DETERMINATION OF THE VELOCITY DISTRIBUTION FUNCTION OF MOLECULES AND ITS MOMENTS FROM TIME-OF-FLIGHT MEASUREMENTS

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INTRODUCTION

Several methods are at present available for measuring the velocity distribution function of molecules in gas flows. These are the mechanical selection method [1], measurements using the Doppler contour of spectral lines excited by a beam of electrons [2], and measurements based on the time taken for the molecules to travel an assigned distance [3]. When using any of these methods the problem arises of interpreting the experimental data, which involves finding a relationship between the results of the measurements and the investigated velocity distribution of the molecules and is common for all the methods used, since in all versions the recorded signal is an integral of the convolution of the distribution investigated with a certain apparatus function. In this paper, using the example of time-of-flight measurements in a molecular beam, we consider two methods of determining gasdynamic parameters related to the moments of the distribution function: the method in which the distribution function is first established using statistical regularization and subsequent calculation of the moments and the method of direct reconstruction of the moments. In the first case the relation between the gasdynamic parameters and the moments of the distribution function are obtained for a distribution of arbitrary form, and in the second it is obtained solely for a Maxwell distribution.

1. Method of Measurement

A block diagram of the system used for time-of-flight measurements is shown in Fig. 1. A narrow packet of molecules is separated from a molecular beam formed by the skimmer 1, using a chopper 2. During the time of flight across the base L this packet becomes blurred in accordance with the velocity distribution function of the molecules. The signal U(t) recorded by the flight-type ionization detector 3 represents the change with time of the density of molecules in the pickup. To increase the signal/noise ratio the time-of-flight curves are stored and averaged in the electronic unit 4. The signal U(t) is the convolution of the distribution function of the molecules f(t) in time space with an apparatus function [4]

$$U(t) = \int f(\tau) A(t-\tau) d\tau + \xi(t), \qquad (1.1)$$

where ξ (t) is the measurement noise which is not eliminated completely by the storage process, and A(t) is the apparatus function of the system which takes into account the chopper function, the dynamic properties of the detector, and the apparatus function of the storage device. The transmission function of the chopper [4] depends on the relation between the effective radius of the molecular beam, the width of the chopper slit, and its speed of rotation.

Methods of processing the results of time-of-flight experiments in order to determine the gasdynamic parameters of the distribution function have been described in a number of papers: in [3], and later in [5], methods are described based on the assumption that the time-of-flight curves are distorted to only a negligible extent by the apparatus function of the chopper and that there is no measurement noise present; in [6] algebraic expressions are obtained between the moments of the recorded time-of-flight signal, the velocity distribution function of the molecules, and the apparatus function. Using a Maxwell distribution function the gasdynamic parameters of the distribution were determined. However, the statistical characteristics of the reconstructed

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TABLE 1

s	<v1>></v1>	$\langle E_1 \rangle$	(v2)	$\langle E_2 \rangle$
0	$\sqrt{\frac{8kT}{\pi m}}$	$\frac{3}{2}kT$	$\sqrt{\frac{2kT}{\pi m}}$	$\frac{1}{2}kT$
0,5	2,76 · w	$2,12 \cdot \frac{1}{2}kT$	1,45 <i>.</i> w	$0.71 \cdot \frac{1}{2}kT$
1	1,63 w	$1,62\cdot\frac{1}{2}kT$	1,11 <i>·w</i>	$0,77 \cdot \frac{1}{2}kT$
2	$1,22 \cdot w$	$1,22.\frac{1}{2}kT$	1,003 · w	$0,98 \cdot \frac{1}{2}kT$
3	1,11 · w	$1,11\cdot\frac{1}{2}kT$	1,00001 · w	$0,9998 \cdot \frac{1}{2}kT$
5	1,04 · w	$1,04\cdot\frac{1}{2}kT$	w+0(w)	$\frac{1}{2}kT + 0\left(\frac{1}{2}kT\right)$
10	1,01 · w	$1,01\cdot\frac{1}{2}kT$	w+0(w)	$\frac{1}{2}kT + 0\left(\frac{1}{2}kT\right)$
8	w	$\frac{1}{2}kT$	w	$\frac{1}{2}kT$

parameters were not considered. In [7], using the same assumptions as in [6], the effect of the transmission function of the chopper and the dynamic function of the detector and its electronic circuit on the time-of-flight signal was estimated, and it was shown that in practical experiments, neglect of apparatus broadening leads to errors when processing and analyzing the experimental results. In none of these papers were the apparatus functions of all the sections taken into account simultaneously nor was the signal reconstructed taking ξ (t) into account. One of the main drawbacks of the above methods is also the need to assume a Maxwell distribution.

