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METHODS FOR DETERMINING THERMAL ACCOMMODATION
COEFFICIENTS FROM FREE MOLECULE FLOW HEAT TRANSFER DATA

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NOMENCLATURE

A	Area
c_v	Specific heat at constant volume
\bar{c}	Average speed
E	Energy
\dot{E}''	Energy flux
F_{ij}	Diffuse shape factor of surface i with respect to surface j
Kn	Knudsen number
k	Boltzmann constant
m	Molecular mass
n	Molecular density or number of surfaces
\dot{n}''	Molecular flux
p	Pressure
\dot{q}_{fmf}''	Free molecule flow heat flux
Q	Total free molecule flow heat flow
R	Gas constant
r	Radius or radial displacement
T	Temperature
α	Accommodation Coefficient
θ, ϕ	Spherical coordinates
γ	Ratio of specific heats

INTRODUCTION

Heat transfer in rarefied gases, a previously little investigated subject, has undergone advances in the past few years due to increased areas of application. Among new areas of application are the insulation of booster propellant storage vessels and heat transfer to exterior surfaces of space vehicles.

Low density heat transfer is subdivided into several regimes with the Knudsen number, Kn (The ratio of mean free path to characteristic dimension of the system) serving as the criteria for designation. At sufficiently low pressures Kn becomes large compared with unity. For Kn greater than about 3, intermolecular collisions in a gas become negligible compared with gas molecule - boundary collisions. This is referred to as the free molecule flow region of gas dynamics and heat conduction. Heat conducted between surfaces separated by a gas with Kn > 3 occurs predominately by the mechanism of thermal exchange by direct molecule - wall collisions. Free molecule flow heat transfer

(hereafter abbreviated fmf heat transfer) may be a large percentage of the total heat flux in a system with Kn in the range 3 to 100. One criteria for the importance of fmf heat flux in a system is the value of the radiation heat flux. The radiation decreases with surface temperatures as the fourth power. Hence it is primarily at lower temperatures, such as occur in cryogenic insulation applications, that the fmf heat flux is of most importance.

To calculate the fmf heat flux in a system it is necessary to have some knowledge of the thermal accommodation coefficients for the gases and surfaces involved. The thermal accommodation coefficient, α , is defined by the relation

$$\alpha = \frac{E_i - E_r}{E_i - E_w} \quad (1)$$

where E_i is the energy carried by an incident molecule, E_r is the energy carried away by a reflected molecule and E_w is the energy that a molecule would possess if in thermal equilibrium at the wall temperature, T_w . Thus α represents the degree to which an incident molecule approaches thermal equilibrium with a surface during a collision. A value of unity for α represents complete accommodation. The thermal accommodation coefficient appears to be a function of the nature of the gas, the nature and temperature of the surface, the Knudsen number and the energy difference between incident molecules and the fully accommodated energy.¹

The purpose of this paper is to describe and compare two techniques for determining the thermal accommodation coefficient for a given gas and surface at a specified thermodynamic state.

ANALYSIS

Two techniques are to be compared; one due to Klett and Irey described in an earlier paper², which utilizes the classical lumped analyses approach, and a method which stems from the analytical work done by Yau Wu^{3,4,5}, in formulating an integral approach to the problem.

Necessary for the application of both techniques is a collection of heat flux data for a gas in a free molecule flow enclosure. The data used for this work were obtained by the use of a two-directional guarded calorimeter. The experimental apparatus and techniques used in collecting the data are described in references 2 and 6. The data consist of values for the fmf heat flow between two concentric copper cylinders separated by a gas at various pressures in the Knudsen number range 2 to 30. The surfaces were held at constant temperatures corresponding to the normal boiling points of liquid nitrogen and liquid Freon 12, i.e. 77.4 K and 243 K respectively. Data were obtained for orientation of the heat flux vector in both the inward and outward normal directions. The heat flow data for air, nitrogen and helium

are shown in Figure 1.

