity u_1. These values are also used in the target molecule velocity distribution in the next iteration.

The kinetic energy per unit mass of a monatomic gas measured relative to the mean flow velocity is equal to the number of degrees of freedom times $(1/2)R_g T$. With this as

the definition of temperature, the following equation can be written for three degrees of freedom:

$$\frac{3}{2} R_g T = \frac{1}{2} \langle V'^2 \rangle = \frac{1}{2} \langle V^2 \rangle - \frac{1}{2} u_1^2 \tag{19}$$

Then, from equation (15)

$$\frac{T_p}{T_{w0}} = \frac{2}{3N\pi^{1/2} C_{w0}} \left(\frac{\rho_p}{\rho_{+0}}\right)^{-1} \left[\sum^{S_+}\left(\frac{V^2}{V_2}\right) - \sum^{S_-}\left(\frac{V^2}{V_2}\right)\right]_p - \frac{2u_{1p}^2}{3C_{w0}^2} \tag{20}$$

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

$$\frac{\left(c_+^2\right)_p}{c_{w0}^2} = \frac{2}{3C_{w0}N\pi^{1/2}} \left(\frac{\rho_{+,p}}{\rho_{+0}}\right)^{-1} \left[\sum^{S_+}\left(\frac{V^2}{V_2}\right)\right]_p - \frac{2}{3}\frac{u_{1+,p}^2}{c_{w0}^2} \tag{21}$$

and similarly for the molecules with $V_2 < 0$

$$\frac{\left(c_-^2\right)_p}{c_{w0}^2} = -\frac{2}{3C_{w0}N\pi^{1/2}} \left(\frac{\rho_{-,p}}{\rho_{+0}}\right)^{-1} \left[\sum^{S_-}\left(\frac{V^2}{V_2}\right)\right]_p - \frac{2}{2}\frac{u_{1-,p}^2}{c_{w0}^2} \tag{22}$$

These values are used in the target molecule velocity distribution in the next iteration.

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

$$(P_{12})_p = [\rho\langle V_1 V_2\rangle]_p = \frac{\rho_{+0}C_{+0}}{N\pi^{1/2}}\left(\sum^{S_+} V_1 - \sum^{S_-} V_1\right)_p \tag{23}$$

The rate at which total energy is transferred across the channel is given by

$$q_{T_p} = \frac{1}{2}\left[\rho\langle V_2(V^2)\rangle\right]_p = \frac{\rho_{+0}C_{w0}}{2N\pi^{1/2}}\left[\sum^{S_+}(v^2) - \sum^{S_-}(v^2)\right]_p \qquad (24)$$

The transfer of the undirected kinetic energy across the channel is $q = 1/2\,\rho\langle V_2'(V'^2)\rangle$ so that equation (24) becomes

$$q = q_T - u_1 P_{12} \qquad (25)$$

The macroscopic quantities of interest are found by using these equations. The values of ρ_+, ρ_-, C_+, C_-, u_{1+}, and u_{1-} are then compared to the assumed values used in the target molecule distribution, and the problem is iterated until they are in agreement. (The initial assumed values are taken from the collisionless solution.) Also obtained at the same time from equations (16) to (25) are the local temperature, density, shear, and energy transfer. Twenty zones of equal size across the channel were used, and it was found that increasing this number had no effect on the results of the present calculations.

RESULTS AND CONCLUSIONS

First the case of stationary walls with a temperature ratio t_{w1} of 0.25 was treated. The local gas temperature divided by the temperature of the hot wall is shown in figure 3. The local density divided by the average density across the channel is given in figure 4. Figure 5 shows the heat flux transferred divided by the heat flux for the collisionless case, which is derived in appendix D.

These results are in good agreement with the results of another Monte Carlo solution by Haviland (ref. 7). The linearized solution of Gross and Ziering (ref. 3) gives very good agreement with the present results except for the temperature profile. In the linearized solution of reference 3 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. 4) 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 are the slip continuum results. These results are obtained by using the fluid temperature near the wall (slip wall temperature) rather than the wall temperature in the continuum equations (appendix E). By using the slip wall temperatures that gave
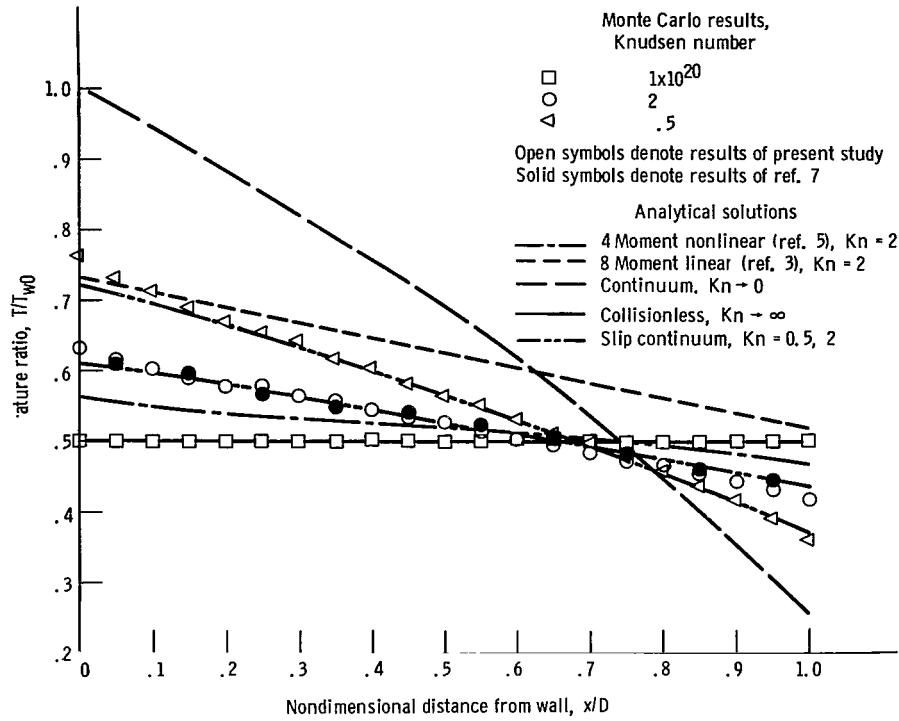
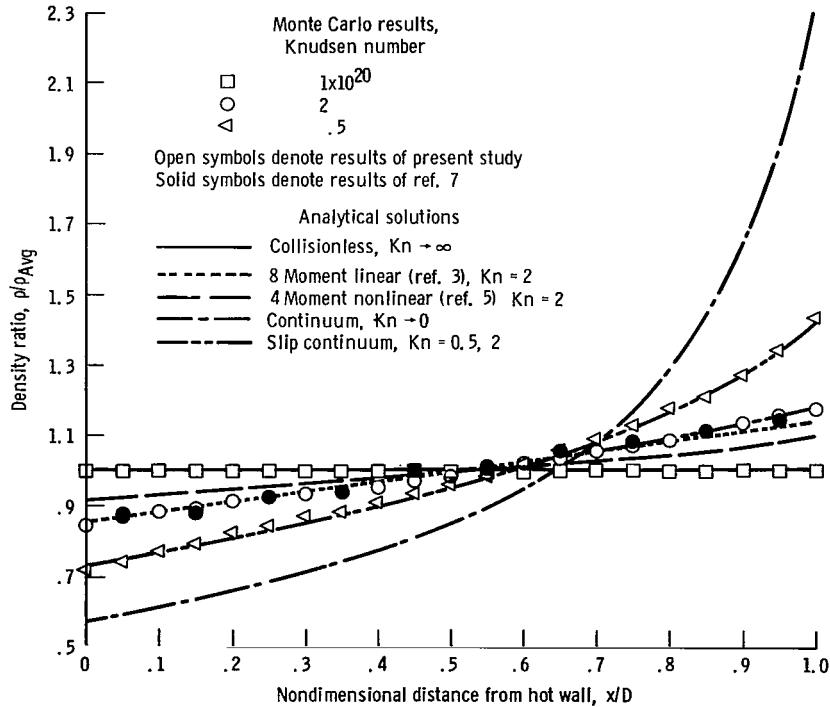Figure 3. - Temperature distributions. Wall-temperature ratio, 0.25; wall Mach number, 0.