In [8], using the Tikhonov method of regularization, the problem of reconstructing the distribution function from measurements using a mechanical selector was solved. The stochastic nature of the physical measurements was not taken into account, and estimates were not made of the errors involved in reconstructing the distribution function.

2. The Relation between the Measured Signal

and the Gasdynamic Parameters

The required function f(t) is proportional to the change in molecular density n(t) as a function of the time of flight t:

$$f(t) = cn(t), \tag{2.1}$$

where c is the apparatus constant. The density n(t) is related to the velocity distribution function F(v) by the expression [5]

$$n(t) = N_0 F(v)/t,$$
 (2.2)

where N_0 is the number of particles in a single packet defined by the chopper. Hence, the dependence of f(t)t on 1/t normalized to unity at the maximum is identical with the dependence of F(v) on v with a similar normalization.

We will write the velocity distribution function in arbitrary form taking into account the anisotropy in directions parallel and perpendicular to the motion of the gas:

$$F(v, \Theta) = c_1 c_2 f_{\parallel}(v, \Theta) f_{\perp}(v, \Theta) v^2, \qquad (2.3)$$

where Θ is the angle between the current lines and the direction to the detector, and c_1 and c_2 are normalization constants. For a Maxwell distribution with directional anisotropy Eq. (2.3) becomes

$$F(v, \Theta) = m/2\pi k T_{\perp} \cdot (m/2\pi k T_{\parallel})^{1/2} \exp\left[-m(v\sin\Theta)^2/2k T_{\perp}\right] \exp\left[-m(v\cos\Theta - w)^2/2k T_{\parallel}\right] v^2,$$

which is identical with the expression for $F(v, \Theta)$ given in [9]. Here k is Boltzmann's constant, m is the mass of the molecule, w is the hydrodynamic velocity, and T_{\parallel} and T_{\perp} are the parallel and perpendicular temperatures [10].

In the case when the detector is placed on the axis of the molecular beam and the solid angle within which the detector is seen from the skimmer is small, Eq. (2.3) can be represented in the simpler form

$$F(v) = c_3 v^2 f_{\parallel}(v), \tag{2.4}$$

where c_3 is a normalization constant, and $f_{\parallel}(v)$ in the case of a Maxwell distribution has the form

$$f_{\parallel}(v) = \exp[-m(v-w)^2/2kT_{\parallel}].$$

Substituting Eqs. (2.2) and (2.4) into Eq. (2.1), we obtain the relation between f(t) and F(v):

$$tf(t) = c_4 F(v) = c_3 c_4 v^3 f_{\parallel}(v), \tag{2.5}$$

where c_4 is a constant.

The information on the distribution function obtained from time-of-flight measurements can be conveniently represented in the form of averaged parameters: the hydrodynamic flow velocity w and the average thermal energy for a direction parallel to the flow E_{\parallel} (equal to $\frac{1}{2}kT_{\parallel}$ under equilibrium conditions). By definition [11], the average velocity and the average thermal energy of the gas have the forms

$$\langle v_{1} \rangle = \frac{\mu_{1} \{F(v)\}}{\mu_{0} \{F(v)\}} = \eta_{1} \{F(v)\} = \frac{\int_{0}^{v} vF(v) \, dv}{\int_{0}^{\infty} F(v) \, dv};$$
(2.6)

$$\langle E_1 \rangle = \frac{m}{2} \frac{\mu_2 \{F(v)\}}{\mu_0 \{F(v)\}} - \frac{m}{2} \Big[\frac{\mu_1 \{F(v)\}}{\mu_0 \{F(v)\}} \Big]^2 = \frac{m}{2} \nu_2 \{F(v)\} = \frac{m}{2} \frac{\int_0^\infty (v - w)^2 F(v) \, dv}{\int_0^\infty F(v) \, dv},$$
(2.7)

