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RARIFIED DIFFUSION BY MODEL SAMPLING

by Morris Perlmutter

Lewis Research Center
Cleveland, Ohio

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16. Abstract

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SUMMARY

The rarefied diffusion of molecules of species α, evaporated or emitted from one plate, through another species β of a different molecular weight enclosed between parallel walls is analyzed by the method of model sampling. The diffusing species is considered sufficiently dilute so that only collisions with nondiffusing molecules are important. Maxwellian collisions are assumed. The results are given over a Knudsen range from free molecule to continuum flow. These results fall along one curve for all molecular mass ratios when the appropriate definition of mean free path is used. The results agreed with the continuum solution limiting case and elementary slip theory was found to give reasonable approximate results.

INTRODUCTION

As more rarefied environments are encountered, an understanding of diffusion processes under noncontinuum conditions becomes of greater importance. Compared to the continuum diffusion, rarefied diffusion has received very little study. The present analysis considers the rarefied diffusion of molecules α evaporated or emitted from a plane surface (see fig. 1). These molecules diffuse through a nondiffusing gas of species β which can be of a different molecular weight. The diffusing molecules are absorbed or condensed when incident on either surface of the enclosure. The diffusing species is considered sufficiently dilute so that only collisions with the nondiffusing molecules are important. The nondiffusing molecules are considered to be in Maxwellian equilibrium at the temperature of the plates, which is constant. Maxwellian collisions are assumed. The results are given for the Knudsen range from free molecule to continuum flow.

The method of solution is model sampling or Monte Carlo. A sample history of a diffusing molecule is generated by randomly choosing from the appropriate distributions

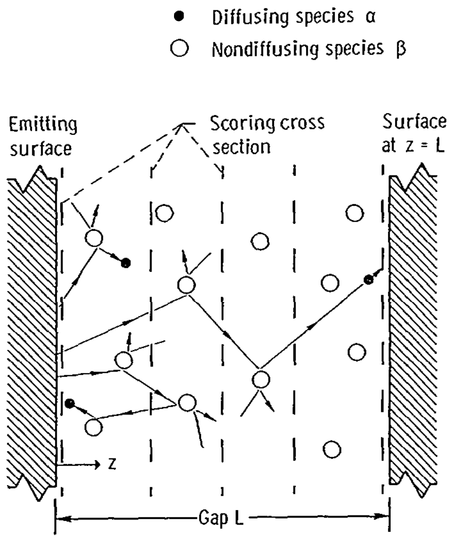

Figure 1. - Analytical model.

at points of decision in the sample history. The sample molecules are scored (i.e., various characteristics are recorded) as they pass scoring positions at specified locations across the gap. These scoring results give the macroscopic flow quantities of interest.

Previous analyses of rarefied gas problems using model sampling were carried out for Couette flow with heat transfer (ref. 1) and the normal shock problem (ref. 2). The present results give the molecular flux and the molecular density profile across the gap.

SYMBOLS

A_1	numerical constant, 2.6595
b	molecular collision parameter
C_α, C_β	thermal velocity; $\left(\frac{2\kappa}{m_\alpha} T\right)^{1/2}$, $\left(\frac{2\kappa T}{m_\beta}\right)^{1/2}$
D	coefficient of diffusion
f	probability distribution function
K	intermolecular force constant, ref. 6
$K\{k^2\}$	factor entering in eq. (30)
L	distance between surfaces
l	dimensionless distance across gap or inverse Knudsen number, L/λ

M	molecular mass ratio, m_α/m_β
m	mass of molecule
N	number of samples leaving surface 0
n	number density
n_i	i^{th} component of unit vector lying in collision plane of two colliding molecules
n_s	slip number density
P_{VP}	vapor pressure
p	scoring position
Q	property of molecule
R	random number chosen from uniform distribution between 0 and 1
T	absolute temperature
V, V_β	velocity of α or β molecules
V_R	relative velocity
v, v^*	normalized velocities of α molecules, V/C_β or V/C_α, respectively
v'	dimensionless velocity after collision
v_R	dimensionless relative velocity, V_R/C_β
v_r^*	dimensionless radial velocity component (normalized by C_α)
v_β	normalized velocity of β molecules, V_β/C_β
Z	coordinate across gap
z	dimensionless distance across gap, Z/L
α	diffusing species
β	nondiffusing species
γ	angle between molecule and z-axis
δ	net sum of Q at scoring position per molecule emitted
ϵ	molecular collision parameter
ζ	dimensionless path length in z direction, λ/λ_β
Θ	collision rate
κ	Boltzmann's constant
λ	path length to first collision in z direction