Figure 4. - Density ratio for various Knudsen numbers. Wall-temperature ratio, 0.25; wall Mach number, 0.
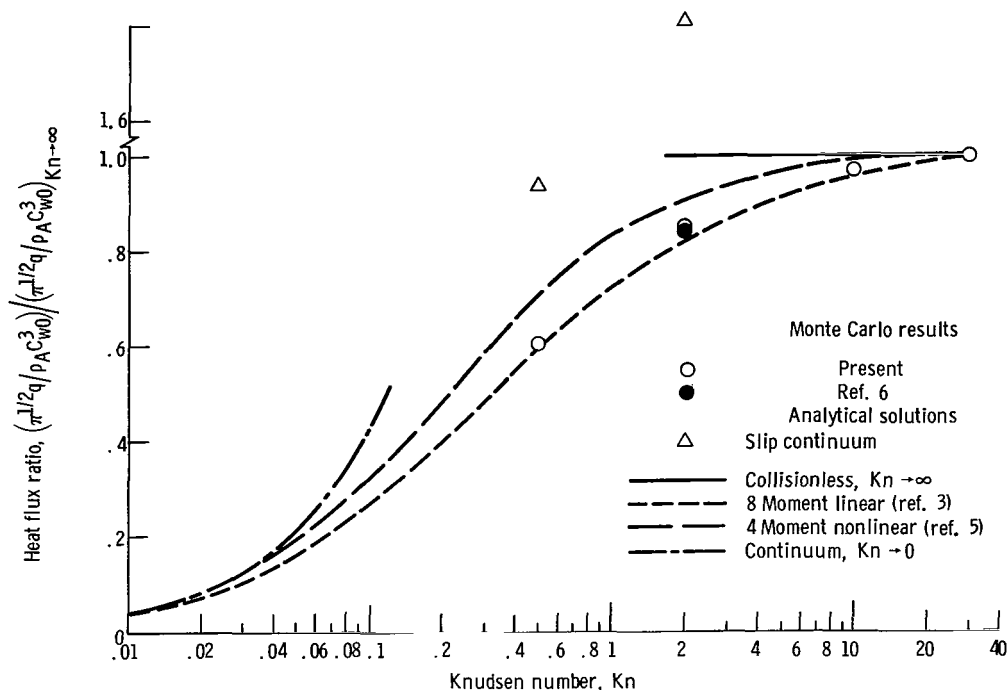
Figure 5. – Dimensionless heat flux as function of Knudsen number. Wall-temperature ratio, 0.25; wall Mach number, 0.

the best fit to both the temperature and the 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 rate was considerably above that from 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 rate at various positions across the channel is shown in figure 6. Theoretically this should be constant at each point across the channel (appendix E), although the present method does not impose this condition by its method of solution. This condition, however, is satisfied by the present results, as can be seen from this figure.

To check the confidence limits of the present results, the solution was carried out for a Knudsen number of 0.5 using 50 000 sample molecules. 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 rate across the channel was about 2 percent of its value. The derivations and equation used in obtaining δ are given in appendix F.

The second case treated is for that in which both walls are at the same temperature but one wall is moving at a wall Mach number, $M_w = u_{w1}/C_{w0}$, of 4. The velocity profile is shown in figure 7. Since the profile is antisymmetric about x/D of 0.5, the re-

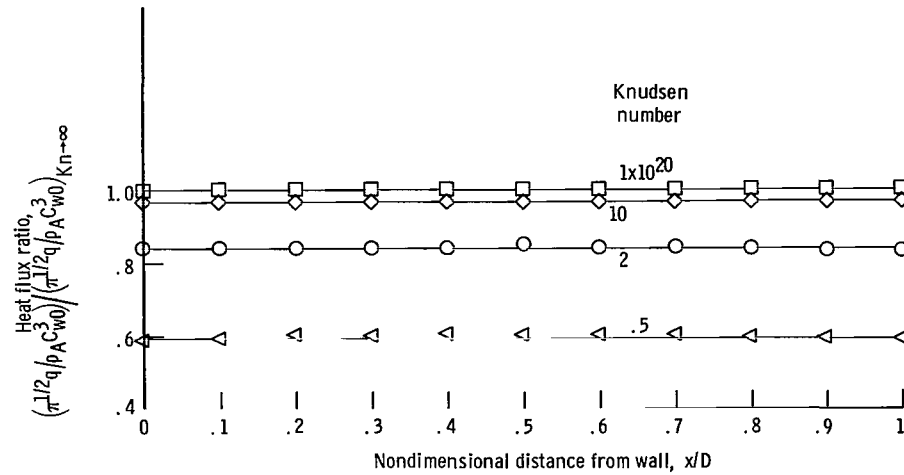Figure 6. – Dimensionless heat flux distribution for various Knudsen numbers. Wall-temperature ratio, 0.25; wall Mach number, 0.
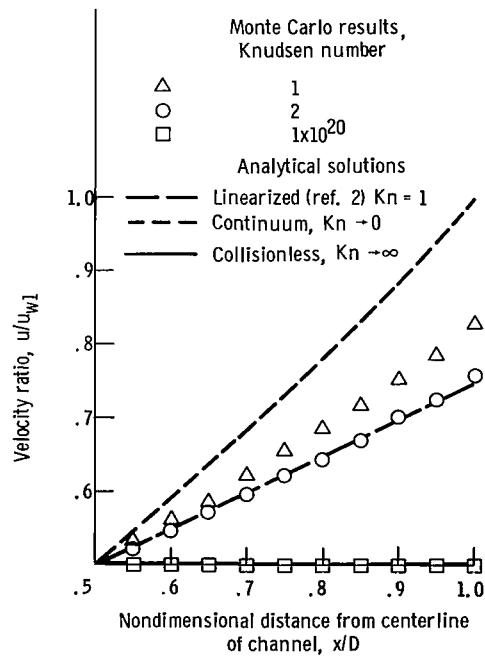

