A BEAM OF FREE MOLECULES EMERGING

FROM A PACKET OF CAPILLARIES

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Introduction

Molecular beams have found wide application in science and technology [1, 2]. The subject of investigations of the parameters of gas streams conducted earlier has been, as a rule, the limiting angular distributions (directional diagrams) [3-14] observed at large distances from the source of the molecular beam. As the source one often takes either individual channels with cross sections of different shapes [3, 6] or tightly packed blocks (packets) of such channels [4, 5, 7-14].

Two principal demands are imposed on molecular beams: high intensity and sharp directionality. Sources in the form of packets of long channels allow one to obtain molecular beams satisfying these demands without the use of additional collimating devices. The intensity of the molecular beam can be increased by increasing the number of channels in the packet [4, 5, 9, 10], by decreasing the distance from the source to the object [12], and by increasing the pressure in the source chamber [3-14] (i.e., in the volume from which the gas enters the channels).

The intensity of a molecular beam is determined by the geometrical characteristics of the source and the intensity of intermolecular collisions. The longer the channels in the source, the narrower the angular distribution of the beam [3]. Because of this many investigations have been confined to the consideration of long channels only [4, 5, 7, 13, 14].

An increase in the channel length leads to a decrease in the beam intensity. Investigations carried out for channels of different lengths are interesting for this reason.

Increasing the pressure in the source chamber leads to an increase in the intensity of a molecular beam, but its directionality is degraded [6] owing to effects of intermolecular collisions.

The purpose of the present work is to investigate the influence of the geometrical characteristics of the source on the molecular beam. Therefore, molecular collisions are not taken into account (a freemolecule mode of flow). In this case the main role is played by the conditions of the interaction of the molecules with the walls of the source, i.e., the boundary conditions for the molecular distribution function. A mathematical model of a multichannel source of a molecular beam is proposed which allows one to calculate the gas parameters at any distances from the source.

A comparison with the results of [12] was made earlier [15]. The incorrectness of such a comparison was noted, since the influence of intermolecular collisions was considerable in the experiment of [12].

The authors of other investigations [4, 5, 7-11, 13, 14] have assumed that the angular distributions of the molecular beams produced by one channel and by a block of such channels coincide. Such an assumption is valid, as calculations show, only at large distances from the source in comparison with its size. The distance between the source and the detector was chosen arbitrarily.

Statement of the Problem

Let us consider the escape of a gas from a large volume through a packet of capillaries of radius r into a vacuum. The gas density in the volume is n_1 and the temperature is T_1 . Henceforth we will use dimensionless quantities, for which we take r, n_1 , $h = \sqrt{2kT_1/m}$, T_1 , and n_1h^{-3} as the units of measurement of distance, number density, velocity, temperature, and the distribution function, respectively, where k is Boltzmann's constant and m is the mass of a molecule. If the dimensional quantities are marked by the sub-

Sverdlovsk. Translated from Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki, No. 5, pp. 31-37, September-October, 1979. Original article submitted June 14, 1978.



Fig. 1

script zero then the relations $l = l_0/r$ and $T = T_0/T_1$, e.g., are valid for the dimensionless quantities, where l is distance and T is temperature. It is assumed that the gas in the volume is in equilibrium and its distribution function equals f_1 , i.e.,

$$f_1 = \exp(-c^2)\pi^{-3/2}$$
.

Supose the gas flows without collisions between molecules through a packet of radius R composed of identical cylindrical capillaries of length L (Fig. 1).

An increase in the number of capillaries in the packet leads to an increase in the size of the source. A mathematical model of the system under consideration must be constructed using the methods of the kinetic theory of gases. The model must allow for the true sizes of both the individual capillaries and of the entire packet.

Mathematical Model

We assume that the gas flows in the direction of the z axis (see Fig. 1), which coincides with the axis of the packet of capillaries. Suppose the exit cross section of the packet, which is in the plane z = 0, emits molecules having a known distribution function f_2 of the form [15]

$$f_2 = \boldsymbol{P} \frac{F(\vartheta)}{\cos \vartheta} f_1,$$

where P is the coefficient of transparency of the source (the ratio of the area of the capillary openings in the exit cross section of the packet to the entire cross sections area); ϑ is the angle between the axis of the source and a ray s directed from some point on the source to the observation point M with the coordinates ρ , z, and $\varphi = 0$; F(ϑ) is the limiting angular distribution for a single capillary [16].

