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ABSTRACT

A discussion of application of the Monte Carlo method to rarefied gas heat transfer is given. A sample problem of heat transfer through a rarefied gas between infinite flat plates is treated. Hard sphere molecular collisions and a wall accomodation coefficient of 1 are assumed. The target molecule distribution is assumed to be Maxwellian. The results are compared to approximate analytical methods and to another Monte Carlo solution.

INTRODUCTION

In rarefied gas transport problems the usual solutions using Navier Stokes' equation for momentum transfer or the Fourier equation for conduction are no longer applicable. This is because these equations assume local isotropy and small gradients compared to the path lengths of the molecules. These assumptions are not valid in the case of rarefied gases. We must then resort to the more fundamental Boltzmann equation. This equation is difficult to treat by the usual analytical procedures because of its complexity. The Monte Carlo method allows us to reduce the complexity of the analysis at the expense of added numerical computation and is not restricted by the many simplifying assumptions generally made to allow analytical solutions.

The Monte Carlo procedure is a model sampling technique. We create a model and then follow histories of sample molecules through this model.

The sample histories are obtained by making choices at points of decision from the appropriate probability distribution. By averaging certain properties of the sample molecules at various positions we can obtain the macroscopic quantities of interest.

For purposes of illustrating the Monte Carlo method let us consider the problems of heat transfer between parallel plates enclosing a rarefied gas. A discussion of much of the previous work on this problem is given in references 1 to 5.

The model is shown in figure 1. The hot wall is considered to be at temperature $T_{w,0}$ and the cold wall at temperature $T_{w,1}$. A rarefied hard sphere molecule gas is contained between the walls.

The sample molecule histories are started at the wall 0 by picking velocity components for the sample molecule leaving the wall from the appropriate distribution of velocities of the absorbed and re-emitted molecules. The space between the walls is divided into zones as shown in figure 1. The sample molecule after leaving the wall will either pass through the first zone or have a collision with a target molecule in this zone. This will depend on whether the path length to collision for the sample molecule is longer or shorter than the distance the sample molecule must travel to pass through the zone. If the sample molecule passes through the first zone with no collision, it is started again at the beginning of the next zone with its velocity components unchanged.

If there is a collision in the zone the point of collision is found at the end of the path length to collision. A target molecule is picked from the distribution of target molecule collision partners in the zone. The distribution of target molecule velocities is assumed uniformly Maxwellian throughout each zone. A collision calculation is then carried out for the sample and target molecule collision partners, and new velocity components for the sample molecules are found. The history of the sample molecule is then continued from the point of collision with the new sample molecule velocity components. The target molecule collision partner is ignored after collision.

A new path length to collision is found for the sample molecule, and this is compared in length to the distance from the point of collision to the next zone. If the path length to collision is greater, the sample molecule is started in the next zone with its velocity components unchanged. In the other case there is a collision in the zone and the collision calculations are repeated as before.

If the sample molecule strikes the upper wall, it is assumed to be absorbed and is reemitted with new velocity components picked from the appropriate distribution of velocities based on the upper wall temperature. After leaving the upper wall it is followed as before. The history is completed when the sample molecule is incident on the lower wall and then a new sample history is begun. This is continued until the desired number of sample histories are completed.

The transport and fluid characteristics of interest are the density distribution, temperature distribution, and heat transfer across the channel. These can be obtained as in reference 6 by locating scoring positions at various locations across the channel (see fig. 1). By scoring the various characteristics of the sample molecules as they pass the scoring cross section, we can obtain the transport properties and fluid characteristics of interest.

The distribution of target molecules, which is assumed uniform in each zone, will greatly affect the results since this will determine the path length to collision for the sample molecule and also the velocity component distribution of the target molecule collision partner in each zone. In the present analysis it was assumed that the target molecules in each zone were in a Maxwellian velocity distribution based on a different local temperature and density in each zone. Then by carrying out the Monte Carlo solution based on this assumed distribution of target molecules the temperature and density in each zone can be found. The Monte Carlo solution is then rerun using the new found local temperature and density in the Maxwellian distribution of target molecules. The problem is iterated in this manner until the density and temperature distribution found from the sample molecule histories agreed with the density and temperature distribution used for the target molecules.

The assumption of a local Maxwellian distribution for the target molecules would be most applicable near equilibrium conditions, that is, cases with small temperature gradients and short mean free paths. It appears possible to extend the analysis to more realistic distributions of target molecules than were used in the present case as for instance a two-sided Maxwellian as used in an analytical solution in reference 5.

In references 1 and 2 a Monte Carlo solution is used to treat a similar problem. In that analysis the solution is carried out with an assumed distribution of target molecules in a tabular form. By scoring the velocities of many sample molecules as they pass through each zone they can obtain the velocity distribution of the molecules in each zone in a tabular form.