LUMPED ANALYSIS

From the classical derivation of the *fmf* heat flux between two concentric cylinders at constant temperatures the following equation is obtained.^{1,6}

$$\dot{q}_{fmf} = k(1 + \gamma) c_v \frac{p}{\sqrt{2\pi RT}} \frac{\alpha_1 \alpha_2 (T_1 - T_2)}{(A_1/A_2)(\alpha_1 \alpha_2 - \alpha_1) - \alpha_2} \quad (2)$$

where *p* is the pressure of the gas separating the cylinders, *T* is the mean temperature of this gas, α_1 , T_1 , A_1 , and α_2 , T_2 , A_2 are the accommodation coefficients, temperatures and areas of the inner and outer cylinders respectively. It can be seen that for given temperatures, pressure and heat flux and unknown accommodation coefficients the equation has two unknowns, α_1 , and α_2 . Thus the necessity for obtaining data for the heat flux vector in two directions; this provides two equations in the two unknowns.

Some discussion on the mean temperature, *T*, of the gas is now necessary. In a free molecule flow situation a gas contained between two constant temperature surfaces will be composed of two streams of molecules, one leaving surface 1 with some reflected temperature T_{r1} and one leaving surface 2 with some reflected temperature T_{r2} . The mean temperature, *T*, then represents some average of these two reflected temperatures and will, in general, be spatially dependent. By employing a radiation analogy and assuming the surfaces to be diffuse reflectors and the two streams of molecules to be Maxwellian, the expression for the mean temperature, *T*, as a function of *r* was found to be⁶

$$\frac{1}{\sqrt{T(r)}} = k \left[\frac{(r_1/r)}{\sqrt{T_{r1}}} + \frac{(2-r_1/r)}{\sqrt{T_{r2}}} \right]$$

where r_1 and r_2 are the radii of the inner and outer cylinders and *r* is the radial distance from the center line.

Taking the average of this expression by integrating over the range from r_1 to r_2 and dividing by $r_2 - r_1$ yields the following expression for the averaged mean temperature.

$$\frac{1}{\sqrt{\bar{T}}} = \frac{1}{2(r_2 - r_1)} \left[\frac{r_1 (\sqrt{T_{r2}} - \sqrt{T_{r1}})}{\sqrt{T_{r1}} \sqrt{T_{r2}}} \right]$$

$$\ln \left(\frac{r_2}{r_1} \right) + \frac{2(r_2 - r_1)}{\sqrt{T_{r2}}} \quad (3)$$

If the values of r_1 and r_2 for the experimental apparatus, i.e. 1.0625 and 1.517 respectively, are put into (3) it becomes

$$\frac{1}{\sqrt{\bar{T}}} = \frac{0.4199}{\sqrt{T_{r1}}} + \frac{0.5801}{\sqrt{T_{r2}}} \quad (4)$$

The reflected temperatures T_{r1} and T_{r2} are found by the classical derivation for the concentric

cylinder geometry to be given by the expressions^{1,6}

$$T_{r1} = \frac{\alpha_2 T_2 (\alpha_1 - 1) - \alpha_1 T_1 \left[(r_1/r_2)^{(1-\alpha_2)} + \alpha_2 \right]}{(r_1/r_2)(\alpha_1 \alpha_2 - \alpha_1) - \alpha_2} \quad (5)$$

and

$$T_{r2} = \frac{\alpha_1 T_1 (r_1/r_2)(\alpha_2 - 1) - \alpha_2 T_2}{(r_1/r_2)(\alpha_1 \alpha_2 - \alpha_1) - \alpha_2} \quad (6)$$

When equations (4), (5), and (6) are combined with the two equations resulting from (2) for the two directions of heat flux, under the constraint that the heat fluxes be compared at equal Knudsen numbers, the result is a set of five equations in the five unknowns α_1 , α_2 , T_{r1} , T_{r2} , and *T*. These equations have been solved on an IBM 360 computer using an iterative scheme. These previously reported results² for the three gases air, nitrogen and helium are shown plotted in Figures 2 through 7 along with the results obtained by the techniques described below.