λ_β	mean free path based on thermal velocity, C_β/Θ
λ_μ	mean free path length to first collision in z direction
μ	molecular flux
φ	angle parameter occurring in two molecule collision
ω	dimensionless molecular collision parameter
ω_m	maximum value of dimensionless collision parameters above which effects of collisions are negligible

Subscripts:

x, y	indicate coordinate directions
0	evaluated at $z = 0$ at emitter plate
+, -	positive, negative z direction

ANALYSIS

Scoring to Find Average Flow Properties

The average quantities of interest at various positions across the gap are the molecular flux μ, which is the number of diffusing molecules crossing the gap per unit area per unit time, and also the molecular density n_α, which is the number of diffusing molecules per unit volume. These values are obtained at the so-called scoring positions in the gap (see fig. 1). If some property of the molecule is designated by Q, the average of Q transported across the scoring position per molecule emitted from the surface 0 can be written as

$$\frac{n\langle Qv_z\rangle}{n_{0,+}\langle v_z\rangle_0} = \langle\delta\rangle = \iint \delta f(\delta, V_{z,0})d\delta\, dv_{z,0}$$

$$= \iint \delta f(\delta \mid v_{z,0})f(v_{z,0})d\delta\, dv_{z,0} \qquad (1)$$

The δ is the sum of Q crossing the scoring position in the positive z direction minus the sum of Q passing the scoring position in the negative z direction for one sample molecule emitted from surface 0 at velocity $v_{z,0}$.

The $v_{z,0}$ is the component of velocity in the positive z direction of the sample molecule leaving surface 0 normalized by the thermal velocity C_β as given in the nomenclature. The joint distribution at the scoring position $f(\delta, v_{z,0})$ can be written as a product of a conditional distribution and a marginal distribution, namely, $f(\delta | v_{z,0}) f(v_{z,0})$. (Dr. Burt Rosenbaum of Lewis aided in the formulation of eq. (1).)

The variance of δ is given as

$$\sigma^2(\delta) = \iint \delta^2 f(\delta | v_{z,0}) f(v_{z,0}) d\delta \, dv_{z,0} - \left[\iint \delta f(\delta | v_{z,0}) f(v_{z,0}) d\delta \, dv_{z,0}\right]^2 \tag{2}$$

By model sampling the integral $\langle \delta \rangle$ in equation (1) (ref. 3, ch. 2) can be approximated as

$$\langle \delta \rangle \approx \bar{\delta} = \frac{1}{N} \sum_{i=1}^{N} \delta_i \tag{3}$$

where N is the number of molecules sampled and δ_i is the net sum of Q crossing the scoring position for the i^{th} sample molecule emitted from surface 0.

As given in the aforementioned references, it is 95 percent certain that the error, which is the difference between the model sampling value $\bar{\delta}$ and the true value of $\langle \delta \rangle$, is less than the so-called 95 percent confidence range given by

$$|\bar{\delta} - \langle \delta \rangle| \leq \frac{1.96}{\sqrt{N}} \sigma(\delta) \tag{4}$$

where

$$\sigma^2(\delta) \approx \frac{1}{N} \sum_{i=1}^{N} \delta_i^2 - \left(\frac{1}{N} \sum_{i=1}^{N} \delta_i\right)^2 \tag{5}$$

Specifically, for the case Q = 1, equations (1) and (3) give

$$\frac{\mu}{\mu_{0,+}} = \frac{1}{N} \sum_{i=1}^{N} \delta_{i,\mu} \tag{6}$$

where $\delta_{i,\mu}$ is the number of times the i^{th} sample molecule passes the scoring position p in the positive direction minus the number of times it passes p in the negative direction. As shown in equation (6), the average gives the diffusing molecular flux passing the scoring position divided by the diffusing molecular flux leaving the surface 0. The 95 percent confidence range is given by equations (4) and (5).