Figure 7. – Velocity ratio distribution for various Knudsen numbers. Wall Mach number, 4; wall temperature ratio, 1.
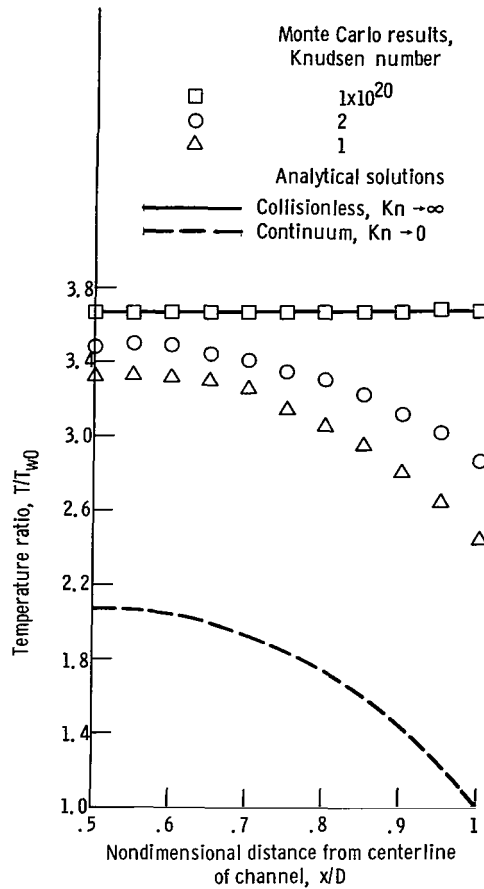
Figure 8. - Temperature distribution for various Knudsen numbers. Wall Mach number, 4; wall-temperature ratio, 1.

sults are only shown for x/D from 0.5 to 1.0. The linearized solution (ref. 2) departs significantly from the present result obtained herein for the nonlinear large wall Mach number case.

The temperature profile across the channel is shown in figure 8. There is a substantial rise in temperature for larger 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 giving the higher temperature.

The shear stress for the channel is shown in figure 9. This has been nondimensionalized by the shear stress for the collisionless case (eq. (D5)). 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. (D6)) gave the same values as the dimensionless shear stress for the cases studied. This is also shown in figure 10, where shear stress and total heat transfer at various positions across the
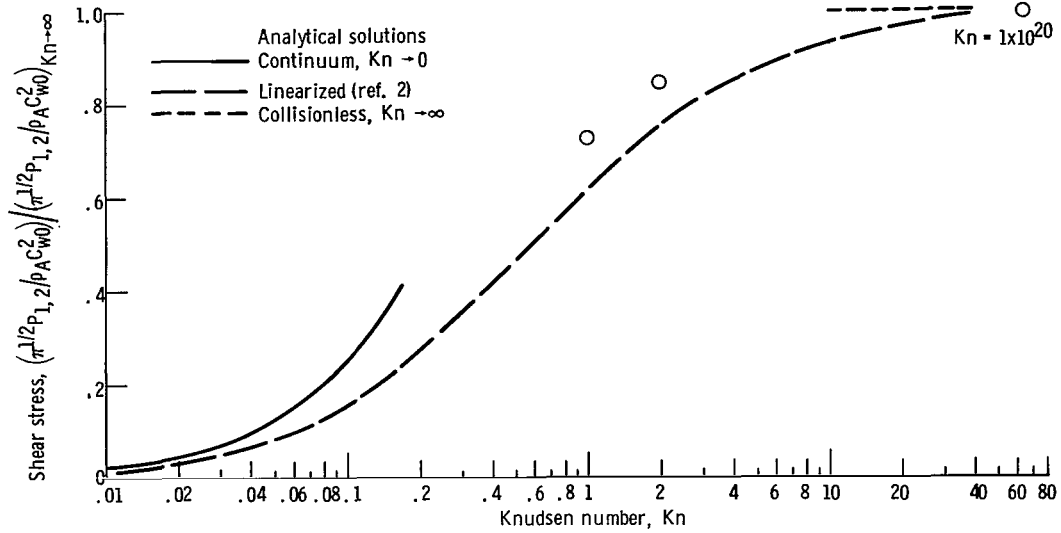
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Figure 9. – Dimensionless shear stress. Wall-temperature ratio, 1; wall Mach number, 4.
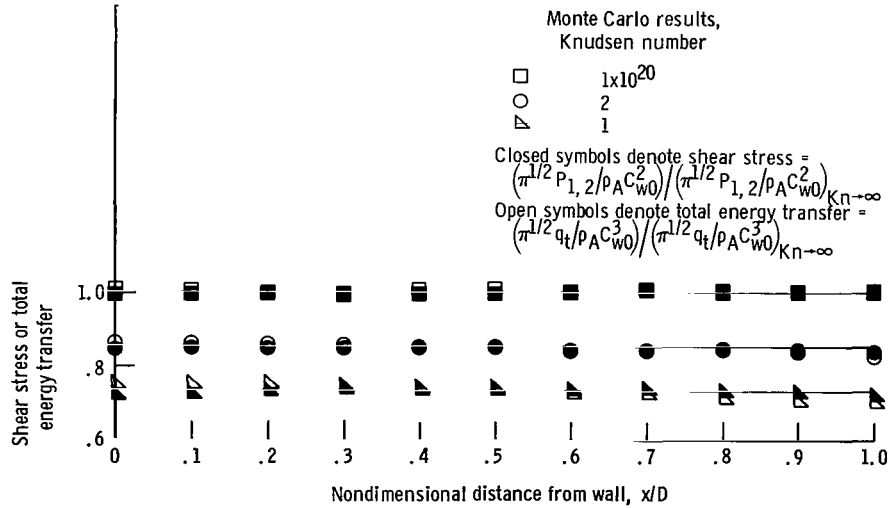

Figure 10. – Dimensionless total energy transfer and shear stress. Wall-temperature ratio, 1; wall Mach number, 4.

channel are plotted. Again, from the 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 analysis, the results in figure 10 indicate that the shear stress and total energy transfer are nearly constant at the different positions across the channel.

