Journal of Engineering Physics and Thermophysics, Vol. 72, No. 2, 1999

DERIVATION AND NUMERICAL SOLUTION OF A SYSTEM OF EQUATIONS FOR THE SINGLE-POINT PROBABILITY DENSITY AND CONVENTIONAL RATE OF DISSIPATION OF TURBULENT PULSATIONS OF A SCALAR FIELD

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UDC 532.517.4

On the basis of the authors' earlier closed equation for the joint probability density function of pulsations of an isotropic turbulent scalar field and its gradient, we derived and solved numerically a system of equations for the single-point probability density and conventional rate of scalar dissipation (CRSD) of fluctuations of a passive scalar field. In closing the equation for the CRSD, the hypothesis that the effect of pulsations of this function on its evolution is of no consequence is adopted. The system includes equations for functions that describe the distribution of turbulent energy and the intensity of scalar pulsations over different length scales.

1. Introduction. The development of theoretical models of turbulent combustion requires rather thorough information about the statistical properties of the gradient of a scalar turbulent field. In [1] a closed equation was derived for the joint probability density function (JPDF) of a reactive scalar field and its gradient. Precisely this level of description of the statistics of the scalar-field gradient is needed to solve many problems of turbulent combustion [2]. However, solution of the equation obtained in [1] for the JPDF seems difficult at present because of the multidimensionality of this function. Therefore, in the present work we attempted to solve a simpler problem, namely, derivation and numerical solution of an equation for the CRSD. This function means the mean value of the rate of dissipation of the intensity of scalar fluctuations calculated at the point $(\vec{x}, t)$, provided that at this point the following value of the scalar-field fluctuation is realized:

$$c(\vec{x}, t) = \Gamma, \tag{1}$$

i.e., actually we deal with calculation of the rate of dissipation on the isoscalar surface defined by (1). The value of the conventional dissipation depends on the parameter Γ. We will denote this function by the symbol $\chi_{\vec{x}, t}(\Gamma)$. The CRSD is related to the JPDF of the scalar and its gradient by the formula

$$\chi_{\vec{x},t}(\Gamma) = D \int\int\int W^2 P_{\vec{x},t}(W, \Gamma)\, d\vec{W}/f_{\vec{x},t}(\Gamma). \tag{2}$$

Here D is the diffusion coefficient; $P_{\vec{x}, t}(W, \Gamma)$ is the joint probability density function of fluctuations of the scalar and its gradient; $f_{\vec{x}, t}(\Gamma)$ is the probability density of scalar-field fluctuations.

The need to study the CRSD is dictated by the demands of the development of various approaches to the problems of turbulent combustion. The flamelet approach to the description of turbulent reactive flows with combustion, which has been developed intensely in recent years [2-4], allows one to take account of the deviation from local chemical equilibrium and to separate effectively the description of the processes of chemical reaction from the description of turbulence. Flamelet models are based on the assumption that a turbulent flame consists of thin one-dimensional zones of reaction (flamelets), each being situated in a locally laminar surrounding. The

Academic Scientific Complex "A. V. Luikov Heat and Mass Transfer Institute of the National Academy of Sciences of Belarus," Minsk, Belarus. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 72, No. 2, pp. 275-288, March-April, 1999. Original article submitted January 22, 1998.

 1062-0125/99/7202-0254$22.00

equations within the framework of these models that describe the mass-mean fractions of the reagents and the mean temperature, as a function that carries information about the turbulence, contain the rate of dissipation of the passive scalar (the coefficient of the mixture), which is calculated on a stoichiometric surface, i.e., actually the CRSD function.

In [5, 6] a new approach to the problem of closing the equations that describe turbulent reactive flows is suggested; it is based on calculation of mean values that are due to the local instantaneous value of the coefficient of the mixture. This system contains the CRSD as an important characteristic of the turbulent scalar field.