INTEGRAL ANALYSIS

It shows that the molecular flux, n'' , in a free molecule flow enclosure with arbitrary wall temperature distribution is an invariant for the system.³ It may be evaluated from the expression

$$\dot{n}'' = \frac{p(\bar{r}) \sqrt{8\pi/mk}}{\int_0^\pi \int_0^{2\pi} \sqrt{\frac{m}{2kT}} \sin\theta d\theta d\phi} \quad (7)$$

where $T_{0\bar{r}}$ is the temperature of the molecules leaving the surface element which subtends the solid angle element $\sin\theta d\theta d\phi$ at the point \bar{r} . The temperature at a point in the system is defined by the average kinetic energy of a molecule

$$E = \frac{3}{2} k T(\bar{r}) = \frac{m\bar{c}^2(\bar{r})}{2}$$

where \bar{c} is the average speed of the molecule. From this

$$T(\bar{r}) = \frac{m\bar{c}^2(\bar{r})}{3k} \quad (8)$$

Upon assuming a Maxwell Boltzmann velocity distribution the expression for the temperature evolves as

$$T(\bar{r}) = \frac{\int_0^\pi \int_0^{2\pi} \sqrt{\frac{m}{2kT}} \sin\theta d\theta d\phi}{\int_0^\pi \int_0^{2\pi} \frac{1}{\sqrt{T}} \sin\theta d\theta d\phi} \quad (9)$$

Writing an energy balance for some point *S* on the enclosure gives

$$E_i''(S) = \int_A \int_X \frac{E_r''(S')}{r} K(S', S) ds' \quad (10)$$

where the subscripts *i* and *r* refer to incident and reflected, and $K(S', S)$ is the probability

that a molecule leaving point S' on the boundary will impinge upon point S . The integral extends over the entire surface, A , of the enclosure.

Assuming constant specific heats, the following expression for the reflected and incident temperatures may be written directly from (10)

$$T_i(S) = \iint_A T_r(S') K(S', S) ds' \quad (11)$$

Equation (1), the definition of α , may be written in the form, providing c_v is constant

$$T_r(S) = (1 - \alpha) T_i + \alpha T_w$$

Now using (11) for T_i this may be written as

$$T_r(S) = (1 - \alpha) \iint_A T_r(S') K(S', S) ds' + \alpha T_w(S) \quad (12)$$

where α is the accommodation coefficient at the point S .

The net heat flux to the point S on the surface is

$$\dot{q}_{fmf}'' = \dot{E}_i'' - \dot{E}_r''$$

or in terms of temperatures

$$\dot{q}_{fmf}'' = m \dot{n}'' (c_v + \frac{1}{2}R) (T_i(S) - T_r(S))$$

Through the use of (11) and (12) this may be written as

$$\dot{q}''(S) = m \dot{n}'' (c_v + \frac{1}{2}R) \alpha \cdot \left[\iint_A T_r(S') K(S', S) ds' - T_w(S) \right] \quad (13)$$

Now, if the enclosure consists of n constant temperature segments, the heat flux to the i th segment is

$$\dot{q}_i'' = m \dot{n}'' (c_v + \frac{1}{2}R) \alpha_i \cdot$$

$$\left[\sum_{j=1}^n \iint_{A_j} T_{rj} K(A_j, A_i) dA_j - T_{wi} \right]$$

Under the assumption that the surface A_i is uniformly bombarded the temperature T_{rj} may be considered constant and moved outside the integral. If this expression is integrated over the surface area A_i and it is noted that for a diffuse reflection system

$$\iint_{A_i} \iint_{A_j} K(A_j, A_i) dA_j dA_i = A_i F_{ij}$$

where F_{ij} is the diffuse angle factor, the total heat flow to surface i from all surrounding surfaces becomes

$$Q_i = m \dot{n}'' (c_v + \frac{1}{2}R) \alpha_i A_i \cdot \left(\sum_{j=1}^n F_{ij} T_{rj} - T_{wi} \right) \quad (14)$$