CONCLUDING REMARKS

The Monte Carlo method gives reasonable results for the present problems 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 50 000 sample molecules on an IBM 7094 are 40 minutes for $K_n = 30$, 50 minutes for $K_n = 2$, and 75 minutes for $K_n = 0.5$. The large increase in running time as the Knudsen number is reduced shows that the procedure as presently formulated is not suited to very small Knudsen numbers. Generally, three iterations of 50 000 samples were needed.

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

Lewis Research Center,
    National Aeronautics and Space Administration,
        Cleveland, Ohio, February 20, 1968,
            129-01-11-05-22.

APPENDIX A

VELOCITIES OF MOLECULES LEAVING THE WALL

The normalized Maxwellian distribution of the molecules at the wall w0 with component $V_2 > 0$ is given by

$$f_{w0} \, dV'^3 = \frac{2}{\pi^{3/2} C_{w0}^3} \left[\exp\left(-\frac{V_{w0}'^2}{C_{w0}^2}\right) \right] dV'^3 \tag{A1}$$

(Note that integration of eq. (A1) over all velocity space with $V_2 > 0$ will give unity.)

The distribution of velocities of the molecules leaving the wall w0 per unit time per unit area is given by $V_2 f_w / \langle V_2 \rangle_{+w0}$. This distribution can be transformed to cylindrical coordinates $V_1' = V_r \cos\theta$, $V_2 = V_2$, $V_3 = V_r \sin\theta$ as

$$\frac{V_2 f_{w0} \, dV'^3}{\langle V_2 \rangle_{+w0}} = \frac{2 V_2 V_r}{\pi C_w^4} \left[\exp\left(-\frac{V_r^2 + V_2^2}{C_{w0}^2}\right) \right] d\theta \, dV_2 \, dV_r \tag{A2}$$

Equation (A2) can be written as the product of the following three single variables distribution functions:

$$f_\theta \, d\theta = \frac{d\theta}{2\pi} \tag{A3a}$$

$$f_{V_2} \, dV_2 = \frac{2V_2}{C_{w0}^2} \left[\exp\left(-\frac{V_2^2}{C_{w0}^2}\right) \right] dV_2 \tag{A3b}$$

$$f_{V_r} \, dV_r = \frac{2V_r}{C_{w0}^2} \left[\exp\left(-\frac{V_r^2}{C_{w0}^2}\right) \right] dV_r \tag{A3c}$$

The velocity components of the sample molecule leaving the surface must be picked from these distributions. A convenient way of picking from a distribution for the high-speed

computer is to transform the distribution to a uniform distribution by setting the random number R equal to the cumulative distribution function. For example,

$$R_\theta = \int_0^\theta f_{\theta'} \, d\theta' = \frac{\theta}{2\pi} \tag{A4}$$

Then, by using a high-speed computer to generate a random number R between 0 and 1, θ can be obtained from equation (A4) such that for a large number of samples picked in this manner the distribution in equation (A3a) will be satisfied. This technique is more fully discussed in reference 1.

Similarly, V_2 can be picked from

$$R_{V_2} = \int_0^{V_2} \frac{2V_2}{C_{w0}^2} \left[\exp\left(-\frac{V_2^2}{C_{w0}^2} \right) \right] dV_2 \tag{A5}$$

Or, since picking R is equivalent to picking $1 - R$,

$$V_2 = \left(-C_{w0}^2 \ln R_{V_2} \right)^{1/2} \tag{A6}$$

so that by picking a random number R_{V_2}, V_2 can be obtained from equation (A6). Similarly

$$V_r = \left(-C_w^2 \ln R_{V_r} \right)^{1/2} \tag{A7}$$

A similar procedure is used to generate sample molecules from wall w1 using instead C_{w1} and $V_2 < 0$.

APPENDIX B

EVALUATION OF MEAN FREE PATH

The incremental number of collisions per unit time $d\Theta$ of a sample molecule moving at velocity V_s through target molecules in velocity space increment dV_t^3 for hard sphere molecules is given, in reference 9, as

$$d\Theta = \frac{\rho f_t}{m} V_R S \, dV_t^3 \tag{B1}$$

where V_R is the magnitude of the velocity of the target molecules relative to the sample molecule velocity before collision, $V_{R,i} = V_{t,i} - V_{s,i}$. The term V_R can be written as

$$V_R = \left[(V_{1t} - V_{1s})^2 + (V_{2t} - V_{2s})^2 + (V_{3t} - V_{3s})^2 \right]^{1/2} \tag{B2}$$

If the local mean velocity $u = u_1$ (which is along the x_1-direction) is subtracted from both the sample molecule and the target molecules, the collision rate for a Maxwellian distribution of target molecules can then be written as

$$d\Theta_M = \frac{\rho S}{m\pi^{3/2} C^3} \left(\exp - \frac{V_t'^2}{C^2} \right) V_R \, dV_{1t}' \, dV_{2t} \, dV_{3t} \tag{B3}$$

