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INTERNAL RAREFIED GAS FLOWS WITH BACKSCATTERING
PART 1: THE BACKSCATTERING BOUNDARY CONDITION
AND FREE MOLECULE FLOW IN A LONG CAPILLARY

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Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road, Springfield, Virginia 22151
Price: Printed Copy \$3.00; Microfiche \$0.95

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Date of Issue: June 16, 1971

Report Number: K-1798, Part 1

Subject Category: PHYSICS

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ABSTRACT

A boundary condition designed to simulate the scattering of gas at a real randomly rough surface is proposed to replace the usual assumption of diffuse scattering. A fraction $1 - \alpha$ of incident molecules are assumed to be scattered back along their incident paths while a fraction α are scattered diffusely.

For free molecule flow in a long capillary the modified boundary condition does not affect the gas density or collision density distribution along the capillary. The molecular flux in the capillary is reduced by the same fraction at each radial position, and the molecular flow through the capillary is reduced by an amount $\alpha/(2 - \alpha)$.

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INTRODUCTION

The interaction between a gas molecule and a solid surface is a subject of much current research both experimental and theoretical. This interaction is very complex and no truly satisfactory general model has been obtained to date. For the purposes of aerodynamics it has been conventional to describe the interaction in terms of accommodation coefficients which relate to the interchange of momentum and energy between the gas molecule and the surface during collision. In fact, for the analysis of internal rarefied gas flows, it is usually assumed that molecules striking surface are completely thermally accommodated and are then re-emitted with a Maxwellian distribution of velocities relative to the surface and characterized by the surface temperature. This leads to the familiar "cosine law" scattering or fully diffuse scattering. A modification of this boundary condition which is sometimes used permits a certain fraction of molecules to undergo "specular" reflection while the remainder are scattered diffusely.

It is fortunate that most surfaces which have undergone no special preparation exhibit approximately diffuse scattering. Analysis of internal rarefied gas flows in which the cosine law boundary condition has been used leads to predicted flows which are in reasonable agreement with experimental observations. Furthermore, the use of the diffuse scattering boundary condition leads to a tractable problem which, at least for flows in simple geometries, can be solved without excessive labor.

In recent years, experimental observations have been made by Huggill [1], Lund and Berman [2,3,4], Davis, Levenson, and Milleron [5], and by Maegley and Berman [6] which indicate significant deviations between observed flows and flows predicted with the diffuse scattering boundary condition. In general, flows in the free molecule and near free molecule regimes are

lower than those predicted. For long capillaries the difference approaches 10% at the free molecule limit.

Lund and Berman [4] conjectured that such deviations resulted from nondiffuse scattering due primarily to wall roughness and furnished experimental evidence to support this conjecture. Since observed flows were lower than predicted flows, the inclusion of some specular reflection would only increase the discrepancy. DeMarcus [7] treated the free molecule flow in a rough walled channel with prescribed regular wall roughness and with diffuse scattering relative to the local surface normal. He found that by proper selection of the roughness the free molecule flow through such a channel could be reduced sufficiently to bring about agreement between predicted and observed free molecule flows.

Although it leads to a tractable free molecule problem, the assignment of a particular regular wall roughness does not seem to be very feasible for the analysis of internal rarefied gas flows over the whole range of Knudsen numbers. Instead, it would be advantageous to have a scattering boundary condition which in principle is as simple as the cosine law or specular reflection models but which leads to a flow reduction in the free molecule and near free molecule regimes. Such a boundary condition and its effect on internal rarefied gas flows are the subject matter of this report.

The presentation will be organized as follows:

Part 1 will detail the proposed boundary condition and its effect on free molecule flow in very long tubes.

In Part 2 the analysis of free molecule flow in finite length tubes will be presented, and the experimental data of Lund and Berman [4] will be used to evaluate the single parameter in the modified boundary condition. This value of the parameter will be used in the subsequent parts of this report.

Part 3 is devoted to the Kramer problem and the effect of the modified boundary condition on the slip coefficient.

Part 4 presents the analysis for plane "Poiseuille" flow at arbitrary Knudsen number.

Part 5 treats the general case of flow in a long one-dimensional system of constant cross section with special application to tubes and annuli.