At the present time the CRSD is used successfully to describe supersonic turbulent combustion [7]. On the basis of the flamelet concept effective methods for predicting ejections of nitrogen oxides have been developed [8]. As is known [9], the CRSD determines the evolution of the single-point of probability distribution density (PDD) of scalar fluctuations $f_{\vec{x}, t}(\Gamma)$. However, even now there is no generally accepted model for this function, which is widely used in the theory of turbulent reactive flows. What has just been said allows the conclusion that the CRSD is required in various approaches to the description of turbulent reactive flows.

An expression for the CRSD was obtained in [10, 11] using the method of a mapping function. In this approach the form of the function of the conventional rate of dissipation obtained in [10] and in at least one of the variants of [11] turned out to be independent of time. At the same time, the results of a calculation of the CRSD carried out on the basis of direct numerical simulation of a turbulent scalar field show that during the evolution of a mixing scalar field the form of this function undergoes substantial changes [12]. This is confirmed by an experimental study of the CRSD in various turbulent flows [13-15].

In [16] an explanation is suggested for the complicated transformation of the form of the CRSD using the assumption of characteristic modes of a turbulent scalar field that change during evolution. More important, however, is the problem of constructing a statistical model for the CRSD that is based on the use of averaged characteristics of turbulence.

We made an attempt to derive a closed system of equations to calculate the evolution of the CRSD during the mixing of a passive scalar field by an isotropic turbulent field of velocity on the basis of the equation that was obtained in [1] for the JPDF of the values of fluctuations of a scalar field and its gradient. The equation for the CRSD turns out to be associated with the single-point PDD of the magnitudes of fluctuations of the scalar $f_t(\Gamma)$. Therefore, for this function the well-known equation that also contains $\chi_t(\Gamma)$ is written [9, 11].

The equations for $\chi_t(\Gamma)$ and $f_t(\Gamma)$ together with auxiliary equations for the functions $P_t(r)$ and $P_t^{(c)}(r)$, which are required to calculate the coefficients in the equation for $\chi_t(\Gamma)$ and which describe the distribution of turbulent energy and the intensity of scalar fluctuations over different length scales, are solved numerically.

2. Derivation of the Equation for the CRSD from the Closed Equation for the JPDF $P_t(W, \Gamma)$. By definition, the CRSD is related to the JPDF of the scalar gradient and the scalar by formula (2). Since the integrand in (2) is scalar, the three-dimensional integral can be reduced to a one-dimensional one:

$$\int\int\int f(z)\, d\vec{z} = 4\pi \int_0^\infty f(z)\, z^2\, dz\,. \tag{3}$$

With account for this formula, expression (2) acquires the form

$$\chi_t(\Gamma) f_t(\Gamma) = 4\pi D \int_0^\infty W^4 P_t(W, \Gamma)\, dW\,. \tag{4}$$

In the case of a passive scalar field the equation for $P_t(W, \Gamma)$ is given by formula (117) from [1] without the last term, which describes the action of a chemical source. Multiplying the left- and right-hand sides of the equation for $P_t(W, \Gamma)$ by $4\pi D W^4$ and integrating over the variable W from 0 to ∞, we obtain

$$\frac{\partial}{\partial t} \int_0^\infty 4\pi D W^4 P_t(W, \Gamma)\, dW = -4\pi D^2 \int_0^\infty W^6 \frac{\partial^2}{\partial \Gamma^2} P_t(W, \Gamma)\, dW +$$

$$+ 4\pi D \int_0^\infty W^4 \sqrt{\left(\frac{\varepsilon(t)}{15\nu}\right)} \left(3 + W\frac{\partial}{\partial W}\right) \left[\frac{S_{UC}}{2}(t)\left\{1 - \frac{DW^2}{\chi(t)}\right\} P_t(W, \Gamma)\right] dW -$$

$$- 4\pi D^2 N_t(\Gamma) \int_0^\infty W^4 \left[\frac{2}{W}\frac{\partial}{\partial W} + \frac{\partial^2}{\partial W^2}\right] P_t(W, \Gamma)\, dW - 8\pi D^2 \frac{\partial}{\partial \Gamma} \times$$

$$\times \left[X_t(\Gamma) \int_0^\infty W^4 \left(3 + W\frac{\partial}{\partial W}\right) P_t(W, \Gamma)\, dW\right]. \tag{5}$$

