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INTERNAL RAREFIED GAS FLOWS WITH BACKSCATTERING
PART 2: FREE MOLECULE FLOW THROUGH
FINITE CAPILLARIES

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INTERNAL RAREFIED GAS FLOWS WITH BACKSCATTERING
PART 2: FREE MOLECULE FLOW THROUGH FINITE CAPILLARIES

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ABSTRACT

The effect of backscattering on the free molecule flow in capillaries of finite length is investigated. Backscattering decreases the transport through such systems (relative to the transport with fully diffuse scattering) by an amount which depends upon the probability of backscattering and the length-to-radius ratio of the capillary.

Comparison with observed flows in short capillaries leads to an estimate of 0.04 for the probability of backscattering from unprepared randomly rough surfaces.

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INTERNAL RAREFIED GAS FLOWS WITH BACKSCATTERING
PART 2: FREE MOLECULE FLOW THROUGH FINITE CAPILLARIES

INTRODUCTION

In Part 1 of this report a modification of the conventional diffuse scattering boundary condition was suggested. A fraction of the molecules incident on the surface are assumed to be scattered back in the direction from which they came while the remainder are scattered diffusely. The effects of this modified boundary condition on free molecule flow in a long (infinite) capillary were examined. It was found that the modified boundary condition does not affect the gas density or collision density distribution along the capillary. The velocity profile and the flow through the capillary are modified. The mean velocity is decreased by the same multiplicative factor $\alpha/(2 - \alpha)$ at every point in the capillary cross section. Here α is the fraction of diffuse scattering and $1 - \alpha$ is the fraction of backscattering. The transport through the long capillary is decreased due to backscattering by the same factor $\alpha/(2 - \alpha)$.

In this report we examine the effect of backscattering on the free molecule transport through finite capillaries. Comparison with the experimental results of Lund and Berman [1] enables us to select a value for the fraction $(1 - \alpha)$ of backscattering which accounts reasonably well for the observed dependence of free molecule transport on the capillary length-to-radius ratio. This value of α is used in subsequent parts of this report for further studies of the effects of backscattering on internal rarefied gas flows.

FREE MOLECULE FLOW IN FINITE CAPILLARIES*

DeMarcus [2] has shown that if one is interested only in free molecule transport, then it is more convenient to formulate the problem in terms

*Although the presentation in this report is concerned with finite capillaries, the basic ideas and the approach are equally valid for any one-dimensional system, i.e., any system in which the collision density can be described in terms of one space variable.

of an integral equation (the Clausing equation) than to solve the collisionless Boltzmann equation for the distribution function and take appropriate moments to find the flow.

DeMarcus [3] has also solved the problem of free molecule flow in finite capillaries with an arbitrary amount of specular reflection at the walls. He showed that if one focuses attention on the particles which undergo diffuse collisions with the capillary walls, then a Clausing equation for the "diffuse collision density" can be written. In an analogous fashion, one can treat the free molecule flow through short capillaries with back-scattering.

In what follows, we use essentially the approach of DeMarcus [3]. In the case of backscattering, however, it is possible for some molecules which are diffusely scattered at some point on the capillary wall to return to that point and be diffusely scattered again without an intermediate diffuse scattering event at some other wall point. The probability for this sequence of events is zero for a scattering law which allows only diffuse and specular reflection.

Let x be the space coordinate along the capillary axis. The front face of the capillary is taken as $x = 0$ and the exit plane is located at $x = \ell$. Without loss of generality we assume a given gas density outside the capillary at $x = 0$ and zero gas density outside the capillary face of $x = \ell$.

In the following definitions all probabilities are considered to be normalized for one particle per second entering the capillary at $x = 0$.

$s(x)dx$ = rate of diffuse collisions at x (normalized collision rate).

$s_1(x)dx$ = probability that a particle entering the system at $x = 0$ makes its first diffuse collision in dx at x .

$\equiv n_1(x)dx$ for $\alpha = 1$ (pure diffuse scattering).