where μ_0 , μ_1 , μ_2 are the zero, first, and second unnormalized, and η_1 and ν_2 are the first and second normalized, central moments of the arbitrary distribution F(v). For a Maxwell distribution function, as a result of integrating Eqs. (2.6) and (2.7) we obtain

$$\langle v_{1} \rangle = w \left\{ 1 + 2 \left[2S^{2} + \frac{1 + \Phi(S)}{1 + \Phi(S) + (\pi)^{-1/2} S^{-1} e^{-S^{2}}} \right]^{-1} \right\};$$
(2.8)

$$\langle E_1 \rangle = \frac{m\gamma^2}{4} \left\{ 1 + \frac{1}{s^2 + \frac{1}{2} + (\pi)^{-1/2} s \, \mathrm{e}^{-S^2} \left[1 + \Phi \left(S \right) \right]^{-1}} \right\},\tag{2.9}$$

where $\gamma = \sqrt{2kT/m}$ is the most probable velocity of random motion, $S = w/\gamma$ is the velocity ratio, and $\Phi(S) = \frac{2}{\sqrt{\pi}} \int_{0}^{S} e^{-x^{2}} dx$ is the probability integral. (Here and henceforth we will omit the subscript on the tem-

perature and functions of it.) When there is no directional flow (w = S = 0) Eqs. (2.8) and (2.9) become

$$\langle v_{\mathbf{i}} \rangle = \sqrt{8kT/\pi m}; \langle E_{\mathbf{i}} \rangle = (3/2) kT$$

and represent the average velocity and the average energy of random motion of the molecules. In the other limiting case when $S \rightarrow \infty$ (T \rightarrow 0), we obtain from Eqs. (2.8) and (2.9)

$$\langle v_1 \rangle = w; \langle E_1 \rangle = (1/2)kT$$

i.e., the hydrodynamic flow speed and the energy of thermal motion.

Table 1 shows values of $\langle v_1 \rangle$ and $\langle E_1 \rangle$ for several values of the velocity ratio. As follows from the table, as S increases the parameters $\langle v_1 \rangle$ and $\langle E_1 \rangle$ approach their limiting values extremely slowly, and only for S > 10 is the error of the approximation $\langle v_1 \rangle = w$ and $\langle E_1 \rangle = \frac{1}{2} kT$ less than 1%.

Replacing the function F(V) by $f_{\parallel}(v)$ in Eqs. (2.6) and (2.7), we have

$$\langle v_{2} \rangle = \eta_{1} \{ f_{\parallel} (v) \} = \frac{\int_{0}^{\infty} v f_{\parallel} (v) dv}{\int_{0}^{\infty} f_{\parallel} (v) dv};$$
(2.10)

$$\langle E_2 \rangle = \frac{m}{2} v_2 \{ f_{\parallel}(v) \} = \frac{m}{2} \frac{\int\limits_0^\infty (v - w)^2 f_{\parallel}(v) \, dv}{\int\limits_0^\infty f_{\parallel}(v) \, dv}.$$
(2.11)

Integrating the new expressions, we obtain

$$\langle v_2 \rangle = w \{ 1 + (\pi)^{-1/2} S^{-1} e^{-S^2} [1 + \Phi(S)]^{-1} \}; \langle E_2 \rangle = \frac{m\gamma^2}{4} \{ 1 - 2(\pi)^{-1/2} S e^{-S^2} [1 + \Phi(S)]^{-1} \}.$$