For the case $Q = 1/v_z$, equations (1) and (3) yield

$$\frac{n}{n_{0,+}\langle v_z\rangle_{0,+}} = \frac{1}{N}\sum_{i=1}^{N} \delta_{i,n} \tag{7}$$

where $\delta_{i,n}$ is the sum of the absolute values of the reciprocals of the velocities (a sample molecule can cross a given scoring position any number of times) with which the i^{th} sample molecule passes the scoring position. Inasmuch as the average molecular velocity leaving the surface 0 is assumed to be given by

$$\langle v_z\rangle_0 = (\pi M)^{-1/2} \tag{8}$$

where M is the molecular mass ratio m_α/m_β; and since the flux is merely $n_{0,+}\langle v_z\rangle_0$, equation (7) becomes

$$\frac{n}{n_{0,+}} = \frac{1}{(\pi M)^{1/2}N}\sum_{i=1}^{N} \delta_{i,n} \tag{9}$$

By using equation (5), the variance can be seen to be

$$\sigma^2\left(\frac{\delta_{i,n}}{(\pi M)^{1/2}}\right) \approx \frac{1}{(\pi M)}\left[\frac{1}{N}\sum_{i=1}^{N} \delta_{i,n}^2 - \left(\frac{1}{N}\sum_{i=1}^{N} \delta_{i,n}\right)^2\right] \tag{10}$$

which can be used to calculate the 95 percent confidence range (eq. (4)).

Relation Between Mass Flux Leaving Surface and Vapor Pressure

The molecular flux evaporating from the surface can be found by relating the molecular density $n_{0,+}$ of the molecules leaving the surface to their vapor pressure P_{VP}. The number density of the molecules leaving the surface $n_{0,+}$ can be related to the vapor pressure P_{VP} of the diffusing α molecules by the ideal gas law, $n_{0,+} = P_{VP}/2\kappa T$ (as given in ref. 4, Sec. 1.6).

Choosing Velocity Components for Emitted Sample Molecules

The molecular flux leaving the surface 0 in velocity increment d^3v^* is given by

$$\frac{2n_{0,+}v_z^*}{\pi^{3/2}}\exp(-v^{*2})d^3v^* \tag{11}$$

where $v^* = V/C_\alpha$. If expression (11) is divided by the total molecular flux leaving the surface $n_{0,+}\langle v_z^*\rangle_0 = n_{0,+}/\sqrt{\pi}$, the result is the velocity probability distribution function for the sample molecules leaving the surface

$$f_0(v^*) = \frac{2v_z^*}{\pi}\exp(-v^{*2}) \tag{12}$$

This can be written in cylindrical coordinates as the product of

$$f\left(v_z^*\right) = 2v_z^*\exp\left(-v_z^{*2}\right) \tag{13a}$$

and

$$f\left(v_r^*\right) = 2v_r^*\exp\left(-v_r^{*2}\right) \tag{13b}$$

Following the method of choosing randomly from a distribution as given in reference 3 (ch. 7. Sec. 4) yields

$$R = \int_0^{v_z^*} 2v_z^*\exp\left(-v_z^{*2}\right)dv_z^* \tag{14}$$

where R is a random number generated by the computer from a uniform distribution in the interval [0, 1]. This equation can be integrated to give

$$v_z^* = v_z\sqrt{M} = (-\ln R)^{1/2} \tag{15}$$

so that by having the computer generate a random number which is substituted into equation (15) we can solve for v_z, the velocity component for the sample leaving the surface 0 normalized by C_β. A similar equation applies for the radial velocity component v_r for the sample molecule leaving the surface.

PATH LENGTH TO COLLISION

After the sample molecule leaves the surface, it is necessary to calculate its path length to first collision. The probability distribution function for path length to collision can be shown to be (ref. 1, p. 460).

$$f(\lambda) = \frac{\exp\left(-\dfrac{\lambda}{\lambda_\mu}\right)}{\lambda_\mu} \tag{16}$$

where λ is the distance in the z direction that the sample molecule will travel before collision. The mean free path in the z direction λ_μ is given by

$$\lambda_\mu = \frac{v_z C_\beta}{\Theta} = v_z \lambda_\beta \tag{17}$$

where $\lambda_\beta = C_\beta/\Theta$.