Rewriting equation (12) for n constant temperature surfaces and integrating over A_i in a similar fashion yields an expression for the reflected temperatures.

$$T_{rj} = (1 - \alpha_i) \sum_{j=1}^n F_{ij} T_{rj} + \alpha_i T_{wi} \quad (15)$$

In the present case of concentric cylinders with flat bottoms the enclosure was divided into four lumped constant temperature surfaces. Thus (15) becomes a set of four linear algebraic equations. Combining these with (14) for the two cases of reversed heat flux gives a set of six equations in the four unknown reflected temperatures and two unknown accommodation coefficients.*

Since \dot{n}'' is invariant in a free molecule flow enclosure it may be evaluated at the point of pressure measurement so long as this point is a part of the free molecule flow system. For instance, if the pressure is measured externally by a McLeod gage connected to the system by a free molecule flow passage, the pressure and temperature of the gage, p_g and T_g respectively, are used in (7) which then becomes

$$\dot{n}'' = \frac{p_g}{\sqrt{2\pi m k T_g}} \quad (16)$$

However this fortunate situation was not present in the experimental arrangement. The pressures recorded in the data were the average pressures within the fmf enclosure. It is therefore necessary to know the mean temperature, T , as before. Performing the integrals in equation (9) at the point T corresponding to the averaged value of T given in equation (4) results in an expression for the mean temperature from the integral approach.

$$T = \frac{0.986 T_{r1} \sqrt{T_{r2}} + 2.156 T_{r2} \sqrt{T_{r1}}}{0.986 \sqrt{T_{r2}} + 2.156 \sqrt{T_{r1}}} \quad (17)$$

Equations (4) and (17) are both expressions for the mean temperature at a point in the gas for the specific geometry at hand. Implicit in the derivation of (4) are a pair of logical but arbitrary definitions of the average molecular number density and the average molecular flux in terms of the two types of molecules present, i.e. those with temperature T_{r1} and those with

*The accommodation coefficients are assumed to be the same on like surfaces at the same temperature.

temperature T_{r7} . Equation (17) is based solely on the definition of the mean kinetic energy of a molecule and is therefore less arbitrary and more nearly correct. The only deviation from exactness in this expression is the approximation in the reflected temperature distribution used in performing the integration.

The solution of equations (14) and (15) is accomplished on the computer by assuming starting values for the accommodation coefficient, solving the set (15) and using the values of T_{r1} , so found, to calculate new values of α from (14).

To separately investigate the influences of the mean temperature and the number of lumped surfaces several variations in data reduction were tried. The previously reported values of the accommodation coefficients which were obtained from equation (2) with equation (4) for the mean temperature are compared in Figures 2 through 7 with the values obtained by the following methods:

- A) Equation (14) considering four lumped surfaces was used with equation (17) for the mean temperature.
- B) Equation (14) considering four lumped surfaces was used with equation (4) for the mean temperature.
- C) Equation (14) considering two lumped surfaces was used with equation (17) for the mean temperature.
- D) Equation (14) considering two lumped surfaces was used with equation (4) for the mean temperature.

DISCUSSION OF RESULTS

It may be seen from Figures 2 through 7 that the previously reported values differ by as much as 0.10 from the values calculated by method (A), i.e., by using the equations derived from the integral analysis and assuming four lumped surfaces. The largest difference occurs with helium when $T_w=243$ K. The same trend with surface temperature, i.e. α decreases with increasing T_w , occurs in both cases as it does, in fact, in all of the cases tried. The trend with Knudsen number is the same for both these techniques with the exception of nitrogen for 243 K. In this instance the previously reported values decrease with Kn whereas the method (A) values increase with Kn.

Studying the results from the other reduction schemes reveals that increasing the number of lumped surfaces tends to decrease the difference in the computed values for the two surface temperatures. A similar effect is noted for the influence of the mean temperature. The use of equation (3) reduces the differences in the accommodation coefficient due to surface temperature over those found by the use of equation (17), holding constant the number of lumped surfaces considered.