These are then used as the target molecule distributions in the next iteration. This process is continued until the sample molecule distribution found agrees with the target molecule distribution assumed. Then from the distributions in each zone the macroscopic quantities of interest can be found by numerical integration of the moments of the distribution. The present method, however, avoids the finding and storing of entire distributions of target molecule for each increment.

In the Monte Carlo method since the distribution of target molecules is an approximation to the true distribution only conservation of mass is satisfied exactly since molecules are not allowed to "disappear" in transit between the walls. Conservation of momentum and energy can only be considered in an average sense because the collision partners are not recorded.

NOMENCLATURE

C	average thermal velocity $(2kT/M)^{1/2}$
D	channel height
erf(x)	error function, $(2/\sqrt{\pi}) \int_0^x e^{-u^2} du$
f	probability distribution function
f_+, f_-	probability distribution function of molecules moving in positive, negative V_2 direction
Kn	Knudson number, $\lambda_m/D = M/\sqrt{2}\, S\rho_A D$
k	Boltzmann constant
M	mass of molecule
N	number of sample molecules emitted from surface 0 in Monte Carlo run, proportional to the flux of molecules leaving surface 0

P	pressure
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 $\int Qf_+\ d^3V$
R	random number between 0 and 1
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
V	molecular velocity
V^*	velocity after collision
x_1,x_2,x_3	coordinates
γ	defined by eqs. (B6) and (B7)
η	defined by eqs. (B6) and (B7)
Θ	collision rate of sample molecule with target molecules
λ	path length to collision
$\lambda_{\mu,s}$	mean free path length
μ	dimensionless velocity, V/C
$\mu_{R,A}$	defined by eq. (A5)
ρ	mass density
σ	diameter of hard sphere molecule
φ	angle between sample molecule and target molecule velocities

Subscripts:

A	averaged
p	increment number
p_f	last increment
R	relative velocity
s	sample molecule
t	target molecule
w,0;w,1	at wall 0, 1
0,1	evaluated next to wall 0, 1
1,2,3	coordinate directions
+,-	positive or negative direction

ANALYSIS

Start of Sample Molecule History at the Wall

The sample molecule history will begin at the surface with temperature $T_{w,0}$. To pick the components of velocity of the molecules leaving the surface the simplest assumption is that the molecules incident on the wall are perfectly accommodated, that is, are in a Maxwellian distribution at the wall based on the wall temperature. This assumption is discussed in reference 3. The normalized Maxwellian velocity distribution of the molecules moving away from the wall ($V_2 > 0$) is given as

$$\frac{\rho_{+,0}}{M} f_{+,0}\, d^3V = \frac{2\rho_{+,0}}{M\pi^{3/2}C_0^3}\left[\exp\left(-\frac{V^2}{C_0^2}\right)\right]dV_1\, dV_2\, dV_3 \quad \text{where} \quad V_2 > 0 \tag{1}$$

The $\rho_{+,0}/M$ is the number density of molecules moving away from the wall, and C_0 is the thermal velocity $\left(\frac{2k}{M} T_{w,0}\right)^{1/2}$. If we consider the positive

x_2 direction normal to the wall, the distribution of velocities of the molecules leaving the wall per unit time per unit area is $V_2 f_{+,0}$ (refs. 1, 2, and 6). This can be transformed to cylindrical coordinates $V_2 = V_2$, $V_1 = V_r \cos\theta$, $V_3 = V_r \sin\theta$ and normalized by $\langle V_2 \rangle_{+,0} = C_0/\sqrt{\pi}$ (ref. 1) to give

$$f(\theta,V_2,V_r) = \frac{V_2 f_{+,0}\, d^3V}{\langle V_2 \rangle_{+,0}} = \frac{2V_2}{\pi C_0^4}\left[\exp\left(-\frac{V^2}{C_0^2}\right)\right] V_r\, d\theta\, dV_2\, dV_r = f_\theta f_{V_2} f_{V_r}\, d\theta\, dV_2\, dV_r \tag{2}$$

The distributions for $f_\theta f_{V_2} f_{V_r}$ can be written separately as

$$f_\theta\, d\theta = \frac{d\theta}{2\pi} \tag{3}$$

$$f_{V_2}\, dV_2 = \frac{2V_2}{C_0^2}\left[\exp\left(-\frac{V_2^2}{C_0^2}\right)\right] dV_2 \tag{3b}$$

$$f_{V_r}\, dV_r = \frac{2V_r}{C_0^2}\left[\exp\left(-\frac{V_r^2}{C_0^2}\right)\right] dV \tag{3c}$$

The velocity components of our sample molecule leaving the surface must be picked from these distributions. This same result was used in references 1 and 6. A convenient way of picking from a distribution for the high speed computer is to transform the distribution to a uniform distribution in R by setting the random number R equal to the cumulative distribution function. For instance

$$R = \int_0^\theta f_\theta\, d\theta = \frac{\theta}{2\pi} \tag{4}$$

Then by using a high speed computer to generate a random number R

between 0 and 1, we can obtain θ from equation (4) such that for a large number of samples picked in this manner the distribution in equation (3a) will be satisfied.