Wherever possible in the discussion of each problem, comparison is made with existing experimental data to assess the utility of the proposed boundary condition modification.

THE BACKSCATTERING BOUNDARY CONDITION

We seek a scattering boundary condition which will result in decreased transport at high Knudsen numbers and which will have very little effect on the transport at low Knudsen numbers. The boundary condition should be simple enough so that it can be readily incorporated into the approximate methods of analysis which are useful for rarefied gas flows. Hopefully, it should also simulate, in some sense, the scattering of gas molecules from a real surface.

As mentioned in the Introduction, reduction of transport seems to be associated primarily with surface roughness. In a system in which a gas density gradient is driving the flow, such roughness results in a greater fraction of molecules being scattered back towards the direction of increasing density than would be the case for a mathematically smooth surface with cosine law or with specular scattering. A scattering boundary condition which is simple and which simulates this property of a rough surface is the following.

We assume that, of all the molecules striking a surface, a fraction α leave the surface with a Maxwellian distribution relative to the surface and characterized by the surface temperature (diffusely scattered), while

a fraction $1 - \alpha$ leave the surface with their incident velocity vector reversed. The latter are said to be backscattered.

Let $f(\vec{c}, \vec{r}) d\vec{c} d\vec{r}$ be the number of molecules in the volume element $d\vec{r}$ about $\vec{r}$ which have velocities in the range $d\vec{c}$ about $\vec{c}$. For considerations in the neighborhood of a surface it is convenient to split the distribution function $f(\vec{c}, \vec{r})$ into two parts and write

$$f(\vec{c}, \vec{r}) = f^+(\vec{c}, \vec{r}) + f^-(\vec{c}, \vec{r}) \quad (1)$$

where, if $\hat{n}$ is the local unit normal directed from the surface into the gas,

$$\begin{aligned} f^+(\vec{c}, \vec{r}) &= 0 \quad \text{for} \quad \hat{n} \cdot \vec{c} < 0 \\ f^-(\vec{c}, \vec{r}) &= 0 \quad \text{for} \quad \hat{n} \cdot \vec{c} > 0. \end{aligned} \quad (2)$$

Thus, $f^+(\vec{c}, \vec{r})$ is the distribution function for molecules leaving the surface, and $f^-(\vec{c}, \vec{r})$ is the distribution function for molecules about to strike the surface.

If a fraction α of molecules are diffusely scattered from a surface and a fraction $(1 - \alpha)$ are backscattered, then the proposed boundary condition at the surface can be written as

$$f^+(\vec{c}, \vec{r}) = \frac{\alpha A}{(2\pi RT)^{3/2}} e^{-c^2/2RT} + (1 - \alpha)f^-(\vec{c}, \vec{r}) \quad (3)$$

where R is the gas constant per gram, T is the surface temperature at the scattering point $\vec{r}$, and A is chosen so that there is no accumulation of molecules on the surface.

It is easy to see that a surface which scatters molecules according to (3), if exposed to a gas at equilibrium at the surface temperature, would emit molecules with an equilibrium Maxwellian distribution.

The boundary condition (3) is not new but is attributed by Clausing [8] to Gaede. Gaede, however, proposed this boundary condition to explain the decrease in transport, from its free molecule value, with increasing

pressure (which he observed in his experimental study of rarefied gas flow between parallel flat plates). He conceived of a smooth surface becoming microscopically rough due to gas adsorption with the subsequent backscattering leading to decreasing flow with increasing pressure. Current theoretical analyses successfully account for this flow behavior even with fully diffuse scattering at the surface.

In the following section of this report we examine the effect of the backscattering condition (3) on the free molecule flow through a very long tube of circular cross section.

FREE MOLECULE FLOW IN AN INFINITE CAPILLARY

Consider a capillary of radius a . Its length is taken great enough so that the contributions to the collision density at any point on the wall of the capillary from molecules which have entered the capillary ends can be ignored. In addition, the gas density is low enough so that intermolecular collisions inside the capillary can be neglected. The capillary wall temperature is assumed constant and equal to the gas temperature. A gas density difference imposed across the capillary ends results in a free molecule transport through the capillary.