In equality (5) the terms that describe the effect of the rate of chemical reaction are omitted, since the aim of the present work is restricted to the derivation of a closed equation for the conventional rate of dissipation of fluctuations of a passive scalar field. Let us write equality (5) in symbolic form:

$$\frac{\partial}{\partial t}(0) = (\mathrm{I}) + (\mathrm{II}) + (\mathrm{III}) + (\mathrm{IV}). \tag{6}$$

We transform each of the terms of equalities (5) and (6). Use of (4) gives the following relation:

$$(0) = 4\pi D \int_0^\infty W^4 P_t(W, \Gamma)\, dW = \chi_t(\Gamma) f_t(\Gamma). \tag{7}$$

For (I) we have

$$(\mathrm{I}) = - 4\pi D^2 \int_0^\infty W^6 \frac{\partial^2}{\partial \Gamma^2} P_t(W, \Gamma)\, dW = - \frac{\partial^2}{\partial \Gamma^2} 4\pi \int_0^\infty W^2 (DW)^2 P_t(W, \Gamma)\, dW. \tag{8}$$

We introduce the notation

$$4\pi \int_0^\infty W^2 (DW^2)^2 P_t(W, \Gamma)\, dW = \overline{\chi_t^2(\Gamma)} f_t(\Gamma). \tag{9}$$

As is seen from the definition, the function $\overline{\chi_t^2(\Gamma)}$ is the mean square of the conventional rate of scalar dissipation. With account for (9), the expression for (I) takes the form

$$(\mathrm{I}) = - \frac{\partial^2}{\partial \Gamma^2} \left[\overline{\chi_t^2(\Gamma)} f_t(\Gamma)\right]. \tag{10}$$

For (II) we obtain

$$(\mathrm{II}) = 4\pi D \sqrt{\left(\frac{\varepsilon(t)}{15\nu}\right)} \int_0^\infty W^4 \left(3 + W\frac{\partial}{\partial W}\right) \frac{S_{UC}(t)}{2} \left\{1 - \frac{DW^2}{\chi(t)}\right\} P_t(W, \Gamma)\, dW =$$

$$= \sqrt{\left(\frac{\varepsilon(t)}{15\nu}\right)} \frac{S_{UC}(t)}{2} \left[3 \cdot 4\pi D \int_0^\infty W^4 \left\{1 - \frac{DW^2}{\chi(t)}\right\} P_t(W, \Gamma)\, dW +\right.$$

$$\left. + 4\pi D \left\{W^5 \left\{1 - \frac{DW^2}{\chi(t)}\right\} P_t(W, \Gamma)\right|_{W=0}^{W=\infty} - 5 \cdot 4\pi D \int_0^\infty W^4 \left\{1 - \frac{DW^2}{\chi(t)}\right\} P_t(W, \Gamma)\, dW \right\}\right]. \tag{11}$$

The second term on the right-hand side of (11) is equal to zero, and therefore

$$(\mathrm{II}) = -S_{UC}(t)\sqrt{\left(\frac{\varepsilon(t)}{15\nu}\right)}\,4\pi D\int_0^\infty W^4\left(1-\frac{DW^2}{\chi(t)}\right)P_t(W,\Gamma)\,dW =$$

$$= -S_{UC}(t)\sqrt{\left(\frac{\varepsilon(t)}{15\nu}\right)}\left[\chi_t(\Gamma)-\frac{\overline{\chi_t^2(\Gamma)}}{\chi(t)}\right]f_t(\Gamma). \tag{12}$$

In writing (12), use was made of notation (9). The term (III) has the form

$$(\mathrm{III}) = -4\pi D^2 N_t(\Gamma)\int_0^\infty W^4\left[\frac{2}{W}\frac{\partial}{\partial W}+\frac{\partial^2}{\partial W^2}\right]P_t(W,\Gamma)\,dW =$$

$$= -4\pi D^2 N_t(\Gamma)\left\{2\left[W^3 P_t(W,\Gamma)\Big|_{W=0}^{W=\infty}-3\int_0^\infty W^2 P_t(W,\Gamma)\,dW\right]-\right.$$

$$\left.-\left[W^4\frac{\partial}{\partial W}P_t(W,\Gamma)\Big|_{W=0}^{W=\infty}-4\int_0^\infty W^3\frac{\partial}{\partial W}P_t(W,\Gamma)\,dW\right]\right\}. \tag{13}$$