Now an expression for the mean collision frequency Θ has to be determined. The collisions between an α and a β molecule are assumed, for simplicity, to be Maxwellian in type; that is, the intermolecular force law between colliding molecules can be described by

$$F = \frac{K}{r^5} \tag{18}$$

where r is the distance between colliding molecules and K is a constant. It is shown, for example (ref. 5, p. 170), that the angle through which a molecule is deflected in a Maxwellian collision depends on the nondimensional quantity

$$\omega = b\left(\frac{M}{M+1} V_R^2 \frac{m_\beta}{K}\right)^{1/4} \tag{19a}$$

where large values of ω correspond to small angles of deflection. Here V_R is the relative velocity before collision and b is the minimum separation distance between the two colliding molecules if they were not deflected from straight line paths by the collision. If the angle of deflection effected by a collision is taken as a measure of the degree of perturbation in the path of the diffusing molecule, then only those collisions in which the angles of deflection are larger than some small value need be considered significant. Equivalently, a maximum value of ω denoted as ω_m may be established where collisions with values of ω larger than ω_m may be ignored. Thus, equation (19a) with ω replaced by ω_m constitutes the definition of b_{max}

$$b_{max} = \omega_m\left(\frac{M+1}{M}\frac{K}{V_R^2 m_\beta}\right)^{1/4} \tag{19b}$$

where b_{max} is the largest value of b for which a significant collision takes place.

Proceeding as in reference 6 (p. 154) reveals that the mean collision frequency Θ is given by

$$\Theta = n_\beta \int f_\beta(V_\beta)V_R\, d^3V_\beta \int_0^{b_{max}} b\, db \int_0^{2\pi} d\epsilon \tag{20a}$$

which can be easily integrated to yield the expression

$$\Theta = n_\beta \pi \omega_m^2 \left[\left(\frac{M+1}{2M}\right)\left(\frac{2K}{m_\beta}\right)\right]^{1/2} \tag{20b}$$

Acceptable values of ω_m were found by carrying out the analysis for different values of ω_m until an increase in ω_m did not significantly change the results. This aspect of the problem is discussed below and in reference 6 (p. 122).

Substituting equation (20b) into equation (17) gives

$$\lambda_\beta = C_\beta\left(\frac{2M}{M+1}\right)^{1/2} \Big/ n_\beta \pi \omega_m^2 \left(\frac{2K}{m_\beta}\right)^{1/2} \tag{21}$$

If ζ is defined as λ/λ_β, equation (16) becomes

$$f_\zeta\left(\frac{\zeta}{v_z}\right) = \exp\left(-\frac{\zeta}{v_z}\right) \tag{22}$$

To randomly choose a normalized distance ζ to collision, proceed as before

$$\zeta = -v_z \ln R \tag{23}$$

The dimensionless distance or number of path lengths across the gap is then given as

$$l_\beta = L/\lambda_\beta \tag{24}$$

where l_β is the inverse of the usual definition of Knudsen number.

SAMPLE MOLECULE VELOCITY AFTER COLLISION

To find the velocity components of the sample molecule after collision, first pick velocity components for a collision partner. For Maxwellian collision the probability that a collision partner will have a velocity v_β in d^3v_β is given by (ref. 1, p. 469)

$$\frac{d\Theta}{\Theta} = f_\beta\, d^3V_\beta = \frac{1}{\pi^{3/2}} \exp\left(-v_\beta^2\right) d^3v_\beta \tag{25}$$

where f_β is the velocity probability distribution function of the nondiffusing β molecules. The function f_β can be written in cylindrical coordinates as

$$f(v_{\beta r}) = 2v_{\beta r} \exp\left(-v_{\beta r}^2\right) \qquad 0 \leq v_{\beta r} \leq \infty \tag{26a}$$

$$f(\theta) = \frac{1}{2\pi} \qquad 0 \leq \theta < 2\pi \tag{26b}$$

$$f(v_{\beta z}) = \frac{1}{\sqrt{\pi}} e^{-v_{\beta z}^2} \qquad -\infty \leq v_{\beta z} \leq \infty \tag{26c}$$

The target molecule velocity components can be picked using

$$v_{\beta r} = (-\ln R_r)^{1/2} \tag{27a}$$

$$v_{\beta z} = (-\ln R_z)^{1/2} \cos(R_2\pi) \tag{27b}$$

$$\theta = 2\pi R_\theta \tag{27c}$$

Now having the sample molecule and target molecule components of velocity before collision allows the velocity after collision as shown in references 6 (p. 163) and 5 (p. 57) to be calculated. Calling the velocity after collision v' enables the following to be written:

$$v_i' - v_i = -\left(\frac{2}{M + 1}\right)\left(v_R n_i \cos \varphi \sin \varphi + v_{Ri} \cos^2 \varphi\right) \tag{28}$$