Because of symmetry it is sufficient to locate any point P in the capillary cross section by giving its axial position Z , measured from any arbitrary axial reference point ($Z = 0$), and its distance r from the axis.

For completely diffuse reflection ($\alpha = 1$) the boundary condition at a wall point located at axial station Z would be

$$f^+(\vec{c}, Z) = \frac{\psi(Z)}{2\pi(RT)^2} e^{-c^2/2RT}$$

where $2\pi a \psi(Z) dZ$ is the number of molecules colliding in one second with the capillary wall in the ring of length dZ at Z .

The boundary condition (3) can thus be written

$$f^+(\vec{c}, Z) = \frac{\alpha\psi(Z)}{2\pi(RT)^2} e^{-c^2/2RT} + (1 - \alpha)f^-(-\vec{c}, Z) . \quad (4)$$

Since there are no intermolecular collisions, the distribution function at any point $P(Z, r)$ in the capillary cross section is

$$f(\vec{c}, Z, r) = f^+(\vec{c}, Z') = \frac{\alpha\psi(Z')}{2\pi(RT)^2} e^{-c^2/2RT} + (1 - \alpha)f^-(-\vec{c}, Z') \quad (5)$$

where Z' is the axial position of the wall point obtained by extending the velocity vector $\vec{c}$ at P backwards until it intersects the capillary wall. The point Z' depends in general on the location of P and on the choice of velocity $\vec{c}$ at P .

If Z'' is the axial location of the wall point obtained by extending the velocity vector $\vec{c}$ at P forward until it intersects the wall, then using the boundary condition (4) we can write

$$f^-(-\vec{c}, Z') = f^+(\vec{c}, Z'') = \frac{\alpha\psi(Z'')}{2\pi(RT)^2} e^{-c^2/2RT} + (1 - \alpha)f^-(\vec{c}, Z'') \quad (6)$$

and

$$f^-(\vec{c}, Z'') = f^+(\vec{c}, Z') = \frac{\alpha\psi(Z')}{2\pi(RT)^2} e^{-c^2/2RT} + (1 - \alpha)f^-(-\vec{c}, Z') . \quad (7)$$

Elimination of $f^-(\vec{c}, Z'')$ from equations (6) and (7) gives for $f^-(\vec{c}, Z')$

$$f^-(\vec{c}, Z') = \left[\frac{1 - \alpha}{2 - \alpha} \psi(Z') + \frac{1}{2 - \alpha} \psi(Z'') \right] \frac{1}{2\pi(RT)^2} e^{-c^2/2RT}$$

and substitution of this result into (5) provides the distribution function at any point in the capillary in terms of $\psi(Z')$ and $\psi(Z'')$.

$$f(\vec{c}, Z, r) = \left[\frac{1}{2 - \alpha} \psi(Z') + \frac{1 - \alpha}{2 - \alpha} \psi(Z'') \right] \frac{1}{2\pi(RT)^2} e^{-c^2/2RT} . \quad (8)$$

If $\psi(Z')$ and $\psi(Z'')$ were known, quantities of physical interest could be obtained by taking suitable moments of the distribution function $f(\vec{c}, Z, r)$.

The collision density $\psi(Z)$ is given by

$$\psi(Z) = - \int_{\hat{n} \cdot \vec{c} < 0} \hat{n} \cdot \vec{c} f d\vec{c} \quad (9)$$

where $\hat{n}$ is the unit normal from surface to gas, and the integration is over all velocity space such that $\hat{n} \cdot \vec{c} < 0$. The gas density n is given by

$$n = \int_{\vec{c}} f d\vec{c} \quad (10)$$

where the integration extends over all velocity space. The molecular flux $n \langle w \rangle$ is given by

$$n \langle w \rangle = \int_{\vec{c}} w f d\vec{c} \quad (11)$$

where w is the axial component of molecular velocity. Finally, the molecular flow Γ is given by

$$\Gamma = 2\pi \int_0^a n \langle w \rangle r dr. \quad (12)$$

Equation (9) leads to an integral equation for the collision density $\psi(Z)$ whose solution then completes the determination of the distribution function $f(\vec{c}, Z, r)$.