In order to carry out the integration to obtain Θ_M, the reference coordinate system is rotated so that V_s' lies along the new 2-direction. This is accomplished by employing Eulerian angles (refs. 9 and 11) (see fig. 1(b)). The rotation can be considered to be a two-step process whereby the coordinate system is first rotated by the angle φ counterclockwise with axis along the 3-direction, where

$$\cos \varphi = \frac{V_{2s}'}{V_{rs}}, \quad \sin \varphi = - \frac{V_{1s}'}{V_{rs}}$$

and $V_{rs} \equiv \left(V_{1s}'^2 + V_{2s}^2 \right)^{1/2}$. After this rotation of the 1, 2-reference plane, the plane containing the velocity vector V_s' of the sample molecule and the new 2-direction is perpendicular to the new 1-direction so that another rotation counterclockwise about an axis along the new 1-direction by the angle θ where

$$\cos\theta = \frac{V_{rs}}{V'_s}, \quad \sin\theta = \frac{V_{3s}}{V'_s}, \quad V'_s = \left(V_{rs}^2 + V_{3s}^2\right)^{1/2}$$

places the 2-direction along V'_s. The matrices corresponding to the preceding transformation and its inverse are

$$V'_{it} = A_{ij}^{-1} V''_{it} \tag{B4a}$$

where

$$A_{ij}^{-1} = \begin{pmatrix} \dfrac{V_{2s}}{V_{rs}} & \dfrac{V'_{1s}}{V'_s} & \dfrac{-V_{3s}V'_{1s}}{V_{rs}V'_s} \\[2em] \dfrac{-V'_{1s}}{V_{rs}} & \dfrac{V_{2s}}{V'_s} & \dfrac{-V_{3s}V_{2s}}{V_{rs}V'_s} \\[2em] 0 & \dfrac{V_{3s}}{V'_s} & \dfrac{V_{rs}}{V'_s} \end{pmatrix} \tag{B4b}$$

and

$$V''_{it} = A_{ij} V'_{jt} \tag{B5a}$$

where

$$A_{ij} = \begin{pmatrix} \dfrac{V_{2s}}{V_{rs}} & \dfrac{-V'_{1s}}{V_{rs}} & 0 \\[2em] \dfrac{V'_{1s}}{V'_s} & \dfrac{V_{2s}}{V'_s} & \dfrac{V_{3s}}{V'_s} \\[2em] \dfrac{-V_{3s}V'_{1s}}{V_{rs}V'_s} & \dfrac{-V_{2s}V_{3s}}{V_{rs}V'_s} & \dfrac{V_{rs}}{V'_s} \end{pmatrix} \tag{B5b}$$

Then equation (B3) becomes

$$d\Theta_M = \frac{\rho S}{m\pi^{3/2}C^3} \left(\exp - \frac{V_t''^2}{C^2}\right) \left[V_{1t}''^2 + (V_{2t}'' - V_s')^2 + V_{3t}''^2\right]^{1/2} dV_t''^3 \tag{B6}$$

Transforming into spherical coordinates

$$V_{1t}'' = V_t' \cos\theta \sin\varphi, \quad V_{2t}'' = V_t' \cos\varphi, \quad V_{3t}'' = V_t' \sin\theta \sin\varphi \tag{B7a}$$

results in

$$d\Theta_M = \frac{c\rho S}{m\pi^{3/2}} \left[\exp\left(-\mu_t^2\right)\right] \mu_t^2 \mu_R \sin\varphi \, d\varphi \, d\theta \, d\mu_t \tag{B7b}$$

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

$$\mu_R = \left(\mu_t^2 + \mu_s^2 - 2\mu_t\mu_s \cos\varphi\right)^{1/2} \tag{B8}$$

To obtain the total collision rate for the target molecules over all velocities, equation (B7b) must be integrated over φ, θ, and μ_t. Integrating over θ from 0 to 2π and over φ from 0 to π gives

$$d\Theta_M(\mu_t) = \frac{4\rho CS}{m\pi^{1/2}} \left[\exp\left(-\mu_t^2\right)\right] \mu_t^2 \mu_{R,A} \, d\mu_t \tag{B9}$$

where $\mu_{R,A} = \int_0^\pi \mu_R (\sin\varphi/2) d\varphi$ or

$$\mu_{R,A} = \begin{cases} \mu_s + \dfrac{\mu_t^2}{3\mu_s} & \text{if } \mu_s > \mu_t \\[4mm] \mu_t + \dfrac{\mu_s^2}{3\mu_t} & \text{if } \mu_t > \mu_s \end{cases} \tag{B10}$$

Integrating equation (B9) over μ_t from 0 to ∞ yields the total collision frequency Θ_M for a sample molecule moving at velocity μ_s through a Maxwellian gas:

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$$\Theta_M = \frac{\rho SC}{m} \left[\frac{\exp -\mu_s^2}{\pi^{1/2}} + (\text{erf } \mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right) \right] \tag{B11}$$

The nondimensional mean free path is then found, as discussed in reference 10, by dividing the sample molecule velocity by the total collision rate and using the hard-sphere definition of Knudsen number Kn to give for the dimensionless mean free path

$$\frac{\Lambda_M}{D} = \frac{V_s}{\Theta_M D} = \frac{\sqrt{2} \, V_s Kn}{C \frac{\rho}{\rho_A} \left\{ \frac{1}{\pi^{1/2}} \left[\exp\left(-\mu_s^2\right) \right] + (\text{erf } \mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right) \right\}} \tag{B12}$$

If there were two different Maxwellian gases in the incremental volume in space, distributed over velocity space by the functions $f_{M\alpha}$ and $f_{M\beta}$, respectively, the total collision rate would be given by the collision rate for the molecules from $f_{M\alpha}$ plus the collision rate for the molecules from $f_{M\beta}$, $\Theta = \Theta_{M\alpha} + \Theta_{M\beta}$, where $\Theta_{M\alpha}$ and $\Theta_{M\beta}$ are given as in equation (B11) with appropriate densities and mean thermal velocities. Since λ_s is given by V_s/Θ,

$$\lambda_s = \frac{1}{\dfrac{\Theta_{M\alpha}}{V_s} + \dfrac{\Theta_{M\beta}}{V_s}} = \frac{1}{\dfrac{1}{\lambda_{M\alpha}} + \dfrac{1}{\lambda_{M\beta}}} \tag{B13}$$

APPENDIX C

TARGET-MOLECULE COLLISION PARTNER

The distribution of target-molecule collision partners in velocity space for a sample molecule passing through target molecules in a Maxwellian distribution is given by dividing equation (B7b) by equation (B11):

$$\frac{d\Theta_M}{\Theta_M} = \frac{\left[\exp\left(-\mu_t^2\right)\right]\mu_t^2 \mu_R \sin\varphi \; d\varphi \; d\theta \; d\mu_t}{\pi\left[\exp\left(-\mu_s^2\right)\right] + \pi^{3/2}(\mathrm{erf}\;\mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right)} \tag{C1}$$