where i = 1, 2, and 3 correspond to the x, y, and z components, respectively, and

$$n_x = -\left(v_{Ry}^2 + v_{Rz}^2\right)^{1/2} \frac{\sin \epsilon}{V_R} \tag{29a}$$

$$n_y = \frac{v_{Rx} v_{Ry} \sin \epsilon - v_R v_{Rz} \cos \epsilon}{v_R \left(v_{Ry}^2 + v_{Rz}^2\right)^{1/2}} \tag{29b}$$

$$n_z = \frac{v_{Rx} v_{Rz} \sin \epsilon + v_R v_{Ry} \cos \epsilon}{v_R \left(v_{Ry}^2 + v_{Rz}^2\right)^{1/2}} \tag{29c}$$

and the v_R is given by

$$v_R = \left(v_{Rx}^2 + v_{Ry}^2 + v_{Rz}^2\right) \tag{29d}$$

where

$$v_{Rx} = v_x - v_{\beta x} \tag{29e}$$

and so forth. The value of φ as shown in reference 6 (p. 158) is given by

$$\varphi = \left(1 + \frac{2}{\omega^4}\right)^{-1/4} K\left\{\frac{1}{2}\left[1 - \left(1 + \frac{2}{\omega^4}\right)^{-1/2}\right]\right\} \tag{30a}$$

where

$$K\{k^2\} = \int_0^{\pi/2} \left(1 - k^2 \sin^2 \theta\right)^{-1/2} d\theta \tag{30b}$$

The values of ϵ and ω are obtained by random selection as explained in reference 6 (p. 161) from the relations

$$\epsilon = 2\pi R_\epsilon \tag{31a}$$

$$\omega = \omega_m R_\omega^{1/2} \tag{31b}$$

Although the value of ω_m is theoretically infinite, as explained previously, collisions with values larger than some value of ω_m would have a negligible effect on the results. In references 2 and 6, where $M = 1$, a value of $\omega_m = 1.5$ gave good results. This value was used in the present analysis for $M = 1$. However, for $M = 0.1$ and $M = 0.01$, it was found that the larger value for ω_m of 2 was needed; whereas, for $M = 10$, a value of $\omega_m = 1.5$ was used although a somewhat smaller value would have been acceptable.

MAXWELL'S CONTINUUM SOLUTION

The continuum diffusion equation from reference 7 (p. 247) can be written as

$$\frac{\mu}{\mu_{0,+}} = \frac{-D\pi^{1/2}}{LC_\alpha} \frac{\partial\left(\frac{n}{n_{0,+}}\right)}{\partial z} \tag{32a}$$

where z equals Z/L. The coefficient of diffusion D is given in reference 7 (p. 247) as

$$D = \frac{C_\alpha^2}{2A_1 n_\beta}\left[\frac{(M+1)Mm_\beta}{K}\right]^{1/2} \tag{32b}$$

where A_1 is given in reference 7 (p. 239) as 2.6595. This can be written in terms of the mean free path as

$$D = \pi\left(\frac{M+1}{2\sqrt{M}}\right)C_\alpha\left(\frac{\omega_m^2}{A_1}\right)\lambda_\beta = \pi C_\alpha\left(\frac{2.25}{A_1}\right)\lambda_M \tag{33}$$

where

$$\lambda_M = \left(\frac{M+1}{2\sqrt{M}}\right)\left(\frac{\omega_m}{1.5}\right)^2 \lambda_\beta \tag{34}$$

Substituting equation (33) into equation (32) and letting $l_M = L/\lambda_M$ give for the continuum solution

$$\frac{\mu}{\mu_{0,+}} = -\frac{\pi^{3/2}}{l_M}\left(\frac{2.25}{A_1}\right)\frac{\partial\left(\frac{n}{n_{0,+}}\right)}{\partial z} = -\frac{4.711}{l_M}\,\frac{\partial\left(\frac{n}{n_{0,+}}\right)}{\partial z} \tag{35}$$

For the continuum solution, there is a no slip at the boundary so that, at $z = 0$, $n/n_{0,+} = 2$ and, at $z = 1$, $n/n_{0,+} = 0$. Hence, $\partial(n/n_{0,+})/\partial z = -2$ and the continuum solution from equation (35) is equal to

$$\left(\frac{\mu}{\mu_{0,+}}\right)_{l\to\infty} = \frac{9.422}{l_M} \tag{36a}$$

This continuum solution is plotted in figure 2. It is evident that it is only a function of the number of free paths across the gap when based on a free path length λ_M (solid line). These results apply regardless of molecular mass ratios M and temperature of the system T.