For use in what follows, the coordinate systems in physical and velocity space indicated in Figure 1 are used. In the figure, u and v are the x and y components, respectively, of velocity $\vec{c}$ and lie in the plane of the cross section. The Z component of molecular velocity is parallel to the capillary axis. All quantities with subscript s are projections in the plane of the cross section. Thus $\vec{c}_s$ is the projection of the molecular velocity $\vec{c}$ at P in the plane of the cross section. A molecule leaving the wall at axial station Z' with velocity $\vec{c}$ travels a distance δ' to reach point P and a distance δ'' to get from P to the wall point at Z'' .

Figure 1
COORDINATE SYSTEMS FOR THE CAPILLARY

Simple geometry furnishes the relations

$$\delta_s' = r \sin \theta + \sqrt{a^2 - r^2 \cos^2 \theta} \quad (13)$$

$$\delta_s'' = -r \sin \theta + \sqrt{a^2 - r^2 \cos^2 \theta} \quad (14)$$

The time τ' required for a molecule leaving the wall at Z' with velocity $\vec{c}$ to reach P is given by

$$\tau' = \frac{\delta_s'}{c} \equiv \frac{Z - Z'}{w} \equiv \frac{\delta_s'}{c_s}$$

and the time τ'' required to go from P to the wall at Z'' is

$$\tau'' = \frac{\delta_s''}{c} \equiv \frac{Z'' - Z}{w} \equiv \frac{\delta_s''}{c_s}$$

These equations furnish the following relationships between the points Z, Z' , and Z'' .

$$Z' = Z - \frac{w\delta_s'}{c_s} ; \quad Z'' = Z + \frac{w\delta_s''}{c_s} \quad (15)$$

We can now obtain the integral equation for the collision density.

Collision Density

From equations (8) and (9) we have

$$\psi(Z) = - \int_{\hat{n} \cdot \vec{c} < 0} \hat{n} \cdot \vec{c} \left[\frac{1}{2 - \alpha} \psi(Z') + \frac{1 - \alpha}{2 - \alpha} \psi(Z'') \right] \frac{1}{2\pi(RT)^2} e^{-c^2/2RT} d\vec{c}$$

To determine the collision density, we select the point P on the wall of the capillary so that $r = a$. This gives $\delta_s' = 2a \sin \theta$, $\delta_s'' = 0$ so that $Z' = Z - (2aw \sin \theta)/c_s$ and $Z'' = Z$. Also for the coordinate system chosen in Figure 1, $\hat{n} \cdot \vec{c} = -v = -c_s \sin \theta$, $c_s^2 = u^2 + v^2$, and $c^2 = c_s^2 + w^2$. The integral equation for the collision density becomes

$$\begin{aligned} \psi(Z) = & \frac{1 - \alpha}{2 - \alpha} \frac{\psi(Z)}{2\pi(RT)^2} \int_{v > 0} v e^{-c^2/2RT} d\vec{c} \\ & + \frac{1}{(2 - \alpha)2\pi(RT)^2} \int_{v > 0} v \psi\left(Z - \frac{2awv}{u^2 + v^2}\right) d\vec{c} \end{aligned} \quad (16)$$

Equation (16) is a homogeneous integral equation for the collision density $\psi(Z)$ and possesses a solution

$$\psi(Z) = A + BZ \quad (17)$$

where A and B are constants. That (17) is a solution of (16) may be verified readily by trial. The collision density varies linearly with axial position as might have been expected from the fact that the capillary is taken to be infinite in the Z direction.

Gas Density

The gas density variation in the capillary is determined from equation (10).

$$\begin{aligned} n = \int_{\vec{c}} f \, d\vec{c} = & \frac{1}{(2 - \alpha)2\pi(RT)^2} \int_{\vec{c}} \left(A + BZ - \frac{Bw\delta_s'}{c_s} \right) e^{-c^2/2RT} d\vec{c} \\ & + \frac{1 - \alpha}{2 - \alpha} \frac{1}{2\pi(RT)^2} \int_{\vec{c}} \left(A + BZ + \frac{Bw\delta_s''}{c_s} \right) e^{-c^2/2RT} d\vec{c} . \end{aligned} \quad (18)$$

The portions of the integrals in equation (18) involving the axial component of velocity w vanish since they are odd in w. The remaining integrals are readily evaluated to give

$$n(Z) = (A + BZ) \sqrt{\frac{2\pi}{RT}} = \sqrt{\frac{2\pi}{RT}} \psi(Z) \quad (19)$$

so that $A = n(0) \sqrt{RT/2\pi}$ and $B = (dn/dZ) \sqrt{RT/2\pi}$. We see that the gas density varies linearly with Z and does not depend on radial position r. We note that the presence of backscattering does not affect the gas density or collision density in the capillary which are the same as in the case of purely diffuse scattering ($\alpha = 1$).