Comparing the previously reported values with those found by method (D) illustrates the fact that equation (14) for two lumped cylindrical surfaces becomes equivalent to the classical expression, equation (2).

CLOSURE

Two approaches to the problem of fmf heat flux between two concentric cylinders have been presented. Discussed first were the results of a lumped analysis for the particular geometry and then a general integral analysis good for any configuration. The integral analysis provides the most useful tool for making heat transfer calculations and, in a reverse sense, for determining thermal accommodation coefficients from heat flux data. It allows any system geometry and surface temperature distribution although for a very complicated configuration the determination of the shape factors may become intractable.

For the system geometry employed in this work the integral technique must be considered more inherently accurate due to the finite length of the cylinders giving rise to end effects not accounted for in the lumped analysis. Its use is therefore recommended for making calculations and for data reduction.

If fmf heat flow data are to be obtained for purposes of determining thermal accommodation coefficients it is recommended that the pressure sensing device, if external to the system, be connected by a free molecule flow passage. Thus the necessity of evaluating equation (9) with the attendant introduction of some degree of approximation and uncertainty is avoided.

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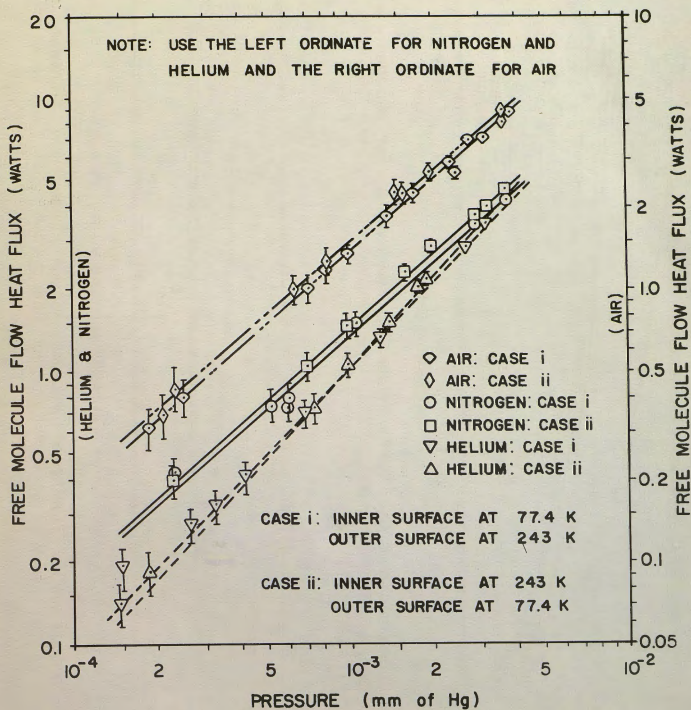


Fig. 1 — Free Molecule Flow Heat Flux Versus Pressure

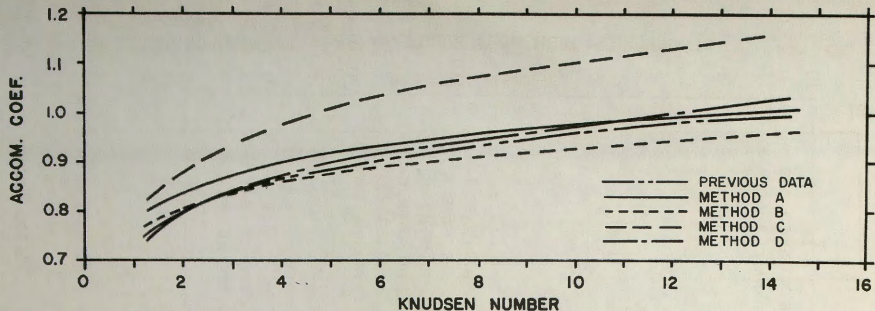


Fig. 2 — Accommodation Coefficient Versus Knudsen Number For Nitrogen On Copper At 77.4 K