Table 1 also shows the quantities $\langle v_2 \rangle$ and $\langle E_2 \rangle$ as a function of S. It should be noted that for $S \ge 2$ the quantities $\langle v_2 \rangle$ and $\langle E_2 \rangle$ can be approximated with small error by their limiting values w and $\frac{1}{2}kT$, respectively. Hence, in experiments in measuring the distribution function using the time-of-flight method for $S \ge 2$ for calculations of the gasdynamic parameters of the distribution of w and E_{\parallel} it is convenient to use Eqs. (2.10) and (2.11). Substituting $f_{\parallel}(v)$ from Eq. (2.5) into Eqs. (2.10) and (2.11), we obtain expressions for calculating the average parameters of a distribution function of arbitrary form from the results of time-of-flight experiments:

$$\langle v \rangle = \eta_1 \{ f_{\parallel}(v) \} = \frac{\int_0^\infty Lf(t) dt}{\int_0^\infty tf(t) dt};$$

$$\langle E \rangle = \frac{m}{2} v_2 \{ f_{\parallel}(v) \} = \frac{m}{2} \frac{\int_0^\infty \left(\frac{L}{t} - \langle v \rangle\right)^2 tf(t) dt}{\int_0^\infty tf(t) dt};$$

where L is the distance from the chopper to the detector.

3. Reconstruction of the Distribution Function

To solve the integral equation (1.1) we will use the procedure employed in [12, 13], which differs from other computational procedures employed to solve ill-posed problems.

First, the use of a discrete Fourier transform in this procedure enables one to construct a unique computational basis for obtaining a statistically regularized solution, enables one to choose the regularization parameter, and also enables one to estimate the error characteristics of the solution. This enables one to reduce the number of computational operations required to construct the regularized solution by 2-3 orders.

Second, consideration of the stochastic nature of the results of the measurements enables one to use mathematical statistics to choose the regularization parameter and to introduce statistical models of the solution errors. Thus, to obtain the regularization parameter which largely determines the success of regularization methods, we used a statistical criterion of optimality [13], on the basis of which we constructed an algorithm which calculates the optimum value (in the sense of the minimum mean-square reconstruction error) of the regularization parameter.

The regularized solution f_{α} , which is a P-dimensional vector, enables us to write

$$f_{\alpha} = f_{+} + \xi_{\alpha}, \qquad (3.1)$$

where f_+ is the solution vector of Eq. (1.1) when there is no measurement noise. The random vector ξ_{α} is interpreted as the solution noise, the vector of the mathematical expectation m_{ξ} and the correlation matrix $R_{\xi\xi}$ of which are calculated from the relations given in [13]. A knowledge of these statistical characteristics of the element ξ_{α} enables one not only to estimate the mean-square error of the solution and to construct confidence regions for the vector f_+ , but also enables one to calculate the errors of the integral characteristics determined from the vector f_{α} .

$$\mu_{k}^{*} = \sum_{j=1}^{P} f_{\alpha}(j) (j\Delta_{i})^{k} \omega_{j}, \qquad (3.2)$$

where Δ_t is the discreteness interval and ω_j are the coefficients of the quadrature formula, are random quantities and may differ considerably from the estimates μ_k , calculated from the vector f_+ :

$$\mu_{k} = \sum_{j=1}^{P} f_{+}(j) (j\Delta_{t})^{k} \omega_{j}.$$

Taking Eq. (3.1) into account, the mathematical expectation and the variance of the moments μ_0^* , μ_1^* , μ_2^* are given by the relations

$$\begin{split} M \left[\mu_{h}^{*} \right] &= \mu_{h} + \Delta \mu_{h}, \quad k = 0, 1, 2; \\ \Delta \mu_{h} &= \sum_{j=1}^{P} m_{\xi}(j) \left(j \Delta_{i} \right)^{h} \omega_{j}; \\ D \left[\mu_{h}^{*} \right] &= \sum_{i=1}^{P} \sum_{j=1}^{P} R_{\xi\xi}(i, j) \left(i \Delta_{i} \right)^{h} \left(j \Delta_{i} \right)^{h} \omega_{i} \omega_{j}. \end{split}$$
(3.3)

When the duration $T_f = P\Delta_t$ the distribution function f(t) is considerably less (by 1.5-2 orders of magnitude) than the correlation interval of the noise of the solution

$$\tau_{\xi} = \frac{\sum_{j=1}^{P} R_{\xi\xi}(1, j) \omega_{j}}{R_{\xi\xi}(1, 1)}$$

and we use the following simpler expression to calculate $D[\mu_k^*]$:

$$D\left[\mu_{k}^{*}\right] \simeq \frac{\tau_{\xi}T_{f}^{2k+1}}{2k+1}, \quad k=0,1,2.$$