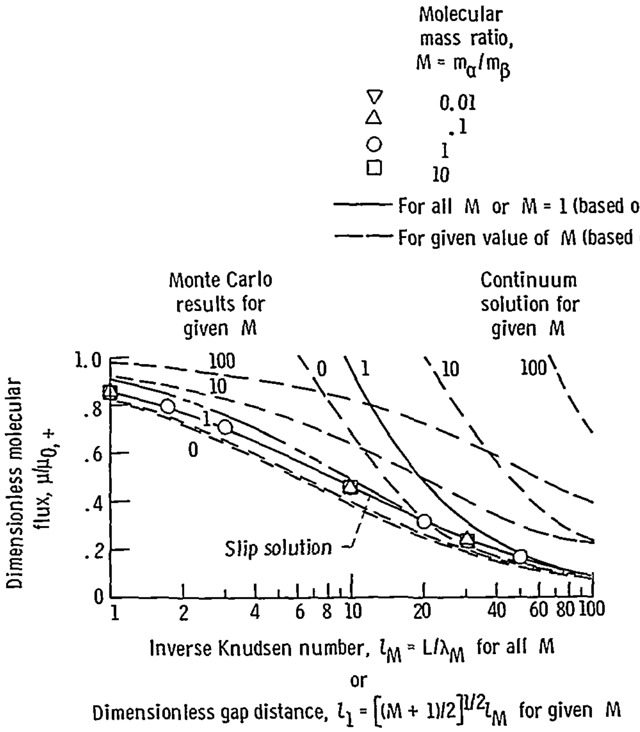

Figure 2. - Molecular flux across gap divided by molecular flux from evaporating surface for various mass ratios.

The effects of varying the molecular masses on the diffusion rate can be shown by defining a dimensionless gap distance l_1, which is independent of the molecular masses. Using equations (21) and (34) results in

$$l_1 = \left(\frac{2}{M + 1}\right)^{1/2} l_M = 2.25\,\pi n_\beta \left(\frac{K}{\kappa T}\right)^{1/2} L \tag{36b}$$

Assuming that K, the term in the intermolecular force law (eq. (18)), is independent of M means equation (36a) can be written as

$$\left(\frac{\mu}{\mu_{0,+}}\right)_{l\to\infty} = \frac{9.422}{l_1}\left(\frac{M + 1}{2}\right)^{1/2} \tag{36c}$$

This result is plotted in figure 2 as the dashed lines for different values of M. The results indicate that, for larger values of the mass of the diffusing molecules compared to the mass of the nondiffusing molecules (i.e., increasing M), the diffusion rate across the channel increases, again assuming that the intermolecular force constant K is unaffected by the change in mass ratio.

Elementary Slip Theory

For conditions close to continuum, a common method of analysis is the slip approximation. The usual continuum equations are assumed to apply in the gap but a discontinuity in density is assumed to occur at the wall; that is, $n_o \neq n_s$ where $n_o = 2n_{0,+}$ and n_s is the density in the gas next to the wall.

Consider some plane z_p located somewhere in the gas. The molecular flux of diffusing α molecules crossing the plane in the positive z direction can be written as (ref. 5, p. 307)

$$(n\langle v_z\rangle)_{+p} = \frac{C_\alpha}{\pi^{3/2}} \iiint n\, e^{-\left[v_x^2+v_y^2+(v_z-\langle v_z\rangle)^2\right]}\, v_z\, d^3v \tag{37}$$

where the limits of integration are v_x and v_y from $-\infty$ to $+\infty$ and v_z from 0 to $+\infty$. Expanding the molecular density in a Taylor series around point z_p as described in reference 5 (p. 307) results in

$$n(z) = n(z_p) - \lambda_s \cos\gamma \left(\frac{\partial n}{\partial z}\right)_{z_p} \tag{38}$$

where λ_s is some average mean free path and γ is the angle between the z axis and the incident molecule. Then equation (37) can be integrated to obtain

$$(n\langle V_z\rangle)_{+p} = \frac{n_p}{2}\left(\frac{C_\alpha}{\sqrt{\pi}} + \langle V_z\rangle\right) - \frac{\lambda_s}{3}\left(\frac{\partial n}{\partial z}\right)_p \left(\frac{C_\alpha}{\sqrt{\pi}}\right) \tag{39}$$