Similarly we can pick V_2 from

$$R_{V_2} = \int_0^{V_2} \frac{2V_2}{C_0^2}\left[\exp\left(-\frac{V_2^2}{C_0^2}\right)\right] dV_2 \tag{5}$$

or, since picking R is equivalent to picking 1 - R,

$$V_2 = (-C_0^2 \ln R_{V_2})^{1/2} \tag{6}$$

so that by picking R_{V_2} we can obtain V_2 from equation (6). The velocity V_r is obtained in the same manner and is given by

$$V_r = (-C_0^2 \ln R_{V_r})^{1/2} \tag{7}$$

The V_2, V_r, and θ picked then give the direction and velocity of the sample molecule as it leaves the wall. This same result was used in references 1 and 6.

The sample molecule is then followed through the first zone until either a collision occurs with another molecule or the sample molecule passes through the zone. This will depend on whether the path length of the sample molecule to collision is shorter or longer than the path length through the zone.

Calculation of the Path Length λ to Collision for the Sample Molecule

The probability that a sample molecule will collide in the incremental path length λ to $\lambda + d\lambda$ is given in reference 7 as

$$f_\lambda = \frac{\exp\left(-\lambda/\lambda_{\mu,s}\right)}{\lambda_{\mu,s}} \tag{8}$$

where $\lambda_{\mu,s}$ is the mean free path to collision of the sample molecule moving at velocity V_s in that zone.

We can then pick a path length to collision for the sample molecule from this distribution by using the same procedure described earlier

$$\lambda = -\lambda_{\mu,s} \ln R_\lambda \tag{9}$$

To use this relationship, we must first calculate the mean free path $\lambda_{\mu,s}$ in the zone.

As shown in appendix A the mean free path of a sample molecule moving at velocity V_s through a Maxwellian gas at density ρ with a thermal velocity C is (eq. (A8))

$$\frac{\lambda_{\mu,s}}{D} = \frac{2^{1/2}\,\mathrm{Kn}\,\mu_s}{\dfrac{\rho}{\rho_A}\left[\dfrac{\exp(-\mu_s^2)}{\pi^{1/2}} + (\mathrm{erf}\,\mu_s)\left(\mu_s + \dfrac{1}{2\mu_s}\right)\right]} \tag{10}$$

where μ_s is the velocity of the sample molecule nondimensionalized by the thermal velocity of the zone ($\mu_s = V_s/C$), D is the distance across the channel and Kn is the usual definition of Knudson number for hard sphere molecules in a Maxwellian distribution

$$\mathrm{Kn} = \frac{\lambda_M}{D} = \frac{M}{\sqrt{2}\,S\rho_A D} \tag{11}$$

Equation (10) can then be used in equation (9) to obtain the distance to collision for the sample molecule in the zone. If there is a collision in the zone, the next step is to pick a collision partner and calculate the new direction and velocity of the sample molecule after collision.

Calculating New Sample Molecule Velocity Components and Direction After Collision

The distribution of target molecules hit by the sample molecule is given in appendix B following the derivation in reference 7. From this distribution we pick a target molecule collision partner. The new velocity of the sample molecule after collision with the target molecule is given following the derivation in reference 1.

$$\left.\begin{aligned} V^*_{2s} &= \frac{1}{2}(V_{2s} + V_{2t}) + \frac{1}{2} V_R(1 - 2b^2) \\ V^*_{1s} &= \frac{1}{2}(V_{1s} + V_{1t}) + V_R(1 - b^2)^{1/2}\, H \\ V^*_{3s} &= \frac{1}{2}(V_{3s} + V_{3t}) + V_R(1 - b^2)^{1/2}\, \Xi \end{aligned}\right\} \tag{12}$$

where

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

The values of H and Ξ are obtained as discussed in reference 1 by picking two random numbers and using them in the following equations

$$H = 2R_H - 1,\ \Xi = 2R_\Xi - 1,\ \text{and}\ \ b^2 = H^2 + \Xi^2 \tag{13}$$

where b^2 must be less than one. If b^2 is greater than one, a new set of random numbers must be chosen to find H and Ξ.

Completion of Sample Molecule Histories

After collision a new path length to collision is found and this is compared to the distance the sample molecule must travel in its new direction to leave the zone. If this distance is smaller than the new path length to collision, the molecule is then started through the next zone as shown in figure 1. This process is continued until the sample molecule returns to the wall 0 and then a new sample molecule history is started. This process is continued for the desired number of sample histories.

