THE INITIAL DISTRIBUTION OF TEST PARTICLES IN NEAR-FREE MOLECULE FLOW

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Received December 19, 1977

Presented by Prof. Dr. J. ANTAL

Introduction

In the free molecule region the molecules move independently of each other. In the near-free molecule region the number of collisions between molecules is commensurable to the number of collisions with the wall but the conditions of the continuum approximation fail. The regions are marked out by the Knudsen number Kn, the ratio of mean free path λ to the characteristic geometrical dimension D. (In the case of a cylindrical tube of radius R_0 Kn equals $\lambda/2R_0$). The flow is free molecular for $Kn > 10$ and near-free molecular for $0.1 < Kn < 10$.

The geometrical conditions and the gas-surface interaction determine the free molecule flow. The independence of molecule paths facilitates the theoretical considerations when $Kn > 10$. Taking the binary collisions between the molecules into account difficulties arise: one has to deal with the collision dynamics and to solve the problem of the initial distribution with respect to the iteration procedures.

The subsequent problems of the axial symmetrical near-free molecule flow will be discussed from the aspect of test particle method of Monte Carlo calculations. Treatment of collision dynamics problems and some results of calculations have been published elsewhere [1]. Here only the problem of the initial distribution of near-free molecule flow around circular orifices as well as in and around cylindrical tubes is investigated. From the aspect of collisions the initial distribution is free molecular in the tube and near the tube exit in the vacuum side. The real difficulties appear at the start of the test particles.

Different approximations

In the case of free molecule flow from the vessel containing a gas of number density n_0, the flow is steady and the rate of emission through the

orifice within the solid angle $d\Omega$ which makes an angle ϑ with the normal to the plane of the orifice and within the velocity interval v and $v + dv$ is

$$\Phi_{\vartheta,v}\, d\Omega dv = v \cos\vartheta\, f_0(v) v^2\, d\Omega dv \tag{1}$$

where f_0 is the distribution function of the uniform gas in the vessel far from the orifice:

$$f_0(v) = \frac{n_0}{v_0^3 \pi^{3/2}} \exp\left[-\, v^2/v_0^2\right] \tag{2}$$

where v_0 is the most probable velocity. Normalizing Eq. (1) by the total flux Φ_0;

$$\Phi_0 = \frac{1}{4} n_0 \langle v \rangle \tag{3}$$

where $\langle v \rangle$ is the mean velocity, we get the dimensionless relative flux in the form

$$\frac{1}{\Phi_0} \Phi_{\vartheta,v}\, d\Omega dv = F(\vartheta)\, \gamma(v)\, d\Omega dv \tag{4}$$

where the angular distribution is

$$F(\vartheta) d\Omega = \frac{1}{\pi} \cos\vartheta\, d\Omega \tag{5}$$

and the probability density function for the velocity magnitudes is

$$\gamma(v) dv = \frac{2v^3}{v_0^4} \exp\left[-\, v^2/v_0^2\right] dv\,. \tag{6}$$

By means of Eqs (5) and (6) the direction and magnitude of the velocity of molecules emerging uniformly distributed from the orifice cross section can be selected.

Let us investigate a circular aperture of negligible lip thickness. Collisions between the molecules impair the isotropy in the vessel: in the direction of the orifice the mean free path elongates and an inward flow appears toward the vessel from the vacuum side because of the collisions near the orifice. The flux will be greater than Φ_0 in Eq. (3). Since the change of the mean free path depends on the direction of the velocity of molecule to the orifice, Eqs (5) and (6) give distributions wrong. The local flux will change as a function of the distance R from the centre of the orifice in the aperture plane. For deter-

mining the flux it is necessary to know the distribution function $f(r = 0, \bar{v})$ across the orifice:

$$\Phi_{\vartheta, v}\, \mathrm{d}\Omega\, \mathrm{d}v = f(r = o, \bar{v}) v \cos \vartheta v^2\, \mathrm{d}\Omega \mathrm{d}v \tag{7}$$

where the condition $r = 0$ refers to the flux in the aperture plane. At different distances R from the centre of the orifice the distribution function assumes different values, and the distances r are measured in direction $\bar{v}$ from the plane of the aperture.