The nonintegral terms in (13) are equal to zero, and therefore

$$(\mathrm{III}) = -4\pi D^2 N_t(\Gamma)\left\{-6\int_0^\infty W^2 P_t(W,\Gamma)\,dW-4\left[W^3 P_t(W,\Gamma)\Big|_{W=0}^{W=\infty}\right]+\right.$$

$$\left.+12\int_0^\infty W^2 P_t(W,\Gamma)\,dW\right\} = -6D^2 N_t(\Gamma)\,4\pi\int_0^\infty W^2 P_t(W|\Gamma)f_t(\Gamma)\,dW. \tag{14}$$

Account for the normalization condition $4\pi\int_0^\infty W^2 P_t(W/\Gamma)dW = 1$ brings (14) to the following form:

$$(\mathrm{III}) = -6D^2 N_t(\Gamma) f_t(\Gamma). \tag{15}$$

For the term (IV) we obtain

$$(\mathrm{IV}) = -8\pi D^2\frac{\partial}{\partial\Gamma}\left[X_t(\Gamma)\int_0^\infty W^4\left(3+W\frac{\partial}{\partial W}\right)P_t(W,\Gamma)\,dW\right] =$$

$$= -8\pi D^2\frac{\partial}{\partial\Gamma}\left[X_t(\Gamma)\left(3\int_0^\infty W^4 P_t(W,\Gamma)\,dW+W^5 P_t(W,\Gamma)\Big|_{W=0}^{W=\infty}-\right.\right.$$

$$\left.\left.-5\int_0^\infty W^4 P_t(W,\Gamma)\,dW\right)\right]. \tag{16}$$

The nonintegral term in (16) is equal to zero, and therefore

$$(\mathrm{IV}) = 4D\frac{\partial}{\partial\Gamma}\left[X_t(\Gamma)\left(4\pi D\int_0^\infty W^4 P_t(W,\Gamma)\,dW\right)\right]. \tag{17}$$

Using (4), we have

$$(\mathrm{IV}) = 4D\frac{\partial}{\partial\Gamma}\left[X_t(\Gamma)\chi_t(\Gamma)f_t(\Gamma)\right]. \tag{18}$$

Substituting the calculated expressions (0)-(IV) into (6), we obtain the equation

$$\frac{\partial}{\partial t}\left[\chi_t(\Gamma) f_t(\Gamma)\right] = -\frac{\partial^2}{\partial \Gamma^2}\left[\overline{\chi_t^2(\Gamma)} f_t(\Gamma)\right] - S_{UC}(t)\sqrt{\left(\frac{\varepsilon(t)}{15\nu}\right)} \times$$

$$\times\left[\chi_t(\Gamma) - \frac{\overline{\chi_t^2(\Gamma)}}{\chi(t)}\right] f_t(\Gamma) - 6D^2 N_t(\Gamma) f_t(\Gamma) + 4D\frac{\partial}{\partial \Gamma}\left[X_t(\Gamma)\chi_t(\Gamma) f_t(\Gamma)\right]. \quad (18)$$

As a hypothesis for simulating the unknown expression for the mean square of the CRSD $\overline{\chi_t^2(\Gamma)}$ we adopt the following:

$$\overline{\chi_t^2(\Gamma)} = \chi_t(\Gamma)\chi_t(\Gamma). \quad (20)$$

In writing a formula for $\overline{\chi_t^2(\Gamma)}$ in the form of (20), the effect of pulsations of the CRSD on the evolution of this function is assumed to be unimportant. For further transformation of (19), we shall avail ourselves of equalities (91) for $N_t(\Gamma)$ and (99) for $\chi_t(\Gamma)$ from [1]. As a result we obtain