As calculations show, the proposed model gives the exact limiting angular distribution $F(\vartheta)$ at distances considerably greater than the size of the packet. The condition of conservation of total flux is satisfied, i.e., the integral over the angular distribution of the particles equals the total flux of particles through the packet of capillaries. In addition, the dependence of the distribution function f_2 on the velocity c in the form $\exp(-c^2)$ is exact in the free-molecule mode of flow under consideration. It should be noted that the accuracy of the results is determined by the quantity P, which should be close to unity (i.e., $P \leq 1$). If intermolecular collisions are absent, then it follows from the Boltzmann equation that the distribution function of the molecules is conserved along the flight trajectory of the molecules. Consequently, the function f_2 assigned in the plane of the exit cross section of the packet is the same at any point in the region of gas flow outside the packet.

Thus, the distribution function $f(\vartheta) = f_2(\vartheta)$ of the molecules is known, and to obtain the calculating equations we can use definitions of the macroscopic quantities through the distribution function

$$n(1, \mathbf{u}, T) = \int f\left(1, \mathbf{c}, \frac{2(\mathbf{c} - \mathbf{u})^2}{3}\right) d\mathbf{c}_s$$
(1)

where n is the number density; u is the average velocity; T is the gas temperature; f is the distribution function of the molecules.



Integration in velocity space in (1) is rather complicated, since it is difficult to determine the limits of integration of the dimensionless absolute velocity \mathbf{c} over the components. It is far simpler to determine them in a coordinate system coinciding with \mathbf{c} at the exit cross section of the source [15, 17, 18], i.e.,

$$n(\mathbf{1}, \mathbf{u}, T) = \frac{2P}{\pi^{3/2}} \int_{0}^{\pi} \int_{0}^{R} \int_{0}^{\infty} \frac{F(\theta)}{s^{2}} \rho_{1} c^{2} \exp\left(-c^{2}\right) \left(\mathbf{1}, \mathbf{c}, \frac{2(\mathbf{c}-\mathbf{u})^{2}}{3}\right) dc d\rho_{1} d\phi_{1}, \tag{2}$$

where $s^2 = z^2 + \rho^2 + \rho_1^2 - 2\rho\rho_1\cos\varphi_1$, and $\vartheta = \arccos(z/s)$.

Because of the axial symmetry of the gas flow, the macroscopic parameters do not depend on the angle φ . Therefore, it is sufficient to determine their values in the quadrant x0z (see Fig. 1). In accordance with Eq. (2), the flux components nu_z and nu_x in the axial and radial directions are calculated from the equation

$$n(u_{z}, u_{x}) = \frac{P}{\pi^{3/2}} \int_{0}^{\pi} \int_{0}^{R} \frac{F(\vartheta)}{s^{3}} (z, \rho - \rho_{1} \cos \varphi_{1}) \rho_{1} d\rho_{1} d\varphi_{1}.$$
(3)

For purposes of simplification of notation, Eqs. (2) and (3) represent systems of equations for the determination of three (density, total flux, and temperature) and two (x and z components of the total flux) parameters of the molecular beam, respectively.

As a rule, the principal result in an investigation of molecular beams is the determination of the angular distribution of the beam of molecules emerging from the source,

$$F_1(\theta) = nu(\theta)/nu(0), \ l_2 = \text{const},$$

where θ is the angle between the axis of the source and the ray l (see Fig. 1); $nu(\theta)$ is the component of the total molecular flux in the direction of the ray l; l_2 is the distance from the center of the exit cross section of the packet to the observation point.

Simple geometrical relations lead to the following expression for $nu(\theta)$:

$$nu(\theta) = nu\cos(\varphi_2 - \theta), \quad \varphi_2 = \operatorname{arctg}(u_x/u_z), \quad u = \sqrt{u_x^2 + u_z^2}$$

The calculations of $F_1(\theta)$ were made by an ALGOL program compiled on an M-222 computer. The average time needed to calculate the macroscopic parameters (2) of the gas at one point of the flow field is about 10 sec. Some of the results of the calculations are presented in Figs. 2 and 3.

Experimental Technique

In the experiment we used two packets of capillaries, or so-called capillary sieves, having a transmittance of 87%, a radius $R_0 = (0.278 \pm 0.001)$ cm, and a length $L_0 = 7.70$ and 14.29 cm, respectively, consisting of bundles of thin-walled glass capillaries obtained by baking them with subsequent drawing. The relative lengths of the packets were L = 153 and 283, where $L = L_0/r$. Dimensional quantities are marked by a zero subscript.