Scoring to Find the Macroscopic Flow Properties

The macroscopic fluid characteristics we must obtain are the density distribution and temperature distribution across the channel since these are needed in the target molecule distribution. Also of interest is the net heat transferred across the channel. These properties are obtained as follows. Scoring positions are located at various distances across the channel as shown in figure 1. The average quantity of Q transported across the scoring cross section p in the positive x_2 direction by the sample molecules crossing it can be written as

$$\frac{\left(\sum_{S_+} Q\right)_p}{S_{+,p}} \approx \frac{\left(\int QV_2 f_+ \, d^3V\right)_p}{\left(\int V_2 f_+ \, d^3V\right)_p} \equiv \frac{\left(\rho_+ \langle QV_2\rangle_+\right)_p}{\left(\rho_+ \langle V_2\rangle_+\right)_p} \tag{14}$$

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

$$\frac{\left(\sum_{S_-} Q\right)_p}{S_{-,p}} \approx \frac{\left(\rho_- \langle QV_2\rangle_-\right)_p}{\left(\rho_- \langle V_2\rangle_-\right)_p} \tag{15}$$

Since there is no net flow across the channel and since all sample histories start and end at the wall 0,

$$S_{+,p} = S_{-,p} \tag{16a}$$

and

$$\left(\int V_2 f_+ \, d^3V\right)_p = -\left(\int V_2 f_- \, d^3V\right)_p \tag{16b}$$

We can then write

$$\frac{\rho\langle V_2 Q\rangle_p}{\rho_{+,p}\langle V_2\rangle_{+,p}} = \frac{1}{S_{+,p}}\left(\sum^{S_+} Q - \sum^{S_-} Q\right)_p \tag{17}$$

The number of sample molecules that pass the scoring cross section at p in the positive V_2 direction $S_{+,p}$ divided by the total number of sample molecule histories started at wall 0, N, can be related to the mass flux passing in the positive V_2 direction at p by

$$\frac{S_{+,p}}{N} \approx \frac{\rho_{+,p}\langle V\rangle_{+,p}}{\rho_{+,0}\langle V\rangle_{+,0}} \tag{18}$$

where $\rho_{+,0}\langle V\rangle_{+,0}$ the mass flux leaving wall 0 is equal to $\rho_{+,0}C_{+,0}/\pi^{1/2}$ (ref. 1). Combining equations (17) and (18) results in

$$\rho\langle V_2 Q\rangle_p = \frac{\rho_{+,0}C_{+,0}}{N\pi^{1/2}}\left(\sum^{S_+} Q - \sum^{S_-} Q\right)_p \tag{19}$$

If Q is taken as $1/V_2$, equation (19) becomes

$$\frac{\rho}{\rho_{+,0}} = \frac{C_{+,0}}{N\pi^{1/2}}\left(\sum^{S_+}\frac{1}{V_2} - \sum^{S_-}\frac{1}{V_2}\right) \tag{20}$$

The average density in the channel is then obtained by averaging the density of all the scoring cross sections from $p = 0$ to $p = p_f$

$$\frac{\rho_A}{\rho_{+,0}} = \frac{1}{p_f}\left[\frac{1}{2}\left(\frac{\rho_0}{\rho_{+,0}} + \frac{\rho_{p_f}}{\rho_{+,0}}\right) + \sum_{p=1}^{p_f-1} \frac{\rho_p}{\rho_{+,0}}\right] \tag{21a}$$

As shown in reference 1 the collision solution (Kn → ∞) is given by

$$\left(\frac{\rho_A}{\rho_{+,0}}\right)_{Kn\to\infty} = \frac{\left(\frac{T_{w,1}}{T_{w,0}}\right)^{1/2} + 1}{\left(\frac{T_{w,1}}{T_{w,0}}\right)^{1/2}} \tag{21b}$$

Similarly we can obtain the local pressure from

$$\frac{P}{\langle \rho V^2 \rangle_{+,0}} = \frac{1}{3}\,\rho\,\frac{\langle V_2^2 + V_r^2 \rangle}{\langle \rho V^2 \rangle_{+,0}} = \frac{2}{3C_{+,0}N\pi^{1/2}}\left(\sum^{S_+} \frac{V_2^2 + V_r^2}{V_2} - \sum^{S_-} \frac{V_2^2 + V_r^2}{V_2}\right) \tag{22}$$

since $\langle \rho V_2^2 \rangle_{+,0} = \frac{\rho_{+,0}C_{+,0}^2}{2}$ as given in reference 1 and $V_r^2 = V_1^2 + V_3^2$. Dividing equation (22) by $\rho/\rho_{+,0}$, as obtained from equation (20), then gives the local temperature

$$\frac{T}{T_0} = \frac{\langle V_2^2 + V_r^2 \rangle}{\frac{3C_{+,0}^2}{2}} = \frac{\frac{P}{\langle \rho V_2^2 \rangle_{+,0}}}{\frac{\rho}{\rho_{+,0}}} \tag{23}$$

as shown in reference 1 the collisionless solution (Kn → ∞) is given by

$$\left(\frac{T}{T_0}\right)_{Kn\to\infty} = \left(\frac{T_{w,1}}{T_{w,0}}\right)^{1/2} \tag{24}$$