The values of $D[\mu_k^*]$ obtained were used to determine the variance of the parameters $\langle v \rangle$ and $\langle E \rangle$ calculated in terms of the moments μ_0^* , μ_1^* , μ_2^* :

$$D\left[\langle \nu \rangle\right] \simeq \frac{D\left[\mu_1^*\right]}{(\mu_0^*)^2} + \frac{\langle \nu \rangle\right)^2}{(\mu_0^*)^2} D\left[\mu_0^*\right]; \ D\left[\langle E \rangle\right] \simeq \frac{D\left[\mu_2^*\right]}{(\mu_0^*)^2} + \frac{\langle \langle E \rangle\right)^2}{(\mu_0^*)^2} D\left[\mu_0^*\right].$$

To explain the degree of spread of the estimates of $\langle v \rangle$, $\langle E \rangle$ due to errors in solving Eq. (1.1) we constructed the confidence intervals

$$\begin{split} \Xi_v = [\langle v \rangle - \xi_v, \, \langle v \rangle + \xi_v]; \\ \Xi_E = [\langle E \rangle - \xi_E, \, \langle E \rangle + \xi_E], \end{split}$$

where

$$\xi_v = k(D[\langle v \rangle])^{1/2}; \ \xi_E = k(D[\langle E \rangle])^{1/4}, \ k = 2-3.$$

In processing the results of time-of-flight measurements with reconstruction of the distribution function we can distinguish the following stages:

A. The construction of a regularized solution f_{α} , calculation of the statistical characteristics of the vector ξ_{α} , and estimation of the uniform and Euclidean norms

$$\Delta_{1} = \max_{j} |f_{\alpha}(j) - f_{+}(j)|, \ j = 1, \ P,$$

$$\Delta_{2} = \left(\sum_{j=1}^{P} (f_{\alpha}(j) - f_{+}(j))^{2}\right)^{1/2}$$

of the errors of the solution, respectively.

B. Finding the moments μ_0^* , μ_1^* , μ_2^* with respect to the vector f_{α} (3.2) and calculating their statistical characteristics $M[\mu_k^*]$, $D[\mu_k^*]$.

C. Determination of the parameters $\langle v \rangle$, $\langle E \rangle$ and the construction of the confidence intervals Ξ_v , Ξ_E .



D. Calculation of the "standard" Maxwell function f_s of the distribution with parameters $\langle v \rangle$ and $\langle E \rangle$.

E. Determination of the quantities

$$\Delta_{1\mathbf{S}} = \max_{j} |f_{\mathbf{S}}(j) - f_{\alpha}(j)|;$$

$$\Delta_{2\mathbf{S}} = \left(\sum_{j=1}^{P} (f_{\mathfrak{d}}(j) - f_{\alpha}(j))^2\right)^{1/2},$$

which characterize the norms of the difference between f_{α} and f_{s} .

The last two stages are used when testing the hypothesis with regard to the reconstructed distribution function. Thus, if $\Delta_{1S} \leq \Delta_1$ and $\Delta_{2S} \leq \Delta_2$, the difference between f_{α} and f_S can be explained by the errors in solving the integral equation (1.1), and the hypothesis which states that the reconstructed function f_{α} belongs to the class of Maxwell distributions can be used.

4. The Method of Moments

In those cases when it is known that the velocity distribution of the molecules is Maxwellian one can use, to estimate the gasdynamic parameters, the simpler method of moments [6], which connects by algebraic relations the moments of the distribution function in time space f(t) with the moments of the measured signal U(t) and the apparatus function A(t). Using this method we developed algorithms for reconstructing the parameters of the distribution function (the average speed of directional motion $\langle v \rangle$ and the thermal energy $\langle E \rangle$) taking into account the chopper function and the dynamic function of the detector and its electronic circuit. Unlike [16], these algorithms include a determination of the statistical characteristics of the reconstructed parameters.