To compare the experimental data with theoretical calculations it was necessary to determine the geometrical dimensions of the capillaries, primarily the capillary diameter. For this we used the results of measurements of the total fluxes of molecules in the viscous mode of gas flow in capillaries, where, as is known, the Poiseuille equation is valid for the description of gas flow. The average number of capillaries in a packet was computed from a photograph of a cross section of the capillary sieve and proved to equal N = 2254. The calculated value of the capillary radius (the so-called hydraulic radius) and its standard deviation were $r = (5.05 \pm 0.07) \cdot 10^{-3}$ cm.

The angular distributions (directional diagrams) of the molecular beams formed by the packets of capillaries were investigated on an experimental installation described in [19]. In experiments on the study of the dependence of the shape of the directional diagram of a beam on the distance between the source and the detector it is necessary to provide a constant solid angle through which the entrance opening of the detector is seen from the source. Therefore, in the experiments we used different adapters for the detector, chosen in such a way that the ratio of the diameter of the entrance opening of the detector channel to the distance from the source to the detector remained constant and equal to 0.02. From these considerations we chose the distances between the source and the detector as $l_0 = 17.2$, 5.60, and 1.55 cm.

Discussion of Results

In Fig. 2 we present an experimental directional diagram of a hydrogen molecular beam formed by a capillary sieve with a length L = 283 for the case of a distance $l_0 = 17.2$ cm between the detector and the source in the free-molecule mode of H_2 flow (Knudsen number Kn = 310); directional diagrams of molecular beams calculated from the equations presented above for packets of capillaries with lengths L = 153 and 283 are also presented here for comparison (curves 2 and 1, respectively). As is seen, the experimental points are located somewhat higher than the theoretical curve, which is evidently connected with the fact that a free-molecule mode of gas flow, both along a diameter and along the length of a capillary, was presumed in the theoretical calculations. But in the experiment a free-molecule mode of gas flow along the length of the channel is not guaranteed.

From experimentation on the formation of molecular beams by single channels (see [20], for example) it is known that with an increase in the channel length one observes narrowing of the beam, which is characterized by the half-width of the angular distribution, determined by the size of the angle θ at which the intensity is equal to half the intensity at the beam axis. It is seen from Fig. 2 that an increase in the length of the capillary sieve by almost two times does not give a significant difference in the half-width of the directional diagram of the beam. At the same time, the intensity of the molecular beam decreases in inverse proportion to the increase in the length of the packet owing to the increase in the resistance of the packet.

An analysis of the theoretical solution shows that the narrow directionality of a molecular beam is determined mainly by the ratio of the length of a capillary to its radius, while the beam intensity is determined by the distance between the detector and the source. At large distances, when $l \gg R$, L, it follows from [3, 6, 15] that the molecular flux at an angle θ to the axis is calculated from the equation

$$nu(\theta) = nu = \frac{P}{2\sqrt{\pi}} - \frac{R^2}{l^2}F(\theta), \text{ i.e., } F_1(\theta) = F(\theta),$$
 (4)

where $F(\theta)$ is the limiting angular distribution for a single capillary with the same values of L and r as those in the packet of capillaries. From the obvious equalities

$$\frac{P\pi R_0^2}{\pi r^2} = PR^2 = N$$

and Eq. (4) we find that the beam intensity $nu(\theta)$ is proportional to the number N of capillaries in the packet.

We can estimate the distance at which one observes the same limiting angular distribution $F(\theta)$ for both a packet and a single capillary. As a calculation example we took a source with the parameters R =10, L = 10, and P = 0.8. In the cases of l = 10, 100, 1000, and 10,000 the ratio $[[F_1(\theta) - F(\theta)]/F_1(\theta)] \cdot 100\%$ was 100, 22, 2, and 0.2%, respectively. Consequently, at distances l comparable with the dimensions R and L of the source it is incorrect to use Eq. (4) to determine the flux. Calculations show that a packet of capillaries can be considered as a point source at distances $l \ge (40-50)R$.

