

DETERMINATION OF THE MOLECULAR-VELOCITY  
DISTRIBUTION FUNCTION IN A MOLECULAR BEAM  
BY THE METHOD OF MECHANICAL SELECTION

É. P. Pavlov and V. D. Perminov

UDC 533.6.011.8:539.198.08

Results are presented for the solution of the problem, which is incorrectly formulated according to A. N. Tikhonov, of the establishment of the molecular-velocity distribution function in a molecular beam based on experimental values of the intensity. It is indicated that the distribution function obtained has a non-Maxwellian character.

One of the methods of determining the velocity distribution function  $f(v)$  in a free-molecule flow is the method of mechanical selection [1-3]. A system for determining the function  $f(v)$  by the indicated method consists of a mechanical selector and a detector. The mechanical selector, located in the molecular beam and rotating with velocity  $\omega$ , passes only those molecules of the beam having velocity in a certain range  $[v_0(\omega) - \Delta_1(\omega), v_0(\omega) + \Delta_2(\omega)]$ , the so-called pass band of the selector. The detector, which is behind the selector, records the molecules that pass through it.

A simple mechanical selector, which has a number of advantages compared to selectors used earlier, is described in [4]. In the present paper we describe the method of processing the experimental data obtained using such a selector.

We assume that all the molecules that move toward the slit in front of the selector of the collimator move parallel to its axis. Then the distribution function  $f(v)$ , determined by the method of mechanical selection, is found from the equation

$$\int_{v_0 - \Delta_1}^{v_0 + \Delta_2} H(v_0, v) v f(v) dv = J(v_0) \quad (1.1)$$

Here  $f(v) dv$  is the number of molecules per unit volume having velocity in the interval  $[v, v + dv]$ ;  $J(v_0)$  is the recorded intensity of molecules having velocity from the interval  $[v_0 - \Delta_1, v_0 + \Delta_2]$ ;  $H(v_0, v)$  is the selector transmissivity, equal to the ratio of intensity of molecules of the beam with velocity from the interval  $[v, v + dv]$  at the exit of the selector to their intensity at the entrance to it (outside the interval  $[v_0 - \Delta_1, v_0 + \Delta_2]$  the function  $H(v_0, v) \equiv 0$ ).

For a system that consists of a plane reversible selector and a detecting device, described in [4] and [5], respectively, the function  $H(v_0, v)$  has the form

$$H(v_0, v) = \eta K(v_0, v)$$

Here  $\eta$  is the capture coefficient, equal to the ratio of the intensity of molecules that enter the selector to the intensity of the free-molecule flow in front of the selector (for the flow intensity we take the intensity recorded by the detector in the absence of the selector), and  $K(v_0, v)$  is the transmission function of the selector, equal to the ratio of the intensity of molecules having velocities  $v$  from  $[v, v + dv]$ , passing

---

Moscow. Translated from Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki, No. 4, pp. 57-61, July-August, 1972. Original article submitted July 6, 1971.

© 1974 Consultants Bureau, a division of Plenum Publishing Corporation, 227 West 17th Street, New York, N. Y. 10011. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, microfilming, recording or otherwise, without written permission of the publisher. A copy of this article is available from the publisher for \$15.00.

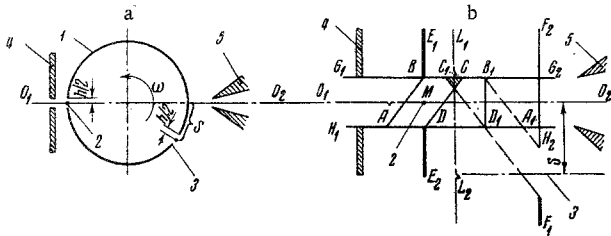


Fig. 1

through the selector, to the intensity of molecules entering the selector (outside the interval  $[v_0 + \Delta_1, v_0 + \Delta_2]$  the function  $K(v_0, v) \equiv 0$ ).

The transmission function of a plane reversible selector practically agrees with the transmission function of a single-ring two-slot selector [4].

Such a selector, schematically presented in Fig. 1a, consists of a thin ring 1 of radius  $R$  with entrance slot 2 and exit slot 3 of width  $h$ . The slot of the collimator of the free-molecule flow 4 and the slot of the detector partition 5, the centers of which together with the center of the ring  $O$  lie on the same axis  $O_1O_2$ , are presented there. The ring rotates with angular velocity  $\omega$ . The axis of rotation of the ring 1 is perpendicular to the  $O_1O_2$  axis, and the length of the twist arc of the selector equals  $s$ .