$$\frac{\partial}{\partial t}\left[\chi_t(\Gamma) f_t(\Gamma)\right] = -\frac{\partial^2}{\partial \Gamma^2}\left[\chi_t^2(\Gamma) f_t(\Gamma)\right] -$$

$$-\sqrt{\left(\frac{\varepsilon(t)}{15\nu}\right)} S_{UC}(t)\left[1 - \frac{\chi_t(\Gamma)}{\chi(t)}\right]\chi_t(\Gamma) f_t(\Gamma) +$$

$$+ D_{CC}^{(IV)}(0, t) D^2 \tilde{N}_t(\Gamma) f_t(\Gamma) + 4D\frac{\partial}{\partial \Gamma}\left[K_t(\hat{\Gamma}) \exp\left(-\alpha(T)\hat{\Gamma}^2\right)\chi_t(\Gamma) f_t(\Gamma)\right]. \quad (21)$$

Here, in conformity with formulas (91), (92), (101), (105), (108), and (109) from [1]

$$\tilde{N}_t(\Gamma) = -\frac{6N_t(\Gamma)}{D_{CC}^{(IV)}(0, t)} = \left[5 - 3T^2(t)\left(1 - \frac{\hat{\Gamma}^2}{4}\right)\right]\exp\left\{-\alpha(t)\hat{\Gamma}^2\right\}; \quad (22)$$

$$T(t) = \frac{\sqrt{2}\chi(t)}{3D\sqrt{\left(\overline{c^2(t)}\right) D_{CC}^{(IV)}(0, t)}}, \quad \alpha(T) = \frac{27T^2(t)}{8\left[5 - 9T^2(t)\right]}; \quad (23)$$

$$K_t(\Gamma) = \frac{\chi(t)}{6D\sqrt{\left(\overline{c^2(t)}\right)}}\kappa(\hat{\Gamma}),$$

$$\kappa(\hat{\Gamma}) = N(n)(2n + 1)\left(\frac{\hat{\Gamma}}{N(n)}\right)^{\frac{2n-1}{2n+1}}\left[2n - (2n + 1)\left(\frac{\hat{\Gamma}}{N(n)}\right)^{\frac{2}{2n+1}}\right]; \quad (24)$$

$$N(n) = \frac{\sqrt{\pi}\,\Gamma(2n + 1)}{\Gamma(2n + 3/2)}, \quad (25)$$

where $\Gamma(x)$ is the gamma function, $\hat{\Gamma} = \Gamma/\sqrt{\overline{c^2(t)}}$.

3. An Equation for the Single-Point Probability Distribution Density of Values of the Scalar. Equation (21) contains the single-point probability distribution density function (PDDF) $f_t(\Gamma)$. For this function, we can write an

equation in a form that contains $\chi_t(\Gamma)$ on the right-hand side as an unknown function. It is obtained from the equation for the JPDF $P_t(W, \Gamma)$ using the formula

$$f_t(\Gamma) = 4\pi \int_0^\infty W^2 P_t(W, \Gamma)\, dW. \tag{26}$$

Multiplying by $4\pi W^2$ the left- and right-hand sides of the equation for $P_t(W, \Gamma)$ with discarded chemical source terms (see (117) in [1]) and integrating over W from 0 to ∞, we can arrive at the following form of the equation for $f_t(\Gamma)$:

$$\frac{\partial}{\partial t} f_t(\Gamma) = -\frac{\partial^2}{\partial \Gamma^2}\left[\chi_t(\Gamma) f_t(\Gamma)\right]. \tag{27}$$

Equation (27) must be solved together with Eq. (21) for $\chi_t(\Gamma)$. In this system the external parameters are: the kinematic coefficient of diffusion of the scalar D; the kinematic coefficient of viscosity ν; the asymmetry of the joint probability density function of the values of the velocity gradient and the scalar gradient $S_{UC}(t)$; the fourth derivative of the structural two-point function of the difference between the concentrations at two points of the isotropic turbulent flow with respect to distance at the zero value of this distance $D_{CC}^{(IV)}(0, t)$; the mean rate of dissipation of the energy of the turbulent velocity field $\varepsilon(t)$; the mean rate of dissipation of the intensity of scalar fluctuations $\chi(t)$; the square of the dispersion of the scalar field $\overline{c^2}(t)$.