The iteration procedure by NARASIMHA [2] and WILLIS [3] enables $f(r = 0, \bar{v})$ to be determined. Their iteration procedure is based on the integral form of the Boltzmann equation. $f^{(n+1)}(\bar{r}, \bar{v})$ at $\bar{r}$ results from the n-th step of the iteration if the distribution function $f^{(n)}(\bar{r}_0, \bar{v})$ is known at $\bar{r}_0$:

$$f^{(n+1)}(\bar{r}, \bar{v}) = f(\bar{r}_0, \bar{v}) \exp\left\{-\int_{\bar{r}_0}^{\bar{r}} \frac{J_2^{(n)}(\bar{l}', \bar{v})}{v}\, \mathrm{d}\bar{l}'\right\} + \\ + \int_{\bar{r}_0}^{\bar{r}} J_1^{(n)}(\bar{l}, \bar{v}) \exp\left\{-\int_{\bar{l}}^{\bar{r}} \frac{J_2^{(n)}(\bar{l}', \bar{v})}{v}\, \mathrm{d}\bar{l}'\right\} \frac{\mathrm{d}\bar{l}}{v}. \tag{8}$$

The collision integrals J_1 and J_2 can be calculated by using the simplifying suppositions of the BGK model equation. The known distribution function at $\bar{r}_0$ is the function f_0 of Maxwell distribution in form of Eq. (2) for the uniform gas in the vessel far away from the orifice. Near to the orifice the known number density $n(\bar{r})$ and the mean molecular velocity

$$\bar{u}(\bar{r}) = \frac{1}{n} \int \bar{v} f(\bar{r}, \bar{v})\, \mathrm{d}\bar{v} \tag{9}$$

are the free molecular values in the zeroth approximation. Using dimensionless form by units v_0, R_0 and n_0, and introducing the quantity $\beta = 1/(1 - 2u^2/3)$, the first approximation for $f(r = 0, \bar{v})$ is

$$f(r = 0, \bar{v}) = f_0 \frac{1}{\sqrt{\pi}\, Kn} \int_0^{\infty} \frac{1}{v} n^2 \beta^{3/2} \exp\{v^2 - \beta(\bar{v} - \bar{u})^2\} \exp\left\{-\frac{1}{\sqrt{\pi}\, Kn} \int_0^{r} n \mathrm{d}r'\right\} \mathrm{d}r \tag{10}$$

Knowing the free molecular distributions $n(\bar{r})$ and $\bar{u}(\bar{r})$, Eq. (10) fairly approximates the distribution function for $Kn > 1$ [4].

In Eq. (10) the coefficient of f_0 is a statistical weight, which gives the intensity of the particle flux emerging from the orifice, unit flux of particles

of velocity v being determined by Eqs (5) and (6). To apply Eq. (10) for $Kn < 1$ it is necessary to determine distributions $n(\bar{r})$ and $\bar{u}(\bar{r})$ of the gas at $Kn = 1$ in the vessel near the orifice by the procedure described above, taking into account the molecules travelling backward because of the collisions. This procedure requires a lot of computer time, so it is worth to deal with simplification possibilities.

In a uniform gas the probability that a molecule reaches a distance greater than x is $\exp(-x/\lambda)$. In the presence of the orifice, less of molecules will travel in the opposite direction, so the probability mentioned above will be greater, and it is proportional to the solid angle $\delta\omega(\vartheta)$, representing the orifice from the given point. The probability may be calculated for $\vartheta = 0$ and as the relation $\delta\omega(\vartheta) = \cos\vartheta\,\delta\omega(0)$ is right far away from the orifice, Wahlbeck [5] has got for the molecule flux:

$$\Phi_\vartheta = \frac{n_0\langle v\rangle}{4\pi}\cos\vartheta\,\{1 + \cos\vartheta\,[\delta\bar{\omega}(0)/2\pi]\} \tag{11}$$

where

$$\frac{\delta\bar{\omega}(0)}{2\pi} = 1 - \frac{\pi}{4Kn}\left[H_1\left(\frac{1}{2Kn}\right) - Y_1\left(\frac{1}{2Kn}\right)\right] + \frac{1}{2Kn}. \tag{12}$$

In Eq. (12) $H_1(x)$ is the Struve function and $Y_1(x)$ is the Bessel function of second kind.

In Wahlbeck's approximation the flux is uniform across the orifice and the velocity distribution is Maxwellian. This approximation gives correct results for $Kn > 1$ and the total flux Φ_0 is accurate enough, again provided $Kn < 1$ because the formula of Φ_0 is fitted to the continuum region:

$$\Phi_0 = \frac{1}{4}n_0\langle v\rangle\left[1 + \frac{2}{3}\,\delta\bar{\omega}(0)/2\pi\right]. \tag{13}$$

It is easy to simplify Eq. (10) by neglecting the change of the velocity distribution; taking simply $v = \langle v\rangle$ and $\bar{u} = 0$. The result is:

$$f(r = 0, \bar{v}) = f_0\frac{1}{2Kn}\int_0^\infty n^2 \exp\left[-\frac{1}{2Kn}\int_0^r n(r')\mathrm{d}r'\right]dr. \tag{14}$$

Eq. (14) gives different weighting factors at different distances from the centre of the orifice. Eq. (14) is handled in the computations similarly to Eq. (10), but the needed computational work is far less.