Using the relation between S and γ and the moments of the function f(t) [6], it can be shown that

$$D(S) = \left(\frac{\partial\Omega}{\partial S}\right)^{-2} \left[\frac{D(v_2\{f(t)\})}{(\eta_1\{f(t)\})^4} + \frac{4v_2\{f(t)\}}{(\eta_1\{f(t)\})^6} D(\eta_1\{f(t)\})\right];$$

$$D(\gamma) = \frac{L^2}{(\eta_1\{f(t)\})^2(S+r)^2} \left[\frac{D(S)}{(S+r)^3} + \frac{D(\eta_1\{f(t)\})}{(\eta_1\{f(t)\})^2}\right],$$
(4.1)

where $\mathbf{r} = (\pi^{1/2} e^{\mathbf{S}^2} (1 + \Phi(\mathbf{S})))^{-1}$; Ω is the time-of-flight [6]; $\eta_1 \{f(t)\} = \int_0^{\lambda} tf(t) dt \Big/ \int_0^{\lambda} f(t) dt$ is the first normalized moment; $\mathbf{v}_2 \{f(t)\} = \int_0^{\lambda} (t - \eta_1 \{f(t)\})^2 f(t) dt \Big/ \int_0^{\lambda} f(t) dt$ is the second normalized central moment; and $D(\eta_1 \{f(t)\})^2$ and

 $D(v_2 \{ f(t) \})$ are the variances of the moments of the function f(t) defined by the expressions

$$D(\eta_{1}\{f(t)\}) \simeq \frac{D(\mu_{1}\{U(t)\})}{(\mu_{0}\{U(t)\})^{2}} + \frac{(\mu_{1}\{U(t)\})^{2}}{(\mu_{0}\{U(t)\})^{4}} D(\mu_{0}\{U(t)\}) - \frac{\mu_{1}\{U(t)\}}{(\mu_{0}\{U(t)\})^{3}} \operatorname{cov}(\mu_{1}, \mu_{0});$$

$$D(\nu_{2}\{f(t)\}) \simeq \frac{D(\mu_{2}\{U(t)\})}{(\mu_{0}\{U(t)\})^{2}} + 4 \frac{(\mu_{1}\{U(t)\})^{2}}{(\mu_{0}\{U(t)\})^{4}} D(\mu_{1}\{U(t)\}) + \left(2 \frac{(\mu_{1}\{U(t)\})^{3}}{(\mu_{0}\{U(t)\})^{3}} - \frac{\mu_{2}\{U(t)\}}{(\mu_{0}\{U(t)\})^{2}}\right)^{2} D(\mu_{0}\{U(t)\}) + 2\left[-\frac{2\mu_{1}\{U(t)\}}{(\mu_{0}\{U(t)\})^{2}}\left(\frac{2(\mu_{1}\{U(t)\})^{2}}{(\mu_{0}\{U(t)\})^{3}} - \frac{\mu_{2}\{U(t)\}}{(\mu_{0}\{U(t)\})^{2}}\right)^{2} \operatorname{cov}(\mu_{1}, \mu_{0}) - 2 \frac{\mu_{1}\{U(t)\}}{(\mu_{0}\{U(t)\})^{3}} \operatorname{cov}(\mu_{1}, \mu_{2}) + \left(2 \frac{(\mu_{1}\{U(t)\})^{2}}{(\mu_{0}\{U(t)\})^{3}} - \frac{\mu_{2}\{U(t)\}}{(\mu_{0}\{U(t)\})^{2}}\right) \frac{1}{\mu_{0}\{U(t)\}} \operatorname{cov}(\mu_{0}, \mu_{2})\right],$$

$$(4.2)$$

where $D(\mu_i)$ is found from Eq. (3.3), when $R_{\xi\xi}(t_i, t_j)$ is the correlation matrix of a noise $\xi(t)$, and $cov(\mu_i, \mu_j)$ is the correlation between the moments μ_i and μ_j .



The variances of the parameters $\langle v \rangle$ and $\langle E \rangle$ are found from Eqs. (4.1) and (4.2):

$$D(\langle v \rangle) \simeq \gamma^2 D(S) + S^2 D(\gamma);$$

$$D(\langle E \rangle) \simeq (m\gamma^2/2)^2 D(\gamma).$$

The algorithms were realized in the form of subprograms in FORTRAN-IV.

It should be noted that the method of moments enables one to determine the hydrodynamic velocity and density of the molecular beam without assuming a Maxwell distribution.