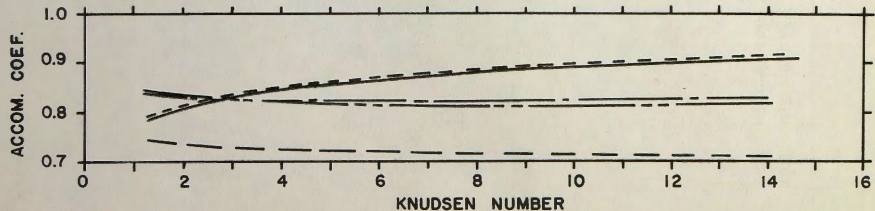


Fig. 3 — Accommodation Coefficient Versus Knudsen Number For Nitrogen On Copper At 243 K

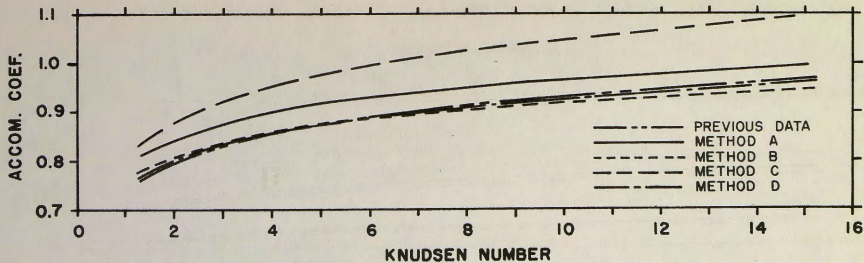


Fig. 4 — Accommodation Coefficient Versus Knudsen Number For Air On Copper At 77.4 K

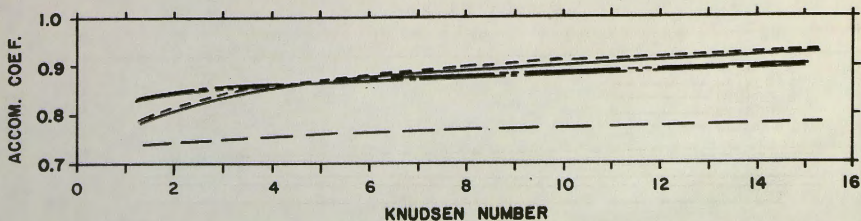


Fig. 5 — Accommodation Coefficient Versus Knudsen Number For Air On Copper At 243 K

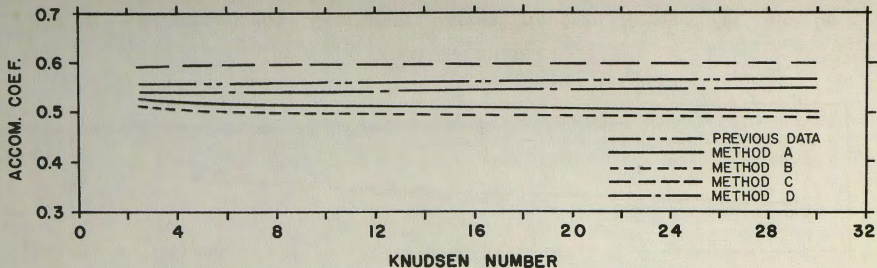


Fig. 6 — Accommodation Coefficient Versus Knudsen Number For Helium On Copper At 77.4 K

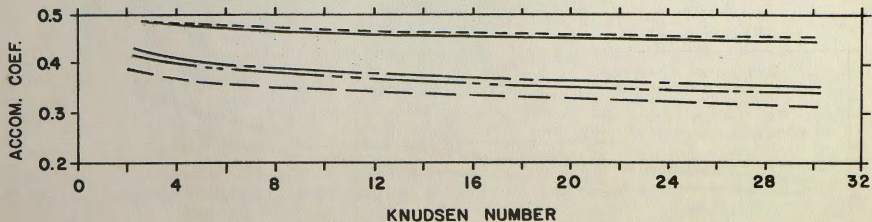


Fig. 7 — Accommodation Coefficient Versus Knudsen Number For Helium On Copper At 243 K