All the external parameters must be assigned. The evolution of the functions $D_{CC}^{(IV)}(0, t)$, $\varepsilon(t)$, $\chi(t)$, and $\overline{c^2}(t)$ is associated with the evolution of the functions $P_t(r)$ and $P_t^{(c)}(r)$, which are the distribution of turbulent energy and the intensity of scalar fluctuations over different length scales (see (127)-(131) in [1]), and the evolution of the function $S_{UC}(t)$ is associated with the evolution of the functions $D_{LCC}''(0, t)$, $\varepsilon(t)$, $\chi(t)$ (see (56) in [1]). To calculate the functions $P_t(r)$ and $P_t^{(c)}(r)$, we will avail ourselves of the closed system of equations (122)-(123) from [1]. Since the evolution of only a passive scalar field is studied, the last term in the equation for $P_t^{(c)}(r)$, which characterizes the influence of chemical reaction on the structure of this function, is not taken into account.

4. The System of Equations in Dimensionless Form. We define dimensionless variables by the following formula:

$$A = \bar{A} A_C, \tag{28}$$

where A_C is the characteristic value of the variable A. We select the following characteristic values: $C_C = |C_{max}|$, the magnitude of the concentration equal to its maximum value; L_C, the length scale; $f_C = 1/C_C$, the value of the single-point PDD; $q_C = \sqrt{q^2(0)}$, the magnitude of the velocity pulsation equal to the initial value of the root-mean-square velocity pulsation; $t_C = L_C/q_C$, the time equal to the time of one revolution of an energy-containing vortex; $\chi_C = C_C^2/t_C$, the magnitude of the scalar dissipation; $\varepsilon_C = q_C^2/t_C$, the magnitude of the rate of dissipation of the turbulent velocity field; $P_C^{(c)} = C_C^2/L_C$, the magnitude of the function $P_t^{(c)}(r)$; $P_C = q_C^2/L_C$, the magnitude of the function $P_t(r)$; $(D_{LCC})_C = q_C C_C^2$, the magnitude of the function $D_{LCC}(r, t)$; $\mathrm{Pe} = q_C L_C/D$, the Peclet number; $\mathrm{Re} = q_C L_C/\nu$, the Reynolds number; $\mathrm{Sc} = \nu/D$, the Schmidt number.

The form of Eq. (27) for $f_t(\Gamma)$ does not change in dimensionless variables. Equations (127)-(131) from [1], which connect auxiliary functions with the functions $P_t(r)$ and $P_t^{(c)}(r)$, in dimensionless form are

$$D_{LCC}(r, t) = \frac{2}{5} r^3 \chi(t) + \frac{4}{\mathrm{Pe}} P_t^{(c)}(r) - \frac{2}{r^2} \frac{\partial}{\partial t} \int_0^r \tilde{r}^2 \int_0^{\tilde{r}} P_t^{(c)}(r')\, dr',$$

$$D_{CC}^{(IV)}(0, t) = 2P_t^{(c)'''}(0), \quad \varepsilon(t) = \frac{15}{\mathrm{Re}} P_t'(0); \tag{29}$$

$$\chi(t) = \frac{3}{\mathrm{Pe}} P_t^{(c)'}(0), \quad \overline{c^2(t)} = \int_0^\infty P_t^{(c)}(\rho)\, d\rho. \tag{30}$$