$S_1(x)$ = probability that a particle entering at $x = 0$ gets past x without an intervening diffuse collision with the wall.

$$\equiv N_1(x) \text{ for } \alpha = 1.$$

$\Gamma(y, x)dx$ = probability that a particle diffusely scattered at y makes its next diffuse collision in dx at x .

$$\equiv K(y, x)dx \text{ for } \alpha = 1.$$

$\tilde{\Gamma}(x, y)dy$ = probability that a particle diffusely scattered at x makes its next diffuse collision at x .*

$\pi(x; 0)$ = probability that a particle diffusely scattered at x leaves the system at $x = 0$ without an intervening diffuse collision.

$$\equiv P(x; 0) \text{ for } \alpha = 1.$$

$\pi(x; \ell)$ = probability that a particle diffusely scattered at x leaves the system at $x = \ell$ without an intervening diffuse collision.

$$\equiv P(x; \ell) \text{ for } \alpha = 1.$$

Q = probability that a particle entering the system at $x = 0$ leaves the system at $x = \ell$; transmission probability.

DeMarcus has shown, for the case of partial specular reflection, that relationships between probabilities similar to those used above can be obtained from their definitions and from mass balance and thermodynamic equilibrium considerations. In a similar way one obtains.

$$S_1(x) = N_1(x) \quad (1)$$

$$s_1(x) = -\alpha(dS_1/dx) = -\alpha(dN_1/dx) \quad (2)$$

$$\pi(x, 0) = -(r_p/2)(dS_1/dx) = P(x, 0) \quad (3)$$

*Note that for pure diffuse and/or specular scattering this probability vanishes. For a finite probability of backscattering, a particle which is diffusely scattered at x can undergo an odd number of backscattering events between dy at y and x so that its next diffuse collision is again at x .

$$\pi(x, \ell) = -(r_p/2)[dS_1(t)/dt]_{t=\ell-x} = P(x, \ell) \quad (4)$$

$$\Gamma(x, y) + \tilde{\Gamma}(x, y) = (r_p/2)[d^2S_1(t)/dt^2]_{t=|x-y|} = K(x, y) \quad (5)$$

The hydraulic radius r_p is defined as twice the cross-sectional area open to flow divided by the total perimeter of the flow cross section.

All the required probabilities follow by differentiation or integration if one of them is known. In particular, one need only compute the probability $N_1(x) = S_1(x)$ for the given geometry and the remaining probabilities can be obtained by differentiation.

For the finite capillary with backscattering, the Clausing equation for the diffuse collision density is

$$s(x) = s_1(x) + \int_0^\ell \Gamma(x, y)s(y)dy + \int_0^\ell \tilde{\Gamma}(y, x)s(x)dy \quad (6)$$

From their definitions it is seen that $\Gamma(x, y)$ and $\tilde{\Gamma}(x, y)$ are related to $K(x, y)$ as follows.

$$\begin{aligned} \Gamma(x, y) &= \alpha K(x, y) + \alpha(1 - \alpha)^2 K(x, y) + \dots \\ &+ \alpha(1 - \alpha)^{2k} K(x, y) + \dots = \frac{1}{2 - \alpha} K(x, y) \end{aligned} \quad (7)$$

$$\begin{aligned} \tilde{\Gamma}(x, y) &= \alpha(1 - \alpha) K(x, y) + \alpha(1 - \alpha)^3 K(x, y) + \dots \\ &+ \alpha(1 - \alpha)^{2k+1} K(x, y) + \dots = \frac{1 - \alpha}{2 - \alpha} K(x, y) \end{aligned} \quad (8)$$

where k is a positive integer.

The integral equation (6) can now be written

$$s(x) = s_1(x) + \int_0^\ell \Gamma(x, y)s(y)dy + \left(\frac{1 - \alpha}{2 - \alpha}\right) s(x) \int_0^\ell K(x, y)dy \quad (9)$$

or using the relation obtained by DeMarcus [4],

$$\int_0^{\ell} K(x,y)dy = 1 - (r_p/2)n_1(x) - (r_p/2)n_1(\ell - x) ,$$

equation (9) becomes

$$s(x) = \Omega(x)s_1(x) + \int_0^{\ell} \Omega(x)\Gamma(x,y)s(y)dy \quad (10)$$

where

$$\Omega(x) = \left\{ 1 - \frac{1-\alpha}{2-\alpha} \left[1 - \frac{r_p}{2} n_1(x) - \frac{r_p}{2} n_1(\ell - x) \right] \right\}^{-1} . \quad (11)$$