It is convenient to consider the interaction of such a selector with a flow for  $h \ll R$ , using the diagram represented in Fig. 1b. Two thin straight strips, which are represented in this figure by the straight lines  $E_1E_2$  and  $F_1F_2$ , perpendicular to the  $O_1O_2$  axis, move in opposite directions with velocity  $\omega R$ . The distance between the strips equals  $2R$ ; the width  $h$  of the entrance slot 2 and exit slot 3 at the strips  $E_1E_2$  and  $F_1F_2$  equals the width of the slot of the collimator 4 and the partition 5. The distance from the center of the exit slot 3 up to the  $O_1O_2$  axis at the moment at which the center of the entrance slot 2 lies on this axis equals  $s$ . The flow boundary between the collimator and the partition is represented by the straight lines  $G_1G_2$  and  $H_1H_2$ .

Since, by assumption, all the molecules that pass into the collimator slit move parallel to the  $O_1O_2$  axis, when the slit 2 passes the slit 4 the selector admits only those molecules having velocities in the range  $[v, v + dv]$ , which occur within the parallelogram  $ABCD$ , whose sides  $AD$  and  $BC$  lie on the flow boundaries and equal  $vh/\omega R$ , and whose height is the diagonal  $BD$ . The parallelogram  $ABCD$  moves as a whole with velocity  $v$  along the  $O_1O_2$  axis.

In Fig. 1b the dotted line plots the trace of the exit slot 3 on a plane that is rigidly coupled with the parallelogram  $ABCD$ . It is clear that through the selector there pass molecules which occur in the hatched portion of the parallelogram  $ABCD$ , lying on the trace of the exit slot 3.

The transmission function of the selector  $K(v_0, v)$  equals the ratio of the hatched area  $S'$  to the total area  $S$  of the parallelogram  $ABCD$  ( $S = h^2v/\omega R$ ). To calculate  $S'$  we note that it is the common part of the parallelograms  $ABCD$  and  $A_1B_1C_1D_1$ , which is obtained for the intersection of the trace of the slit 3 with the boundaries of the flow  $G_1G_2$  and  $H_1H_2$  and is the mirror image of  $ABCD$  with respect to the  $L_1L_2$  axis. If the distance  $MM_1$  between the centers of these parallelograms is denoted by  $x$ , then, as can be easily shown, the area  $S'$  is determined from the expression

$$S' = \begin{cases} h(2a - x)^2/4a, & a \leq x \leq 2a \\ h(2a^2 - x^2)/4a, & -a \leq x \leq a \\ h(2a + x)^2/4a, & -2a \leq x \leq -a \end{cases} \quad (1.2)$$

$$a = AD = A_1D_1 = hv/\omega R$$

The distance  $x$  is determined from the equation

$$x = 2R - sv/\omega R \quad (1.3)$$

We shall call the velocity  $v_0$  for which  $S'$  is a maximum ( $x = 0$ ) the principal velocity of the molecules passed by the selector rotating with angular velocity  $\omega$ :

$$v_0 = 2R^2\omega/s \quad (1.4)$$

Such an expression was obtained in [4] for molecules passed by a selector on which the quantity  $h \rightarrow 0$ .

Using (1.2)-(1.4), we obtain an expression for the transmission function

$$K(y) = \begin{cases} (1 + 2\varepsilon - y)^2/4\varepsilon^2, & 1 + \varepsilon \leq y \leq 1 + 2\varepsilon \\ (2\varepsilon^2 - 1 + 2y - y^2)/4\varepsilon^2, & 1 - \varepsilon \leq y \leq 1 + \varepsilon \\ (1 - 2\varepsilon - y)^2/4\varepsilon^2, & 1 - 2\varepsilon \leq y \leq 1 - \varepsilon \end{cases} \quad (1.5)$$