Using these formulas, it is possible to write Eq. (21) in dimensionless form. Omitting the bars over the dimensionless variables, we obtain

$$\frac{\partial}{\partial t}\left[\chi_t(\Gamma) f_t(\Gamma)\right] = -\frac{\partial^2}{\partial \Gamma^2}\left[\chi_t^2(\Gamma) f_t(\Gamma)\right] - \sqrt{\left(P_t'(0)\right)}\, S_{UC}(t) \times$$

$$\times \left[1 - \frac{\mathrm{Pe}\,\chi_t(\Gamma)}{3P_t^{(c)'}(0)}\right] \chi_t(\Gamma) f_t(\Gamma) + \frac{2P_t^{(c)'''}(0)}{[\mathrm{Re\,Sc}]^2} \widetilde{N}_t(\hat{\Gamma}) f_t(\Gamma) +$$

$$+ \frac{2P_t^{(c)'}(0)}{\mathrm{Re\,Sc}\left[\int_0^\infty P_t^{(c)}(\rho)\, d\rho\right]^{1/2}} \frac{\partial}{\partial \Gamma}\left[\kappa(\hat{\Gamma}) \exp\left\{-\alpha(T)\hat{\Gamma}^2\right\} \chi_t(\Gamma) f_t(\Gamma)\right]. \tag{31}$$

Here the functions $\widetilde{N}_t(\hat{\Gamma})$ and $\kappa(\hat{\Gamma})$ are defined by Eqs. (22) and (24), and the expression for $T(t)$ in dimensionless variables is represented as

$$T(t) = \frac{P_t^{(c)'}(0)}{\sqrt{\left(\int_0^\infty P_t^{(c)}(\rho)\, d\rho\right)} \sqrt{\left(-P_t^{(c)'''}(0)\right)}}. \tag{32}$$

The functions $P_t(\rho)$ and $P_t^{(c)}(\rho)$ can be obtained by solving a coupled system of equations (see (122)-(123) in [1]) that in dimensionless form is

$$\frac{\partial P_t(\rho)}{\partial t} = \frac{\partial}{\partial \rho}\left[\frac{2}{\mathrm{Re}} + 2\gamma \int_0^\rho \sqrt{\left(\tilde{\rho} P_t(\tilde{\rho})\right)}\, d\tilde{\rho}\right]\left(\frac{\partial}{\partial \rho} + \frac{4}{\rho}\right) P_t(\rho), \tag{33}$$

$$\frac{\partial P_t^{(c)}(\rho)}{\partial t} = \frac{\partial}{\partial \rho}\left[\frac{2}{\mathrm{Pe}} + 2\beta \int_0^\rho \sqrt{\left(\tilde{\rho} P_t(\tilde{\rho})\right)}\, d\tilde{\rho}\right]\left(\frac{\partial}{\partial \rho} + \frac{2}{\rho}\right) P_t^{(c)}(\rho). \tag{34}$$

Here $\gamma = 0.24$ and $\beta = 1.08$ are experimental constants.

The system of equations (27), (31), (33), and (34) can be solved under the following boundary and initial conditions:

$$\chi_t(\Gamma)|_{t=0} = \chi_0(\Gamma) = 2\Theta\,1 - |\Gamma|)\,\chi(0)\,(1-\Gamma^2), \quad \chi(0) = \frac{3}{\mathrm{Pe}} P_t^{(c)}(0)|_{t=0} = \frac{6}{\mathrm{Pe}}; \tag{35}$$

$$f_t(\Gamma)|_{t=0} = f_0(\Gamma) = \frac{\Theta(1-|\Gamma|)}{\pi\sqrt{1-\Gamma^2}}, \quad f_t(\Gamma)|_{|\Gamma|=1} = 0; \tag{36}$$

$$P_t(\rho)|_{t=0} = P_0(\rho) = 2\rho \exp(-\rho^2), \quad P_t(0) = 0,$$
$$P_t(\infty) = 0, \quad P_t(\rho) > 0 \quad \text{for} \quad 0 < \rho < \infty; \tag{37}$$

$$P_t^{(c)}(\rho)|_{t=0} = P_0^{(c)}(\rho) = 2\rho \exp(-\rho^2), \quad P_t^{(c)}(0) = 0,$$
$$P_t^{(c)}(\infty) = 0, \quad P_t^{(c)}(\rho) > 0 \quad \text{for} \quad 0 < \rho < \infty. \tag{38}$$