Finally, the heat transfer across the channel can be obtained from

$$q = \frac{1}{2}\,\rho\,\langle(V_z^2 + V_r^2)\rangle = \frac{\rho_{+,0}C_{+,0}}{2\pi^{1/2}N}\left[\sum^{S_{+,p}} (V_z^2 + V_r^2) - \sum^{S_{-,p}} (V_z^2 + V_r^2)\right] \tag{25}$$

This can be nondimensionalized by $q_\lambda = \frac{1}{2}\,(\rho\langle V_z(V_z^2 + V_r^2)\rangle)_{+,0} = \frac{1}{\pi^{1/2}}\,(\rho_{+,0}C_{+,0}^3)$, the heat leaving the wall as given in (ref. 1) and then divided by ρ_+/ρ_A to give

$$\frac{\pi^{1/2}}{\rho_A C_{+,0}^3}\,q = \frac{1}{2NC_{+,0}^2}\left[\sum^{S_{+,p}} (V_z^2 + V_r^2) - \sum^{S_{-,p}} (V_z^2 + V_r^2)\right]\left(\frac{\rho_+}{\rho_A}\right) \tag{26}$$

This can be compared to the collisionless result given in reference 1

$$\left(\frac{\pi^{1/2}q}{\rho_A C_{+,0}^3}\right)_{Kn\to\infty} = \left(\frac{T_{w,1}}{T_{w,0}}\right)^{1/2} - \left(\frac{T_{w,1}}{T_{w,0}}\right) \tag{27}$$

In this manner the local temperature and density in each zone can be obtained. This is compared to the assumed temperature and density distribution used in the local Maxwellian distribution of the target molecules in each zone and the results are iterated till agreement is obtained.

RESULTS AND CONCLUSIONS

The results for the density distributions and temperature distributions are shown in figures 2 and 3. The heat-transfer results are shown in figure 4. These results were compared with the Gross-Ziering eight moment half range solution as given in reference 4 and Haviland and Lavin nonlinear four moment solution given in reference 5 and their Monte Carlo solution given in reference 2.

Both Monte Carlo solutions are in better agreement with the Gross-Ziering solution and poor agreement with the nonlinear four moment solution.

The present technique is very flexible and can be readily extended to different types of molecular collisions and to different boundary conditions. Using the Maxwellian distribution for the target molecules resulted in a nonconstant heat transfer across the channel. This was averaged to obtain the present result. More realistic target molecule distributions, however, can be used in the analysis. An important shortcoming of the present method is the need of a high speed computor and extensive computing time. Each solution required about 1 hour of running time on the IBM 7094.

APPENDIX A

EVALUATION OF MEAN FREE PATH

The number of collisions per unit time $d\Theta(V_R,V_t)$ of a sample molecule moving at velocity V_s through target molecules in velocity volume space d^3V_t for hard sphere molecules is given in reference 6 as

$$d\Theta = \rho f_t V_R S\ d^3V_t \tag{A1}$$

where V_R is the velocity of the target molecules relative to the sample molecule velocity before collision, $V_{R,i} = V_{t,i} - V_{s,i}$, as shown in figure 5, and S is the mutual collision cross section $\pi\sigma^2$ where σ is the diameter of the molecule. The relative velocity V_R as seen from figure 5 can be written as

$$V_R = (V_t^2 + V_s^2 - 2V_sV_t \cos \varphi')^{1/2} \tag{A2}$$

where φ' is the angle between V_t and V_s. For the case of a Maxwellian distribution following the analysis given in reference 7 the collision rate can be written as

$$d\Theta(\mu_t,\varphi',\theta) = \frac{\rho CS}{M\pi^{3/2}} \left[\exp\left(-\mu_t^2\right)\right] \mu_t^2\mu_R \sin \varphi'\ d\varphi'\ d\theta'\ d\mu_t \tag{A3}$$

where μ is the nondimensionalized velocity V/C and the angles φ' and θ' are shown in figure 5. To obtain the total collision rate for the target molecules over all velocities, this must be integrated over φ', θ', and μ_t. We can integrate this over θ' from 0 to 2π and integrate over φ' from 0 to π to give

$$d\Theta(\mu_t) = \frac{4\rho CS}{M\pi^{1/2}} \left[\exp\left(-\mu_t^2\right)\right] \mu_t^2 u_{R,A}\ d\mu_t \tag{A4}$$

where

$$\mu_{R,A} = \int_0^{\pi} (\mu_t^2 + \mu_s^2 - 2\mu_s\mu_t \cos \varphi')^{1/2} \frac{\sin \varphi'}{2} d\varphi'$$

or

$$\mu_{R,A} = \begin{cases} \mu_s + \mu_t^2/3\mu_s & \text{if} \quad \mu_s > \mu_t \\ \mu_t + \mu_s^2/3\mu_t & \text{if} \quad \mu_t > \mu_s \end{cases} \tag{A5}$$