The distribution in θ for the target-molecule collision partners is readily seen to be

$$f_\theta \; d\theta = \frac{d\theta}{2\pi} \tag{C2}$$

where the value of θ can be picked from this distribution as discussed in appendix A by employing the relation

$$\theta = 2\pi R_\theta \tag{C3}$$

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

$$f_{\mu_t} \; d\mu_t = \frac{4\left[\exp\left(-\mu_t^2\right)\right]\mu_t^2 \mu_{R,A} \; d\mu_t}{\left[\exp\left(-\mu_s^2\right)\right] + \pi^{1/2}(\mathrm{erf}\;\mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right)} \tag{C4}$$

The value of μ_t from this distribution is found from

$$R_{\mu_t} = \frac{\gamma(\mu_s, \mu_t) + \epsilon(\mu_s, \mu_t)}{\left[\exp\left(-\mu_s^2\right)\right] + \pi^{1/2}(\mathrm{erf}\;\mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right)} \tag{C5}$$

where

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

$$\left. \begin{array}{c} - \frac{\mu_t}{\mu_s}\left[\exp\left(-\mu_t^2\right)\right] + \frac{\sqrt{\pi}}{2\mu_s} \ (\text{erf } \mu_t) \\ \\ \epsilon = 0 \end{array} \right\} \text{when } \mu_s > \mu_t \qquad \text{(C6)}$$

and

$$\left. \begin{array}{c} \gamma(\mu_s, \mu_t) = \gamma(\mu_s, \mu_s) \\ \\ \epsilon = -2\left[\exp\left(-\mu_t^2\right)\right]\left(\frac{\mu_s^2}{3} + 1 + \mu_t^2\right) + \left[2 \ \exp\left(-\mu_s^2\right)\right]\left(\frac{4\mu_s^2}{3} + 1\right) \end{array} \right\} \text{when } \mu_s < \mu_t \qquad \text{(C7)}$$

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

$$\frac{d\Theta(\mu_t, \varphi)}{\Theta} = f(\mu_t)f(\varphi | u_t) \qquad \text{(C8)}$$

Then φ must be found from the conditional distribution

$$f(\varphi | \mu_t) = \frac{\mu_R \sin \varphi \ d\varphi}{2\mu_{R,A}} \qquad \text{(C9)}$$

The value of φ for a given μ_t is found from

$$R_\varphi = \frac{\mu_R^3 - |\mu_t - \mu_s|^3}{\left(\mu_t^2 + \mu_s^2 + 2\mu_t\mu_s\right)^{3/2} - |\mu_t - \mu_s|^3} \qquad \text{(C10)}$$

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where

$$\mu_R^3 = \left(\mu_t^2 + \mu_s^2 - 2\mu_t\mu_s \cos\varphi\right)^{3/2}$$

After φ, μ_t, and θ are found, the velocity components V''_{1t}, V''_{2t}, and V''_{3t} are found by using the relations given by equation (B7a). Then, from equation (B4)

$$V_{1t} = V''_{1t}\left(\frac{V_{2s}}{V_{rs}}\right) + V''_{2t}\left(\frac{V'_{1s}}{V'_s}\right) - V''_{3t}\left(\frac{V_{3s}V'_{1s}}{V_{rs}V'_s}\right) + u_1 \qquad\qquad \text{(C11a)}$$

$$V_{2t} = -V''_{1t}\left(\frac{V'_{1s}}{V_{rs}}\right) + V''_{2t}\left(\frac{V_{2s}}{V'_s}\right) - V''_{3t}\left(\frac{V_{2s}V_{3s}}{V_{rs}V'_s}\right) \qquad\qquad \text{(C11b)}$$

$$V_{3t} = V''_{2t}\left(\frac{V_{3s}}{V'_s}\right) + V''_{3t}\left(\frac{V_{rs}}{V'_s}\right) \qquad\qquad \text{(C11c)}$$

APPENDIX D

COLLISIONLESS SOLUTION

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

$$
\rho f_\infty = \begin{cases} \dfrac{2\rho_{+0}}{\pi^{3/2} C_{w0}^3} \left[\exp - \left(\dfrac{V_{w0}^{\prime 2}}{C_{w0}^2} \right) \right] & V_2 > 0 \\[3em] \dfrac{2\rho_{-1}}{\pi^{3/2} C_{w1}^3} \left[\exp - \left(\dfrac{V_{w1}^{\prime 2}}{C_{w1}^2} \right) \right] & V_2 < 0 \end{cases} \tag{D1}
$$

where ρ_{+0} is the density of molecules with $V_2 > 0$, while ρ_{-1} is the density of molecules with $V_2 < 0$. The local density is then given by

$$
\rho \langle V_2 Q \rangle_{Q=1/V_2} = \rho \langle 1 \rangle
$$

$$
= \rho = \rho_{+0} + \rho_{-1}
$$

Since there is no net flow across the channel,

$$
\rho \langle V_2 \rangle = \frac{1}{\pi^{1/2}} \left(\rho_{+0} C_{w0} - \rho_{-1} C_{w1} \right) = 0
$$

From the first relation

$$
\left(\frac{\rho_{-1}}{\rho} \right)_\infty = 1 - \frac{\rho_{+0}}{\rho} \tag{D2a}
$$

where, from the second relation

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$$\left(\frac{\rho_{+0}}{\rho}\right)_{\infty} = \left(\frac{1}{1 + \dfrac{\rho_{-1}}{\rho_{+0}}}\right)_{\infty} = \frac{1}{1 + \dfrac{C_{w0}}{C_{w1}}} = \frac{1}{1 + t_{w1}^{-1/2}} \tag{D2b}$$

The flow parallel to the channel wall is given by

$$u_1 = \langle V_1 \rangle = \frac{\rho_{+0}}{\rho} u_{1, w0} + \frac{\rho_{-1}}{\rho} u_{1, w1} \tag{D3}$$

The local temperature as can be seen from equation (19) is given by

$$\frac{T}{T_{w0}} = \frac{2}{3 C_{w0}^2} \langle V^2 \rangle - \frac{2}{3} M^2$$

which when evaluated gives

$$t = \frac{2}{3} \left(\frac{\rho_{+0}}{\rho} M_{w0}^2 + \frac{\rho_{-1}}{\rho} M_{w1}^2 - M^2 \right) + \frac{\rho_{+0}}{\rho} \left(1 + t_{w1}^{1/2} \right) \tag{D4}$$