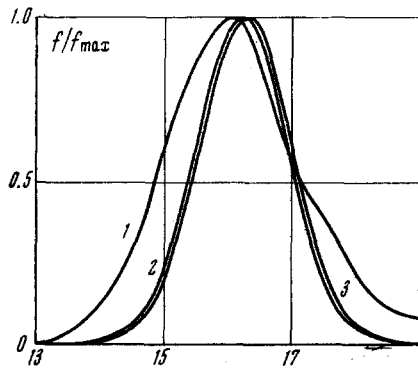


Fig. 2

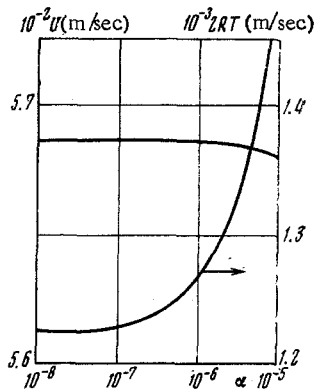


Fig. 3

Here  $y = v_0/v$ , and  $\varepsilon = h/s \ll 1$ . When the change in  $f(v)$  in the range of the pass band is small, the velocity distribution in the flow in front of the selector can be determined directly from the measurement results. Actually, from (1.5) and (1.1) we obtain

$$J(v_0) = \eta v_0^2 f(v_0) \int_{1-2\varepsilon}^{1+2\varepsilon} \frac{K(y)}{y^3} dy = \eta v_0^2 f(v_0) \varphi(\varepsilon)$$

Hence

$$f(v) = \frac{J(v)}{\eta v^2 \varphi(\varepsilon)}, \quad \varphi(\varepsilon) = \frac{1}{4\varepsilon^2} \ln \frac{(1+2\varepsilon)(1-\varepsilon)^2}{(1-2\varepsilon)(1+\varepsilon)^2} \quad (1.6)$$

When it is impossible to neglect the change in  $f(v)$  on the pass band (which is typical for high-velocity molecular beams), we must solve the integral equation (1.1) with kernel (1.5). This initial equation of selection is a particular case of an integral equation of the first kind, the problem of obtaining the solution of which is incorrectly formulated in the general case. Many works (see, e.g., [6-10]) are devoted to methods of solving such problems, which are sometimes called inverse problems.

In the present study, in order to solve the integral equation we use the method of regularization, proposed in [6]. According to this method the family of approximate solutions  $f^\alpha(v)$ , converging for  $\alpha \rightarrow 0$  to the solution (1.1) if the right side of  $J(v_0)$  is given exactly, are extremals of the functional

$$M^\alpha [f, J] = N [f, J] + \alpha \Omega [f]$$

$$N [f, J] = \int_0^\infty \left\{ \eta \int_{v_0-\Delta_1}^{v_0+\Delta_2} K(v_0, v) v f(v) dv - J(v_0) \right\} dv_0$$

$$\Omega [f] = \int_0^\infty \left[ \left( \frac{df}{dv} \right)^2 + f^2 \right] dv$$

Solution (1.1) is assumed to be unique.

For the numerical solution of this variational problem we use a correspondingly modified method of local variations [11], and for the choice of the solution based on the parameter  $\alpha$  we use the method of [9].

As  $J(v_0)$ , we use the given intensities obtained on an MP apparatus, described in [5], for forechamber pressure 155 torr. As the molecular-beam source we use an argon jet, flowing from a sonic nozzle of radius 0.1 mm. The gas in the forechamber is at room temperature (293°K). The distance from the skimmer of the first aperture up to a section of the nozzle for which the interaction with the skimmer did not perturb the velocity distribution functions was selected based on the method proposed in [12]. The parameters of the selector were such that  $\varepsilon = 0.031$ .

The distribution function obtained, normalized to the maximum value, is shown in Fig. 2 (curve 1); along the axis of abscissas we plot a quantity equal to the ratio of the velocity to  $\sqrt{2RT}$ . Figure 3 illustrates the buildup velocity according to  $\alpha$  of the moments of the distribution function of the mean velocity  $u$  and the root-mean-square deviation (dispersion)  $2RT$ .

From the theorems proved in [6], in particular, it follows that to obtain  $f^\alpha(v)$  differing from solution (1.1) by no more than  $\varepsilon'$  the function  $J(v_0)$  must be given with corresponding accuracy, and, inversely, the specifying of  $J(v_0)$  with a certain accuracy does not enable us, for decreasing  $\alpha$ , to obtain  $f^\alpha(v)$  differing from the solution (1.1) by less than  $\varepsilon_0$ . It is thus natural to expect that the accuracy of the solution obtained will be worse than the accuracy of the experimental data. And although the exact dependence between them is not obtained, in trial calculations [13, 9] the accuracy of the solution is approximately 1.5-2 times worse than the accuracy of the initial data.