We can then integrate over μ_t from 0 to ∞ to obtain the total collision frequency for a sample molecule moving at velocity μ_s through a Maxwellian gas as

$$\Theta = \frac{\rho SC}{M}\left\{\frac{\exp\,(-\mu_s^2)}{\pi^{1/2}} + (\text{erf}\ \mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right)\right\} \tag{A6}$$

The dimensionless mean free path is then found as discussed in reference 7 by dividing the dample molecule velocity by the total collision rate to give

$$\frac{\lambda\mu_s}{D} = \frac{V_s}{\Theta} = \frac{\mu_s M}{D\rho S\left\{\frac{1}{\pi^{1/2}}\left[\exp\,(-\mu_s^2)\right] + (\text{erf}\ \mu_s)\ \left(\mu_s + \frac{1}{2\mu_s}\right)\right\}} \tag{A7}$$

Using the definition of Knudson number as given by equation (11) enables us to write

$$\frac{\lambda\mu_s}{D} = \text{Kn}2^{1/2}\mu_s\left(\frac{\rho}{\rho_A}\right)^{-1}\left\{\frac{\left[\exp\,(-\mu_s^2)\right]}{\pi^{1/2}} + (\text{erf}\ \mu_s)\ \left(\mu_s + \frac{1}{2\mu_s}\right)\right\}^{-1} \tag{A8}$$

APPENDIX B

PICKING THE TARGET MOLECULE COLLISION PARTNER

The velocity distribution of target molecules that the sample molecule will collide with is discussed in reference 1 is given by

$$\frac{d\Theta(\mu_t,\varphi',\theta)}{\Theta} = \frac{[\exp\,(-\mu_t^2)]\mu_t^2\mu_R \sin\varphi'\; d\varphi'\; d\theta'\; d\mu_t}{\pi[\exp\,(-\mu_s^2)] + \pi^{3/2}(\mathrm{erf}\;\mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right)} \tag{B1}$$

The distribution in θ' for the target molecules is readily seen to be

$$f_{\theta'}\; d\theta' = \frac{d\theta'}{2\pi} \tag{B2}$$

Then the θ' can be picked from this distribution by

$$\theta' = 2\pi R_\theta \tag{B3}$$

The distribution of μ_t for the target molecules is obtained from the marginal distribution

$$f_{\mu_t}\; d\mu_t = \frac{4[\exp\,(-\mu_t^2)]\; \mu_t^2\mu_{R,A}\; d\mu_t}{\left\{[\exp\,(-\mu_s^2)] + \pi^{1/2}(\mathrm{erf}\;\mu_s)\left(\mu_s + \frac{1}{2\mu_s}\right)\right\}} \tag{B4}$$

We can then pick from this distribution as before

$$R\mu_t = \frac{\gamma(\mu_s,\mu_t) + \eta(\mu_s,\mu_t)}{[\exp\,(-\mu_s^2)] + \pi^{1/2}(\mathrm{erf}\;\mu_s)\left(\mu_s + \frac{1}{\mu_s}\right)} \tag{B5}$$

where when $\mu_s > \mu_t$

$$\gamma(\mu_s,\mu_t) = -2\mu_s\mu_t\left[\exp(-\mu_t^2)\right] + \mu_s\;\sqrt{\pi}\;(\mathrm{erf}\;\mu_t) - \frac{2}{3}\,\frac{\mu_t^3}{\mu_s}\left[\exp(-\mu_t^2)\right]$$
$$- \frac{\mu_t}{\mu_s}\left[\exp\,(-\mu_t^2)\right] + \frac{\sqrt{\pi}}{2\mu_s}\;(\mathrm{erf}\;\mu_t) \tag{B6}$$

$\eta = 0$

and when $\mu_s < \mu_t$

$$\left.\begin{aligned} &\gamma(\mu_s,\mu_t) = \gamma(\mu_s,\mu_s) \\ &\eta = -2\left[\exp\,(-\mu_t^2)\right]\left(\frac{\mu_s^2}{3} + 1 + \mu_t^2\right) + 2\left[\exp\,(-\mu_s^2)\right]\left(\frac{4\mu_s^2}{3} + 1\right) \end{aligned}\right\} \qquad \text{(B7)}$$

To find φ' for the target molecule, we can write the distribution of target molecules as a product of a marginal times a conditional distribution

$$\frac{d\Theta(\mu_t,\varphi')}{\Theta} = f(\mu_t)f(\varphi'|\mu_t) \qquad \text{(B8)}$$

then we must pick φ' from the conditional distribution

$$f(\varphi'|\mu_t) = \frac{(\mu_t^2 + \mu_s^2 - 2\mu_s\mu_t\cos\varphi')^{1/2}\,\dfrac{\sin\varphi'\,d\varphi'}{2}}{\mu_{R,A}} \qquad \text{(B9)}$$