The shear stress (eq. (23)) $P_{12} = \rho \langle V_1 V_2 \rangle$ can be found to be

$$\frac{\pi^{1/2} P_{12}}{\rho 2 R_g T_{w0}} = \frac{\rho_{+}}{\rho} (M_{w0} - M_{w1}) \tag{D5}$$

The total energy transferred is given by equation (25) as $q_T = \rho/2 \, \langle V'^2 V_2 \rangle + u_1 P_{12}$. For the collisionless case, the relation becomes

$$\frac{\pi^{1/2} q_T}{\rho (2 R_g T_{w0})^{3/2}} = \frac{\rho_{+0}}{\rho} - \frac{\rho_{-1}}{\rho} t_{w1}^{3/2} + \frac{\rho_{+0}}{\rho} \frac{M_{w0}^2}{2} - \frac{\rho_{-1}}{\rho} \frac{M_{w1}^2}{2} t_{w1}^{1/2} \tag{D6}$$

APPENDIX E

CONTINUUM SOLUTIONS

Maxwell's equation of transfer for the steady-state condition can be written

$$\frac{\partial}{\partial X_i} (\rho \langle V_i Q \rangle) = m \, \Delta(Q) \qquad \text{(E1)}$$

where the convention is used that repeated subscripts are to be summed over. Here, $\Delta(Q)$ denotes the rate of increase in some molecular quantity Q due to molecular collisions. This term is zero for cases where Q is conserved during collision. This is true when Q is equal to 1, V, or V^2, corresponding to conservation of mass, momentum, or energy, respectively:

$Q = 1$:

$$\frac{\partial}{\partial X_i} (\rho u_i) = 0 \qquad \text{(E2)}$$

$Q = V$:

$$0 = \frac{\partial}{\partial X_i} (\rho \langle V_i V_j \rangle)$$

$$= \frac{\partial}{\partial X_i} \left[\rho \langle (V'_i + u_i)(V'_j + u_j) \rangle \right]$$

$$= \frac{\partial}{\partial X_i} (\rho \langle V'_i V'_j \rangle + \rho u_i u_j)$$

$$= \frac{\partial}{\partial X_i} (\rho \langle V'_i V'_j \rangle) + \rho u_i \frac{\partial u_j}{\partial X_i} + u_j \frac{\partial (\rho u_i)}{\partial X_i}$$

Inasmuch as $\rho \langle V'_i V'_j \rangle \equiv P_{ij}$ and $\partial(\rho u_i)/\partial X_i = 0$ by equation (E2), the preceding equation can be written as

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$$\frac{\partial P_{ij}}{\partial X_i} + \rho u_i \frac{\partial u_j}{\partial X_i} = 0 \qquad (E3)$$

$Q = V^2$:

$$0 = \frac{\partial}{\partial X_i} \left(\rho \langle V_i V^2 \rangle \right)$$

$$= \frac{\partial}{\partial X_i} \left[\rho \langle (V_i' + u_i)(V' + u)^2 \rangle \right]$$

$$= \frac{\partial}{\partial X_i} \left(\rho \langle V_i' V'^2 \rangle \right) + \frac{\partial}{\partial X_i} (u_i P_{jj}) + \frac{\partial}{\partial X_i} (2u_j P_{ij}) + \frac{\partial}{\partial X_i} \left(\rho u_i u^2 \right)$$

By equations (E2) and (E3) the sum of the last two terms of the preceding gives $(2P_i \, \partial u_j / \partial X_i)$, so that

$$\frac{\partial}{\partial X_i} \left(\rho \langle V_i' V'^2 \rangle \right) + \frac{\partial}{\partial X_i} (u_i P_{jj}) + 2P_{ij} \frac{\partial u_j}{\partial X_i} = 0 \qquad (E4)$$

In addition, there exist the two well-known relations for a fluid, namely,

$$q_i \equiv \frac{1}{2} \rho \langle V_i' V'^2 \rangle = -\kappa \frac{\partial T}{\partial X_i} \qquad (E5)$$

$$P_{ij} = \delta_{ij} P - 2\mu \left(\frac{1}{2} \frac{\partial u_i}{\partial X_j} + \frac{1}{2} \frac{\partial u_j}{\partial X_i} - \frac{1}{3} \delta_{ij} \frac{\partial u_k}{\partial X_k} \right) \qquad (E6)$$

Equations (E5) and (E6) serve to introduce the gas conductivity κ, the viscosity μ, and the static pressure P into the relations. In this context, note that the introduction of equation (E6) into equation (E4) yields the Navier-Stokes equations.

With respect to the problem treated herein, where the only changes occur in the X_2- or across-channel-direction, equations (E2) to (E4) become

(E2):

$$\frac{\partial u_1}{\partial X_1} = 0 \qquad \text{or} \quad u_1 = g(x_2) \tag{E7a}$$

(E3):

$$\frac{\partial P_{2j}}{\partial X_2} = 0 \qquad \text{or} \quad P_{12} = -\mu \frac{\partial u_1}{\partial X_2} = \text{Constant} \tag{E7b}$$

where equation (E6) has also been employed,

(E4):

$$\frac{\partial}{\partial X_2}(q_2 + P_{21}u_1) = 0$$

so that by equation (25)

$$q_T = q_2 + u_1 P_{12} = \text{Constant} \tag{E7c}$$

For hard-sphere molecules, the temperature-dependent conductivity and viscosity can be written for the continuum case as (ref. 6)

$$\kappa = \kappa_0 t^{1/2}$$

where

$$\kappa_0 = \frac{75m}{64\sigma^2} \frac{\kappa_g C_{w0}}{(2\pi)^{1/2}} \tag{E8}$$

and

$$\mu = \mu_0 t^{1/2}$$

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where

$$\mu_0 = \frac{5mCw_0}{16\sigma^2(2\pi)^{1/2}} \tag{E9}$$

For the case where both walls are stationary, equation (E7c) becomes

$$q_2 = -\frac{\kappa}{D} \frac{\partial T}{\partial x_2} = \text{Constant} \tag{E10}$$

where the dimensionless coordinate $x_2 = X_2/D$ has been introduced. Substituting equation (E8) into equation (10) and integrating give

$$t_{M=0} = \left[1 - \left(1 - t_{w1}^{3/2}\right)x_2\right]^{2/3} \tag{E11}$$

Because the pressure across the channel is uniform, the ideal gas law becomes

$$\rho t_{M=0} = \text{Constant}$$

Then, employing the relation $\rho_A = \int_0^1 \rho \, dx_2$ shows that

$$\left(\frac{\rho}{\rho_A}\right)_{M=0} = \frac{1 + t_{w1}^{1/2} + t_{w1}}{3t_{M=0}} \tag{E12}$$