Molecular Flux

The number of molecules crossing unit area perpendicular to the Z axis per second is obtained from equation (11).

If one selects a cylindrical coordinate system in velocity space θ, c_s, w in which $d\vec{c} = c_s d\theta dc_s dw$, the integrations over c_s and w are readily

carried out to give

$$n \langle w \rangle = \frac{\alpha}{2 - \alpha} \left(- \frac{dn}{dz} \sqrt{\frac{2RT}{\pi}} \right) \int_0^{\pi/2} \sqrt{a^2 - r^2 \cos^2 \theta} d\theta. \quad (20)$$

This result differs from the molecular flux for purely diffuse scattering only by the multiplicative factor $\alpha/(2 - \alpha)$. Thus the molecular flux at every radial position in the capillary is reduced by the same factor due to backscattering. The integral in (20) can be related to the complete elliptic integral of the second kind. The molecular flux profiles for pure diffuse scattering ($\alpha = 1$) and for 10% backscattering ($\alpha = 0.9$) are shown in Figure 2.

Molecular Flow

The molecular flow Γ is obtained by the integration of (20) over the capillary cross section as indicated in (12):

$$\Gamma = 2\pi \left(\frac{\alpha}{2 - \alpha} \right) \left(- \frac{dn}{dz} \sqrt{\frac{2RT}{\pi}} \right) \int_0^a \int_0^{\pi/2} \sqrt{a^2 - r^2 \cos^2 \theta} r dr d\theta.$$

The double integral represents an integration over a quarter disc of radius a , and is evaluated most easily in a rectangular coordinate system $x = r \cos \theta$, $y = r \sin \theta$, $r d\theta dr = dx dy$. The final result is

$$\Gamma = \left(\frac{8}{3} \pi a^3 \sqrt{\frac{RT}{2\pi}} \frac{\Delta n}{\ell} \right) \left(\frac{\alpha}{2 - \alpha} \right) \quad (21)$$

where Δn is the density difference imposed across the ends of the long tube of length ℓ . Equation (21) can be rewritten in terms of the transmission probability Q defined by

$$Q \equiv \Gamma / \left(\pi a^2 \Delta n \sqrt{\frac{RT}{2\pi}} \right). \quad (22)$$

One obtains

$$Q = \left(\frac{\alpha}{2 - \alpha} \right) \frac{8a}{3\ell}. \quad (23)$$

Backscattering reduces the transmission probability by a factor $\alpha/(2 - \alpha)$. To reduce the transmission probability by 10% requires about 5.5% backscattering, i.e., $\alpha = 0.945$.

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Figure 2
MOLECULAR FLUX PROFILE IN A LONG CAPILLARY

CONCLUSIONS AND SUMMARY

A simple boundary condition at a gas solid interface in a rarefied gas flow has been proposed which results in a reduction of the free molecule flow through a long capillary below that which would be predicted with the more commonly used pure diffuse scattering law (cosine law). The modified boundary condition permits some backscattering along with diffuse scattering and is intended to simulate the scattering at a real randomly rough surface.

For free molecule flow in a long capillary the modified boundary condition does not affect the gas density or collision density distribution along the capillary, reduces the molecular flux in the axial direction by the same amount at each radial position, and reduces the molecular flow (or the transmission probability) by an amount $\alpha/(2 - \alpha)$ where α is the probability of backscattering and $1 - \alpha$ is the probability of diffuse scattering.

In Part 2 of this report we examine the effect of backscattering on the free molecule flow in capillaries of arbitrary length-to-radius ratio. Comparison with experimental data leads to an estimate of the amount of backscattering required to account for dependence of the observed transmission probabilities on length-to-radius ratio.

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