A widely used method of obtaining the distribution function is the method of searching for the solution of Eq. (1.1) in a definite class of functions with one or several unknown parameters [14, 15]. These

parameters are chosen so that the left side of (1.1) in a certain sense differs little from the measured value of  $J(v_0)$ . As is indicated in [10], this method makes sense if and only if the solution of the equation actually belongs to this class.

In studies on the determination of the distribution function in high-velocity molecular beams it is usual to assume that

$$f_n(v) \sim v^{2n} \exp[-(v-u)^2/2RT]$$

Here  $n$ ,  $u$ , and  $T$  are parameters.

Since the direct solution of Eq. (1.1) gives the possibility of finding the distribution function  $f(v)$  and, hence, also its moments  $u$  and  $2RT$ , we can, using the latter, examine how close the functions  $f_n(v)$  approximate the numerical solution of the equation of selection. The functions  $f_n(v)$ , normalized to the maximum value, for  $n = 0$  and  $n = 1$  are given in Fig. 2 (curves 2 and 3). A comparison shows that the molecular-velocity distribution function in the molecular beam is not Maxwellian.

#### LITERATURE CITED

1. H. U. Hostettler and R. B. Bernstein, "Improved slotted disk type velocity selector for molecular beams," *Rev. Sci. Instr.*, **31**, No. 8, 872-878 (1960).
2. J. E. Scott, H. S. Morton, J. A. Phipps, and J. F. Moonan, "Distribution-function measurement in rarefied gas flow through an orifice," in: *Rarefied Gas Dynamics (Adv. in Appl. Mech., Suppl. 3)*, Vol. 2, Academic Press (1960).
3. S. M. Trujillo, P. K. Rol, and E. W. Rothe, "Slotted-disk velocity selector of extended range," *Rev. Sci. Instr.*, **33**, No. 8 (1962).
4. É. P. Pavlov, "Multiple-ring mechanical selector," *Uch. Zap. TsAGI*, **1**, No. 5 (1970).
5. I. S. Borovkov, I. D. Vershinin, É. P. Pavlov, and V. M. Sankovich, "Determination of partial intensities of components of a molecular flow," *Zh. Prikl. Mekhan. i Tekh. Fiz.*, No. 5 (1968).
6. A. N. Tikhonov, "Solution of incorrectly formulated problems and method of regularization," *Dokl. Akad. Nauk SSSR*, **151**, No. 3 (1963).
7. M. M. Lavrent'ev, *Some Incorrect Problems in Mathematical Physics* [in Russian], Izd. SO Akad. Nauk SSSR, Novosibirsk (1962).
8. V. K. Ivanov, "Linear incorrectly formulated problems," *Dokl. Akad. Nauk SSSR*, **145**, No. 2 (1962).
9. A. N. Tikhonov, "Incorrectly formulated problems," in: *Calculation Methods and Programming*, No. 8 [in Russian], Izd. MGU, Moscow (1967).
10. A. N. Tikhonov, V. K. Ivanov, and M. M. Lavrent'ev, "Incorrectly formulated problems," in: *Partial Differential Equations* [in Russian], Nauka (1970).
11. F. L. Chernous'ko, "Method of local variations for numerical solution of variational problems," *Zh. Vychislit. Matem. i Matem. Fiz.*, **5**, No. 4 (1965).
12. J. B. Anderson, R. P. Andres, J. B. Fenn, and G. Maise, "Studies of low-density supersonic jets," in: *Rarefied Gas Dynamics (Adv. in Appl. Mech., Suppl. 3)*, Vol. 2, Academic Press (1966).
13. A. N. Tikhonov and V. B. Glasko, "Approximate solution of Fredholm integral equations of the first kind," *Zh. Vychislit. Matem. i Matem. Fiz.*, **4**, No. 3 (1964).
14. H. G. Nöller, "Approximate calculation of expansion of gas from nozzle into high vacuum," *J. Vacuum Sci. and Technol.*, **3**, No. 4 (1966).
15. J. A. Alcalay and E. L. Knuth, "Molecular-beam time-of-flight spectroscopy," *Rev. Sci. Instr.*, **40**, No. 3 (1969).