If the solution $s(x)$ of (10) is known, then the transmission probability is given by

$$Q = S_1(x) + \int_0^{\ell} \pi(x;\ell)s(x)dx . \quad (12)$$

An alternative form for the transmission probability which will prove useful is obtained by writing

$$Q = 1 - R = 1 - \left\{ (1 - \alpha)[1 - N_1(\ell)] + \int_0^{\ell} \pi(x,0)s(x)dx \right\} \quad (13)$$

where R , the reflection coefficient, is the probability that a particle entering the system at $x = 0$, leaves the system at $x = 0$. With the relationships between the probabilities (1) through (5) one can write

$$Q = 1 - (1 - \alpha)[1 - N_1(\ell)] - \frac{r_p}{2\alpha} \int_0^{\ell} s_1(x)s(x)dx . \quad (14)$$

DeMarcus [4] has discussed a variational method which can be used to obtain a bound on the transmission probability. Consider the functional

$$F\{g(x)\} = \int_0^{\ell} g(x)[2s_1(x) + \int_0^{\ell} L(x,y)g(y)dy - g(x)] dx . \quad (15)$$

If

- a) $L(x,y) \geq 0$; $x,y \in (0,\ell)$
- b) $L(x,y) = L(y,x)$

c) there exists an integer n such that

$$\int_0^{\ell} L^{(n)}(x, y) dy = b(x) < 1 ; x \in (0, \ell)$$

where

$$L^{(n+1)}(x, y) = \int_0^{\ell} L(x, t) L^{(n)}(t, y) dt$$

and

$$L^{(1)}(x, y) = L(x, y) ,$$

then the function $F\{g(x)\}$ is an absolute maximum when $g(x) \equiv s(x)$ where $s(x)$ is the solution of the integral equation

$$p(x) = \phi(x) + \int_0^{\ell} L(x, y) p(y) dy . \quad (16)$$

Further, the maximum value of the functional is given by

$$\max F\{g(x)\} \leq \int_0^{\ell} \phi(x) p(x) dx \quad (17)$$

where the equality holds when $g(x) \equiv p(x)$.

If one defines

$$p(x) = s(x) / \sqrt{\Omega(x)} \quad (18)$$

$$\phi(x) = s_1(x) \sqrt{\Omega(x)} \quad (19)$$

$$L(x, y) = \Gamma(x, y) \sqrt{\Omega(x) \Omega(y)} , \quad (20)$$

then the integral equation (10) is identical to (16) and $L(x, y)$ satisfies the necessary conditions.

Using (17), (18) and (19) we can express the integral in (14) as

$$\begin{aligned} \int_0^{\ell} s_1(x)s(x)dx &= \int_0^{\ell} \frac{\phi(x)}{\sqrt{\Omega(x)}} p(x)\sqrt{\Omega(x)} dx \\ &= \int_0^{\ell} \phi(x)p(x)dx \geq \max F\{g(x)\} \end{aligned}$$

so that a bound for the transmission probability is given by

$$Q \leq 1 - (1 - \alpha)[1 - N_1(\ell)] - (r_p/2\alpha) \max F\{g(x)\} . \quad (21)$$

For $g(x)$ we choose a simple linear trial function

$$g(x) = B - Ax \quad (22)$$

to form $F\{g(x)\}$ as in (15) and maximize with respect to the constants A and B . The maximum value of $F\{g(x)\}$ is found to be

$$\begin{aligned} \max F\{g(x)\} &= A^2(I_1 - \frac{1}{3}\ell^3) + B^2(I_3 - \ell) - 2AI_4 \\ &\quad + 2BI_5 + AB(\ell^2 - 2I_2) \end{aligned} \quad (23)$$

with

$$A = \frac{(\ell - I_3)I_4 - [(\ell^2/2) - I_2]I_5}{(\ell - I_3)[I_1 - (\ell^3/3)] + [(\ell^2/2) - I_2]^2} , \quad (24)$$