In this paper we have described two different approaches to determining parameters from time-of-flight measurements. To compare these approaches both from the point of view of the accuracy of calculating the parameters and from the point of view of the computer time involved in processing the experimental results, we solved the following model problem. We took as the input signal f(t) a Maxwell distribution function with parameters S = 5 and $\gamma = 0.15 \cdot 10^5$ cm/sec. The transmission function A(t) was chosen in the form of a trapezium with a length of the lower base NH. A random process Z(t) simulating the noise of the measuring system with correlation function

$$R_{Z}(\tau) = \sigma^{2} \exp\left(--\beta|\tau|\right)$$

with zero mathematical expectation, where σ^2 is the variance of the noise, was imposed on the output signal U(t), which is the convolution of the functions f(t) and A(t).

To determine the level of noisiness of the output signal we introduced the parameter

 $\zeta = (||Z||/||U||) \cdot 100\%,$

where $||Z|| = \sqrt{\sum_{i=1}^{n} (Z_i)^2}$ and $||U|| = \sqrt{\sum_{i=1}^{n} (U_i)^2}$ are the root-mean-square norms.

Parameters S and γ were reconstructed for values of $\zeta = 2.8$, 10, and 18% for a transmission function A(t) with NH=10.14 for a constant duration NX=70 input signals. Correspondingly, the conditionality numbers P are defined by the relation

$$P = \|H'H\| \|(H'H)^{-1}\|$$

where H is a square matrix which approximates the integral operator (1.1); we took values of P=360, and 17,000.

Figure 2a, b shows the change in the relative errors of the reconstructed parameters $\delta(S)$ and $\delta(\gamma)$ as a function of ζ when using the method of statistical regularization (curves 1 and 3), and the method of moments (curves 2 and 4); the continuous lines are the curves for P=360 and the dashed lines are for P=17,000; it is seen that the errors in reconstructing the parameters by the method of moments are greater than the corresponding errors in calculating the same parameters from the reconstructed distribution function. These differences can be explained by the filtering properties of the regularizing algorithm. The computer time T_c required to calculate the desired quantities on the "Ural-14D" computer using the reconstruction of the distribution function function.

5. Example of Processing of the Experimental Results

Figure 3 shows an example of the reconstruction of the function f(t) from the experimental data. The argument is the time of flight of the molecules across the distance from the chopper to the detector t (sec). Curve 1 is the output signal of the measuring system U(t), and curve 2 is the regularized solution $f_{\alpha}(t)$ of the integral equation (1.1); both curves are normalized with respect to their maximum values. It is seen from Fig. 3 that $f_{\alpha}(t)$ is shifted toward lower values of t with a reduction in its half-width. The regularized function $f_{\alpha}(v)$ replotted on a velocity scale (the dashed line) is shown in Fig. 4. Here we have drawn the "standard" function $f_{s}(v)$ (the continuous curve) and we have also drawn the 95% confidence intervals for $f_{+}(v)$. The norms of the errors are as follows: $\Delta_1 = 0.095$, $\Delta_2 = 0.047$, $\Delta_{1S} = 0.068$, and $\Delta_{2S} = 0.021$.

It follows from the inequalities $\Delta_{1S} < \Delta_1$, $\Delta_{2S} < \Delta_2$ that the difference between $f_{\alpha}(v)$ and $f_{s}(v)$ may be due to errors in solving the integral equation (1.1) and the fact that the function $f_{\alpha}(v)$ is represented as being Maxwellian in the experiment. When processing the signal shown in Fig. 3 (curve 1) by the method of statistical regularization we obtained the estimates $S^*=3.8$ with confidence intervals from 3.4 to 4.2, and $\gamma^*=0.19 \cdot 10^5$ cm/sec with confidence intervals from 0.16 $\cdot 10^5$ to 0.22 $\cdot 10^5$ cm/sec. The method of moments gave results for $S^*=4.2$ and $\gamma^*=0.17 \cdot 10^5$ cm/sec with confidence intervals of 3.4-5.0 and 0.14 $\cdot 10^5$ -0.20 $\cdot 10^5$ cm/sec, respectively.

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