The dependence of the shape of the directional diagram (or the angular distribution $F_1(\theta)$) on the distance *l* between the source and the detector for a capillary with L = 153 is shown in Fig. 3. Here the theoretical curves 2-4 and the experimental points, obtained in the free-molecule limit (Kn ≈ 100), correspond to distances $l_0 = 17.2$, 5.60, and 1.55 cm. Curve 1 is the limiting diagram $F(\theta)$ for a single capillary with the same parameters L and r as for the capillary sieve. As is seen, with an increase in l_0 the directional diagram essentially narrows down to the limiting one. Thus, the satisfactory agreement of the experimental and theoretical results shows that the chosen mathematical model is entirely correct in describing the dependence of the shape of the directional diagram on the distance between the detector and a multichannel source of limited size. It is shown that the use of the angular distribution is incorrect at small distances from the source in comparison with its size.

LITERATURE CITED

- 1. N. F. Ramsey, Molecular Beams, Clarendon Press, Oxford (1956).
- 2. A. M. Brodskii and V. S. Leonas (editors), Research with Molecular Beams (Collection) [Russian translation], Mir, Moscow (1969).
- 3. P. Clausing, "Über die Strahlformung bei der Molekularströmung," Z. Phys., 66, 471 (1930).
- 4. J. A. Giordmaine and T. C. Wang, "Molecular beam formation by long parallel tubes," J. Appl. Phys., <u>31</u>, 463 (1960).
- 5. G. Becker, "Zur Theorie der Molekularstrahlerzengung mit langen Kanalen," Z. Phys., <u>162</u>, No. 3, 290 (1961).
- 6. V. S. Troitskii, "Directionality of a molecular beam formed by the escape of gas from a channel," Zh. Tekh. Fiz., <u>32</u>, No. 4 (1962).
- 7. J. C. Johnson, A. T. Stair, and J. L. Pritchard, "Molecular beams formed by arrays of 3-40 diameter tubes," J. Appl. Phys., <u>37</u>, No. 4, 1551 (1966).
- 8. P. Zugenmaier, "Zur Theorie der Molekularstrahlerzengung mit Hilfe zylindrischer Rohre," Z. Angew. Phys., 20, No. 3, 184 (1966).
- 9. R. H. Jones, D. R. Olander, and V. R. Kruger, "Molecular beam sources fabricated from multichannel arrays. I. Angular distributions and peaking factors," J. Appl. Phys., <u>40</u>, No. 11, 4641 (1969).
- 10. D. R. Olander and V. R. Kruger, "Molecular beam sources fabricated from multichannel arrays. III. The exist density problem," J. Appl. Phys., <u>41</u>, No. 7, 2769 (1970).
- 11. D. R. Olander, R. H. Jones, and W. J. Siekhans, "Molecular beam sources fabricated from multichannel arrays. IV. Speed distribution in the centerline beam," J. Appl. Phys., <u>41</u>, No. 11, 4388 (1970).
- 12. R. K. Goodman and A. L. Hunt, "A cross beam neutralizer for ion beams," Rev. Sci. Instrum., <u>42</u>, No. 9, 1359 (1971).
- R. G. Wilmoth, "Speed distribution measurements of N₂ and Ar molecular beams produced by a multichannel source," J. Vac. Sci. Technol., 9, No. 3, 1121 (1972).
- 14. H. C. Reijerinak and N. F. Verster, "Velocity distribution and angular distribution of molecular beams from multichannel arrays," J. Appl. Phys., <u>46</u>, No. 5, 2083 (1975).
- I. G. Neudachin, B. T. Porodnov, and P. E. Suetin, "Formation of a molecular beam by a packet of cylindrical channels," in: Fourth All-Union Conference on Rarefied-Gas Dynamics, Collection of Annotations [in Russian], Moscow (1975).
- 16. I. G. Neudachin, B. T. Porodnov, and P. E. Suetin, "Formation of narrow molecular beams by cylindrical channels," Zh. Tekh. Fiz., <u>42</u>, No. 5 (1972).
- 17. G. I. Marchuk, Theory and Methods for Nuclear Reactor Calculations, Plenum Publ. (1964).
- 18. I. G. Neudachin, B. T. Porodnov, and P. E. Suetin, "The use of a distribution function to describe freemolecule beams," Zh. Tekh. Fiz., 44, No. 4 (1974).
- 19. A. A. Tarin, S. T. Barashkin, B. T. Porodnov, and P. E. Suetin, "The use of the modulation method to detect molecular beams," Zh. Tekh. Fiz., 46, No. 1 (1976).
- 20. S. T. Barashkin, B. T. Porodnov, and M. F. Chemagin, "Total fluxes and directional diagrams in the escape of gas into a vacuum through capillaries of different lengths," Zh. Prikl. Mekh. Tekh. Fiz., No. 4 (1977).