$$B = \frac{I_5}{\ell - I_3} + \frac{[(\ell^2/2) - I_2](\ell - I_3)I_4 - [(\ell^2/2) - I_2]^2 I_5}{(\ell - I_3)^2[I_1 - (\ell^3/3)] + (\ell - I_3)[(\ell^2/2) - I_2]^2} , \quad (25)$$

$$I_1 = \int_0^{\ell} \int_0^{\ell} xyL(x,y)dxdy , \quad (26)$$

$$I_2 = \int_0^{\ell} \int_0^{\ell} yL(x,y)dxdy , \quad (27)$$

$$I_3 = \int_0^{\ell} \int_0^{\ell} L(x,y)dxdy , \quad (28)$$

$$I_4 = \int_0^{\ell} x\phi(x)dx , \quad (29)$$

and

$$I_5 = \int_0^{\ell} \phi(x)dx . \quad (30)$$

With $\max F\{g(x)\}$ known, equation (21) provides an upper bound for the transmission probability Q .

DETERMINATION OF α

The probabilities required for the estimate of Q provided by (21) have been given by DeMarcus [4] for the case of a capillary with circular cross section. With these, the required integrals were evaluated using numerical quadrature techniques, where required.

Figure 1 shows the results of such calculations for capillaries with various length-to-radius ratios. The ordinate is $1 - (Q_b/Q_d)$ where Q_b is the upper bound for the transmission probability with backscattering ($\alpha < 1$) and Q_d is the upper bound for pure diffuse scattering ($\alpha = 1$). Results are shown for backscattering probabilities of 0.05, 0.06, and 0.07. The points indicated in the figure are the results of the experiments of Lund and Berman [1] for argon flow through nickel capillaries. Other than careful machining, no special surface treatment was used in the preparation of these capillaries.

Note that a choice of α between 0.93 and 0.94 would provide a reasonable fit to the observed deviations from the free molecule flows calculated under the assumption of completely diffuse reflection.

In the shorter capillaries, the observed deviations are probably subject to greater error since a substantial fraction of the molecules can get through the capillary without making a wall collision and are thus

Figure 1
THE EFFECT OF BACKSCATTERING ON
FREE MOLECULE FLOW THROUGH SHORT CAPILLARIES

unaffected by the scattering law at the wall. Hence it is felt that more weight should be assigned to the experimental results for the longer capillaries.

In the subsequent parts of this report a value of $\alpha = 0.94$ will be used.

SUMMARY AND CONCLUSIONS

The effect of backscattering on the free molecule flow in finite capillaries has been determined. Backscattering decreases the free molecule transport from that which would be obtained with fully diffuse scattering. The magnitude of this decrease depends on the probability for backscattering and on the length-to-radius ratio of the capillary. The decrease is greater for greater probability of backscattering and for longer capillaries. In the limit of an infinite capillary we know from Part 1 that the fractional decrease in transport approaches $\alpha/(2 - \alpha)$.

Comparison with experimental data leads to the conclusion that a value of $\alpha = 0.94$ provides a satisfactory description of the observed free molecule flows through short capillaries. This value will be used in subsequent parts of this report.

In Part 3 of this report we depart from considerations of free molecule flow and begin the examination of transport at lower Knudsen numbers with the study of the Kramer problem and the determination of the effect of backscattering on the slip coefficient.

REFERENCES

1. Lund, L. M., and Berman, A. S., J. Appl. Phys., 37, 2496 (1966).
2. DeMarcus, W. C., The Problem of Knudsen Flow - Part I. General Theory, Union Carbide Corporation, Nuclear Division, Oak Ridge Gaseous Diffusion Plant, September 5, 1956 (K-1302, Part I).

3. DeMarcus, W. C., Rarefied Gas Dynamics, Suppl. 1, L. Talbot, ed., New York, Academic Press, 1961, p. 161.
4. DeMarcus, W. C., The Problem of Knudsen Flow - Part III. Solutions for One-Dimensional Systems, Union Carbide Corporation, Nuclear Division, Oak Ridge Gaseous Diffusion Plant, March 19, 1957 (K-1302, Part III).