Similarly, the molecular flux in the negative z direction is given by

$$(n\langle V_z\rangle)_{-p} = \frac{n_p}{2}\left(\frac{C_\alpha}{\sqrt{\pi}} - \langle V_z\rangle\right) + \frac{\lambda_s}{3}\frac{C_\alpha}{\sqrt{\pi}}\left(\frac{\partial n}{\partial z}\right)_p \tag{40}$$

If it is assumed that, close to continuum conditions, the mean diffusion velocity is small compared to the mean thermal velocity, $\langle V_z\rangle / (C_\alpha/\sqrt{\pi}) \ll 1$. The net flux at point p is then given by the difference between equations (39) and (40) as

$$\mu = -\frac{2\lambda_s}{3}\frac{C_\alpha}{\sqrt{\pi}}\frac{\partial n}{\partial z} \tag{41}$$

which can be written in dimensionless form as

$$\frac{\mu}{\mu_{0,+}} = -\frac{2}{3}\left(\frac{\lambda_s}{L}\right)\frac{\partial\left(\frac{n}{n_{0,+}}\right)}{\partial z} \tag{42}$$

To calculate the slip, consider a cross section z adjacent to the surface at z = 0. In that case the mass flux coming off the wall in the positive z direction is given by equation (8). Then

$$(n\langle V_z\rangle)_{+0} = \frac{n_{+0}C_\alpha}{\sqrt{\pi}} \tag{43a}$$

The mass flux in the negative z direction as in equation (40) is now given as

$$(n\langle V_z\rangle)_{-0} = \frac{n_s}{2}\frac{C_\alpha}{\sqrt{\pi}} + \frac{\lambda_s}{3}\frac{C_\alpha}{\sqrt{\pi}}\frac{\partial n}{\partial z} \tag{43b}$$

where n_s is the density of the gas adjacent to the wall. Then the net flux is given by the difference between equations (43a) and (43b) which yields

$$\left(n\langle V_z\rangle\right)_0 = \frac{n_{+0}C_\alpha}{\sqrt{\pi}} - \frac{n_s}{2}\frac{C_\alpha}{\sqrt{\pi}} - \frac{\lambda_s}{3}\frac{C_\alpha}{\sqrt{\pi}}\frac{\partial n}{\partial z} \tag{44}$$

By using equation (41) this can be rewritten as

$$\mu = \frac{C_\alpha}{2\sqrt{\pi}}\left(2n_{0,+} - n_s\right) + \frac{\mu}{2} \tag{45a}$$

or

$$-\frac{1}{2}\frac{\mu}{\mu_{0,+}} = \frac{1}{2}\left(\frac{n_s}{n_{0,+}}\right) - 1 \tag{45b}$$

If it is assumed that the continuum solution as given by equation (35) applies in the gas but that the density adjacent to the wall is now $n_s/n_{0,+}$ instead of 2, the continuum solution with slip would give from equation (35)

$$\frac{\mu}{\mu_{0,+}} = -\frac{4.711}{l_M}\left(\frac{1 - \dfrac{n_s}{n_{0,+}}}{0.5}\right) \tag{46}$$

It can be shown that the results are antisymmetric around the center of the gap $z = 1/2$ so the results will only be carried out for half the gap. Combining equations (45) and (46) results in the following for the molecular flux with slip:

$$\left(\frac{\mu}{\mu_{0,+}}\right)_{\text{slip}} = \left(1 + \frac{l_M}{9.422}\right)^{-1} \tag{47}$$

This result is shown in figure 2 as the dashed double dot line. Similarly from equations (45) and (46) the number density slip can be obtained as follows:

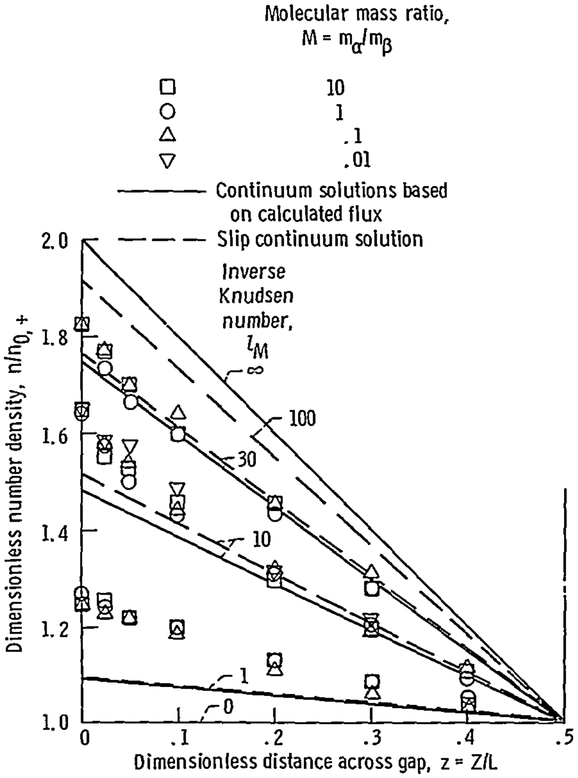

Figure 3. - Number density of diffusing molecules across gap divided by number density of molecules leaving from evaporating surface.

$$\frac{n_S}{n_{0,+}} = \frac{2l_M + 9.422}{l_M + 9.422} \tag{48}$$

This result is shown in figure 3.

RESULTS

The resulting molecular flux for different values of the molecular mass ratio $M = m_\alpha/m_\beta$ are plotted in figure 2 as a function of l_M which is the number of mean free paths across the gap based on the mean free path λ_M. These results were obtained for given values of l_M and M for acceptable values of ω_m. The λ_β was calculated from these values by equation (34). This gave the normalized distance across the channel l_β which was used as input in the calculation (eq. (24)). When the results are plotted as a function of l_M, the molecular flux in figure 2 falls along one curve for all values of the molecular mass ratio M. This curve is shown as the solid line drawn through the results. Also shown is Maxwell's continuum solution as a function of l_M. This also plots along one curve for all values of M. The rarefied solution approaches the continuum solution for large values of l_M.

The effect of varying the molecular mass ratio M of the diffusing to the nondiffusing molecules on the molecular flux can be seen by keeping the dimensionless distance l across the gap independent of the mass ratio M. From equation (36b) it is evident that if the results are replotted as a function of l_1, which is the dimensionless distance across the gap independent of the molecular mass ratio, the effect of the molecular mass ratio on the molecular flux transport across the gap can be observed. These results, which are shown as dashed lines, indicate much higher diffusion rates for heavier molecules. In a similar manner the effect of the temperature of the system can be found, since the number of mean free paths across the gap can be related to the temperature of the system by $(T_2/T_1)^{1/2} = l_1/l_2$ (eq. (36b)). Thus, the square root of a temperature ratio increase equals the decrease in the path length ratio across the gap, thereby giving an increasing molecular flux as the system temperature increases. Also shown in figure 2 is the simple slip solution as a function of l_M. The simple relation given by equation (47) gives a good approximation to the reported numerical result.

In figure 3 the number density of the diffusing α species at various positions across the gap are shown. They are plotted for given values of l_M. The density profiles are equivalent for the same values of l_M for all molecular mass ratios. This is similar to the result found for the molecular flux. The curves were found to be odd functions about the center of the gap. Plotted as solid lines in figure 3 are the linear density results based on the calculated Monte Carlo molecular flux given in figure 2 using the continuum solution of equation (46). Shown as dashed lines in figure 3 are the slip solutions given by equation (48). The slip solution gives good results at the higher values of l_M, but the agreement is poorer for smaller values of l_M.

The amount of time needed to run a given number of sample histories depended strongly on the number of collisions for each sample, so that as the number of mean free paths across the gap increased the computing time increased. Using an IBM 7094 for $M = 0.1$ and 10 000 samples, the results for $l_M = 1.0$ took 2 minutes; for $l_M = 10$, 10 minutes; and for $l_M = 30$, 25 minutes. The parameters that shorten the mean free path will accordingly lengthen the running time. As can be seen from equation (34), both M and ω_m will have an effect on the value of l_M.

The 95 percent confidence range as given by equation (4) was also calculated. The value of $\sigma(\mu/\mu_{0,+})$ was about 0.5 so that for 10 000 samples the 95 percent confidence range for $\mu/\mu_{0,+}$ is about 0.01. For the number density results the variance was higher and about 5. This gave a 95 percent confidence interval for $n/n_{0,+}$ of about 0.1.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, February 13, 1970,
129-01.

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