Also the heat-transfer rate across the channel is

$$(q_2)_{M=0} = -\frac{\kappa}{D} \frac{\partial T}{\partial x_2} = -\frac{\kappa_0 t^{1/2} T_{w0}}{D} \frac{\partial t_{M=0}}{\partial x_2}$$

which upon evaluation becomes

$$\left(\frac{q_2}{\rho_A C_{w0}^3}\right)_{M=0} = \frac{25}{64} (\pi)^{1/2}\left(1 - t_{w1}^{3/2}\right)(Kn) \tag{E13}$$

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For the case where wall w1 is moving at velocity μ_{w1}, equation (25) applies:

$$q_T = q_2 + u_1 P_{12}$$

$$= -\frac{\kappa}{D} \frac{\partial T}{\partial x_2} - \frac{\mu}{D} \frac{\partial u_1}{\partial x_2} u_1$$

$$= -\frac{\kappa}{c_p D} \left(c_p \frac{\partial T}{\partial x_2} + \frac{\mu c_p}{\kappa} \frac{1}{2} \frac{\partial u_1^2}{\partial x_2} \right)$$

Inasmuch as $c_p = 5/2\, R_g$ and $Pr \equiv \mu c_p / \kappa = 2/3$ for a gas, this equation becomes

$$\frac{\partial}{\partial x_2} \left(c_p T + \frac{u_1^2}{3} \right) = -\frac{c_p}{\kappa} D q_T \qquad \text{(E14)}$$

The right side can also be written as a partial derivative with respect to x_2 by making use in turn of the relations $\mu c_p / \kappa = 2/3$ and equations (E7b) and (E7c):

$$-\frac{c_p}{\kappa} D q_T = -\left(\frac{2}{3} \frac{1}{\mu} \right) D q_T$$

$$= \frac{2}{3} \frac{q_T}{P_{12}} \frac{\partial u_1}{\partial x_2}$$

$$= \frac{\partial}{\partial x_2} \left(\frac{2}{3} \frac{q_T}{P_{12}} u_1 \right)$$

Thus, equation (E14) is transformed to

$$\frac{\partial}{\partial x_2} \left(c_p T + \frac{u_1^2}{3} - \frac{2}{3} \frac{q_T}{P_{12}} u_1 \right) = 0$$

Dividing through by $c_p T_{w0} = 5/2\, R_g T_{w0} = 5/4\, C_{w0}^2$ yields

$$\frac{\partial}{\partial x_2}\left(t + \frac{4}{15}M^2 - \frac{8}{15}\frac{q_T}{P_{12}C_{w0}}M\right) = 0 \tag{E15}$$

For the case where both walls are at the same temperature, that is, $t_{w0} = t_{w1} = 1$, integration of equation (E15) gives

$$t = \frac{4}{15}M(M_{w1} - M) + 1 \tag{E16}$$

and the relation

$$q_T = \frac{1}{2}M_{w1}P_{12}C_{w0} \tag{E16a}$$

If equation (E9) is substituted into equation (E7b), the result is

$$P_{12} = -\frac{\mu_0 t^{1/2}C_{w0}}{D}\frac{\partial M}{\partial x_2} = \text{Constant} \tag{E17}$$

Substitution of equation (E16) yields

$$\sqrt{\frac{4}{15}M(M_{w1} - M) + 1}\frac{\partial M}{\partial x_2} = \text{Constant}$$

Integrating the preceding equation gives

$$x_2 = \left(\left(\frac{15}{4} + M_{w1}M - M^2\right)^{1/2}2M - M_{w1} + (15)^{1/2}\frac{M_{w1}}{2} - \left(\frac{M_{w1}^2 + 15}{2}\right)\left\{\sin^{-1}\left[\frac{M_{w1} - 2M}{\left(15 + M_{w1}^2\right)^{1/2}}\right]\right.\right.$$

$$\left.\left. - \sin^{-1}\left[\frac{M_{w1} - 2M}{\left(15 + M_{w1}^2\right)^{1/2}}\right]\right\}\right)\left((15)^{1/2}M_{w1} + M_{w1}^2 + 15\left\{\sin^{-1}\left[\frac{M_{w1}}{\left(15 + M_{w1}^2\right)^{1/2}}\right]\right\}\right)^{-1} \tag{E18}$$

and the relation

$$
-\frac{\pi^{1/2} P_{12}}{\rho_A C_{w0}^2} = \frac{5\pi}{32} \, Kn \left\{ M_{w1} + \frac{\left(M_{w1}^2 + 15 \right)}{(15)^{1/2}} \, \sin^{-1} \left[\frac{M_{w1}}{\left(M_{w1}^2 + 15 \right)^{1/2}} \right] \right\}
\tag{E19}
$$

Equation (E18) gives the velocity profile across the channel and may be used in conjunction with equation (E16) to give the temperature distribution across the channel. The shear stress is given by equation (E19) and the total heat flow by equation (E16a).

APPENDIX F

CONFIDENCE LIMITS OF RESULTS

Following the derivation in reference (1), the confidence limits on the present results can be obtained as follows. For some number of sample molecules a quantity g is obtained. Repeating this process k times will give a sample set of g values. The average of the k values would give $\bar{g}$, which is the average value of the sample set. If an infinite number of values of g were obtained, the average value of g would be the true average denoted as $\langle g \rangle$. It is necessary to determine a value of δ such that the absolute value of the difference between $\langle g \rangle$ and $\bar{g}$ is less than δ with a 95 percent probability. The central limit theorem states that the distribution of sample means $f(\bar{g})$ approaches a normal distribution with a mean value equal to the population mean $\langle g \rangle$ and with a variance equal to the population variance divided by k, the number of measurements used to determine $\bar{g}$. Since the 95 percent confidence interval δ corresponds to twice the standard deviation for the average of k values, $\delta = 2S/(k)^{1/2}$, where S^2 is the approximation to the variance of the population obtained by finding the variance of the sample set

$$ S^2 = \frac{\left[\overline{g^2} - (\bar{g})^2 \right] k}{k - 1} \tag{F1} $$

This gives the 95 percent confidence interval δ as

$$ \left| \langle g \rangle - g \right| \lesssim \delta = 2 \left(\frac{\overline{g^2} - \bar{g}^2}{k - 1} \right)^{1/2} \tag{F2} $$

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