The comparison with the experimental data shows Eq. (11) to give accurate results for $Kn > 1$, but to correct the deviations for high and low values of angle ϑ for $Kn < 1$ Eq. (14) has to be used. This fact is illustrated in Fig. 1, demonstrating the necessity and sufficiency of Eq. (14).

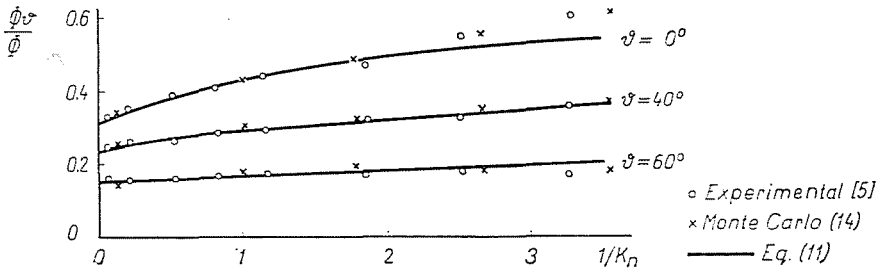

Fig. 1. Relative flux *vs.* the Knudsen number at different angles ϑ

In the case of cylindrical tubes the simplest procedure is to use Eq. (11) to calculate the near-free molecule flow. In this procedure the change of the velocity distribution may be neglected and the anisotropy is determined from the density ratios. Numerical values of three number densities belonging to the given Kn have to be known: the density n_0 in the vessel far away from the entrance plane of the tube; the average density n'_a near the aperture of negligible lip thickness; and the average density n'_t near the entrance of the tube. These number density values yield the factor j:

$$j = \frac{n_0 - n'_t}{n_0 - n'_a} = \frac{1 - n_t}{1 - n_a}$$

where $n_t = n'_t/n_0$ and $n_a = n'_a/n_0$. In Eq. (11) $\delta\bar{\omega}(0)/2\pi$ must be multiplied with this factor j.

Accuracy of calculations is improved by determining the distribution of molecules travelling backward by one or more iteration cycles using Eqs (11) or (10).

Conclusions

The calculation of the initial distribution of test particles in long tubes considerably increases the computer time, but the Monte Carlo method is generally inefficient for long tubes. Table I shows the comparison of the three approaches of different accuracies. The density ratios at characteristic points of the tube are compared; in $n(R, z)$ R and z are measured from the centre of the orifice, R along the radius in R_0 units and z along the axis of the tube of length L. In the same way are presented the ratios of the axial components of mass velocity defined by Eq. (9). Since Eq. (10) gives reliable results on the level of the BGK model equation, Table I shows the percentile deviations of the values calculated by Eqs (11) and (14) from results by Eq. (10).

Table I

	$L/R_0 = 2$	$Kn = 2$	$L/R_0 = 0.5$	$Kn = 0.28$
	Percentile deviations from Eq. (10)			
	(14)	(11)	(14)	(11)
n (0.52, 0.9L)/n (0.52, 0.1L)	2.81	2.17	4.81	13.02
n (0.17, 0.9L)/n (0.17, 0.1L)	3.05	3.27	7.71	15.25
n (0.97, 0.5L)/n (0.17, 0.5L)	2.11	4.83	5.14	8.61
u_z(0.52, 0.9L)/u_z(0.52, 0.1L)	1.67	3.17	6.26	7.75
u_z(0.17, 0.9L)/u_z(0.17, 0.1L)	2.24	2.91	4.75	10.62
u_z(0.97, 0.5L)/u_z(0.17, 0.5L)	2.02	3.71	5.17	12.10
α	2.21	1.98	2.75	33.81

It is understandable that the method taking only the dependence on angle ϑ into account gives considerable deviation for $Kn < 1$. It is noteworthy, however, that the transmission probability α characterizing the mass transfer along the tubes, may be calculated with a minimum error even by Eq. (11). This peculiarity may be attributed to the fitting of the total flux in Eq. (13) to the continuum region.

Taken all in all the expected closeness of every approximation is proportional to the required computer time. When a detailed determination of the flow or $Kn < 1$ is needed — involving density distribution, mass velocity, angular distribution of the emerging particles — Eq. (10) is imposed for maximum accuracy [6]. In other cases even approximations using Eq. (11) or Eq. (14) are satisfactory.

Summary

In the near-free molecule region the collisions between the molecules impair the isotropy near the orifice. The test particle method of the Monte Carlo calculations requires the knowledge of the distribution function in the orifice plane. Various iteration procedures approach the distribution function in the interval of the Knudsen number $0.1 < Kn < 10$. The approximations are compared by way of the characteristic distributions of the axial symmetrical flows.

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