Picking φ' for a given μ_t is found as before from

$$R_{\varphi'} = \frac{(\mu_t^2 + \mu_s^2 - 2\mu_t\mu_s\cos\varphi')^{3/2} - |\mu_t - \mu_s|^3}{(\mu_t^2 + \mu_s^2 + 2\mu_t\mu_s)^{3/2} - |\mu_t - \mu_s|^3} \qquad \text{(B10)}$$

Then components of velocity of the target molecule must still be transposed to the coordinate system of the channel. Taking V_{2t}' in the same direction as the V_s coordinate as shown in figure 5 and V_{3t}' in the same direction as the V_3 coordinate we can obtain the component of velocity for the target molecule in the primed system as

$$\left.\begin{aligned} \mu_{2t}' &= \mu_t\cos\varphi' \\ \mu_{1t}' &= \mu_t\sin\varphi'\cos\theta' \\ \mu_{3t}' &= \mu_t\sin\varphi'\sin\theta' \end{aligned}\right\} \qquad \text{(B11)}$$

Then by a simple rotation of the coordinate system through an angle φ around the V_3 axis the components of velocity of the target molecule in the channel coordinates are given by

$$\left.\begin{aligned}\mu_{3t} &= \mu'_{3t}\\ \mu_{2t} &= \mu'_{2t}\cos\varphi - \mu'_{1t}\sin\varphi\\ \mu_{1t} &= \mu'_{2t}\sin\varphi + \mu'_{1t}\cos\varphi\end{aligned}\right\} \qquad \text{(B12)}$$

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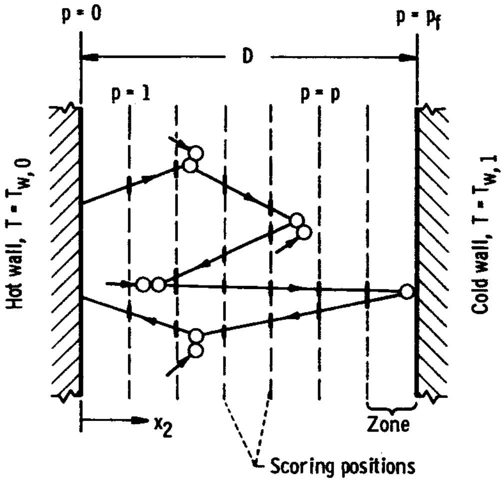

Figure 1. - Model.

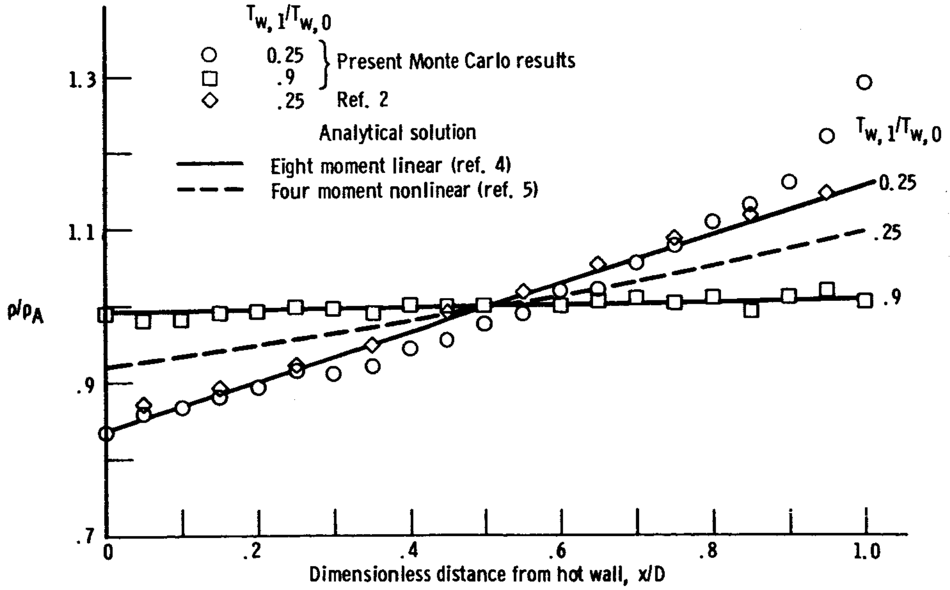

Figure 2. - Density distribution across channel. Knudson number, 2.

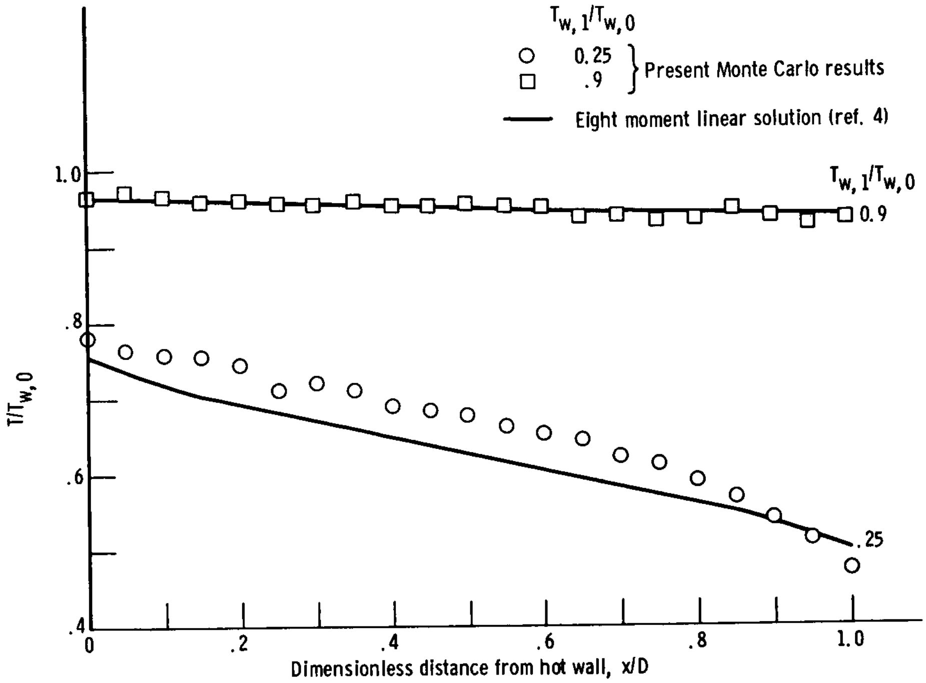

Figure 3. - Temperature distribution across channel. Knudson number, 2.

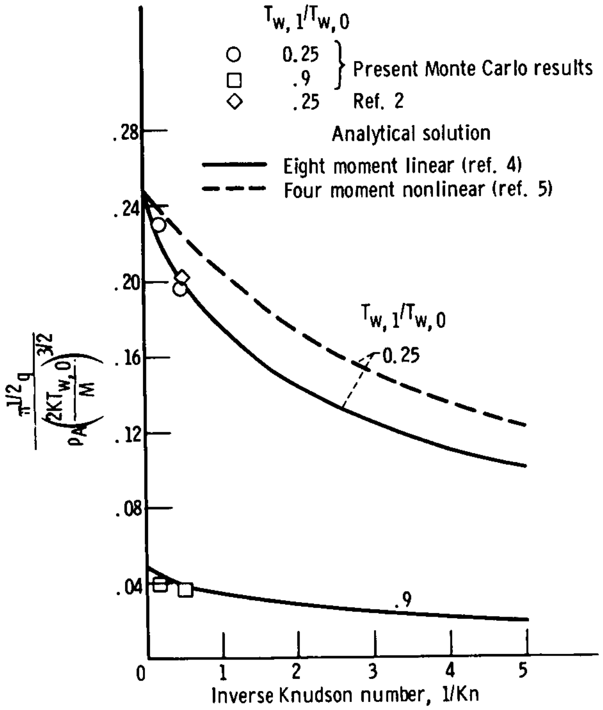

Figure 4. - Heat transfer across channel.

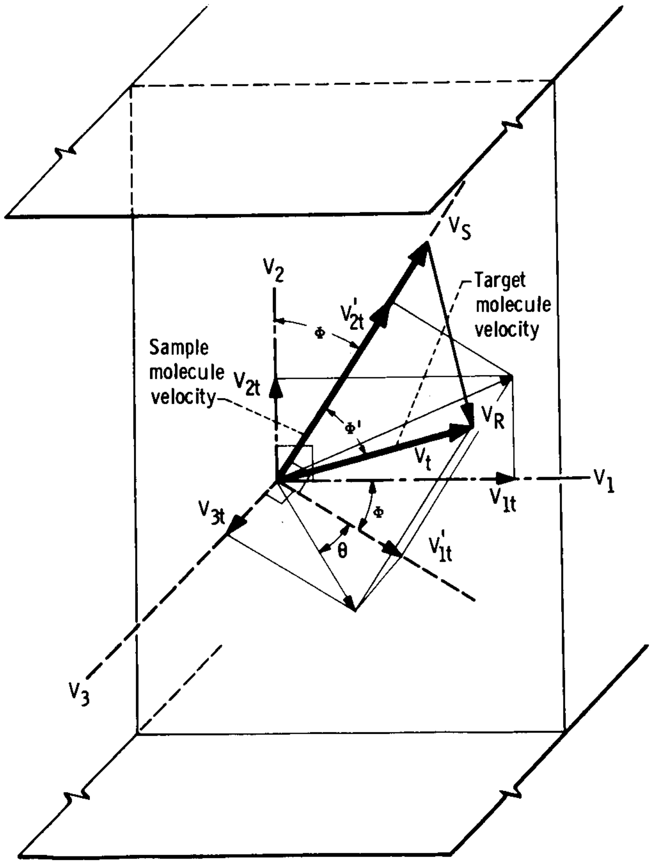

Figure 5. - Velocity of sample and target molecules at collision.