It is convenient to rewrite the system of equations (27), (31) for the functions $\chi_t(\Gamma)$ and $F_t(\Gamma)$, where $F_t(\Gamma) = \int_0^\Gamma f_t(\tilde{\Gamma})\,d\tilde{\Gamma}$ is defined as an integral distribution function. Simple transformation of Eqs. (27), (31) leads to the following system of equations for $\chi_t(\Gamma)$ and $F_t(\Gamma)$:

$$\frac{\partial \chi_t(\Gamma)}{\partial t} = A(t)\chi_t(\Gamma) - B(t)\chi_t^2(\Gamma) - C(t)N_t(\Gamma) - \chi_t(\Gamma)\frac{\partial^2 \chi_t(\Gamma)}{\partial \Gamma^2} +$$
$$+ \left[\frac{\partial F_t(\Gamma)}{\partial \Gamma}\right]^{-1}\left[2\frac{\partial \chi_t(\Gamma)}{\partial \Gamma}\frac{\partial F_t(\Gamma)}{\partial t} + D(t)\frac{\partial}{\partial \Gamma}\left(\kappa(\hat{\Gamma})\exp\left\{-\alpha(T)\hat{\Gamma}^2\right\}\chi_t(\Gamma)\frac{\partial F_t(\Gamma)}{\partial \Gamma}\right)\right], \tag{39}$$

$$\frac{\partial F_t(\Gamma)}{\partial t} = -\frac{\partial}{\partial \Gamma}\left[\chi_t(\Gamma)\frac{\partial}{\partial \Gamma}F_t(\Gamma)\right], \tag{40}$$

where $A(t) = -S_{UC}(t)\sqrt{P_t(0)}$; $B(t) = -S_{UC}(t)\sqrt{P_t(0)}/\chi(t)$; $C(t) = 2|P_t^{(c)''}(0)|/[\mathrm{ReSc}]^2$; $D(t) = \frac{2\chi(t)}{3\sqrt{c^2}}$.

5. Numerical Solution of the System of Equations for the CRSD and the Single-Point Probability Density Function. Taking into account the symmetry of the function $\chi_t(\Gamma)$ and the asymmetry of the function $F_t(\Gamma)$ with respect to the coordinate origin, we will consider half their domain of definition, $0 \le \Gamma \le 1$. The CRSD and the single-point distribution density function are specified by system of equations (39)-(40) with the boundary conditions

$$\left.\frac{\partial \chi_t(\Gamma)}{\partial \Gamma}\right|_{\Gamma=0} = 0, \quad \chi_t(\Gamma)|_{\Gamma=1} = 0; \quad F_t(\Gamma)|_{\Gamma=0} = 0, \quad F_t(\Gamma)|_{\Gamma=1} = 1/2.$$

The selected system of variables $\chi_t(\Gamma)$ and $F_t(\Gamma)$ is more convenient for numerical solution than the variables $\chi_t(\Gamma)f_t(\Gamma)$ and $f_t(\Gamma)$, since the first two functions are smoother. To solve this problem, it is necessary to know the functions of time $A(t)$, $B(t)$, $C(t)$, $D(t)$, $\tilde{N}_t(\Gamma)$, $\kappa_t(\Gamma)$, $\alpha(t)$, and $T(t)$. They are all defined in terms of the functions $P_t(\rho)$ and $P_t^{(c)}(\rho)$, for whose determination Eqs. (33) and (34) are given.

The boundary conditions for the integral distribution function are specified by the conditions of its normalization. The dispersion $c^2(t)$ and the mean rate of dissipation of scalar fluctuations $\chi(t)$, which are calculated from the function $P_t^{(c)}(\rho)$ by Eq. (30), can be calculated also as internal parameters of the problem by the formulas

$$\overline{c^2(t)} = 2\int_0^1 \Gamma^2 f_t(\Gamma)\,d\Gamma, \quad \chi(t) = \int_0^1 \chi_t(\Gamma) f_t(\Gamma)\,d\Gamma. \tag{41}$$

The procedure for numerical solution of the boundary-value problem for the functions $\chi_t(\Gamma)$ and $F_t(\Gamma)$ is complicated by the presence of the terms $-\frac{\partial}{\partial \Gamma}\left[\chi_t(\Gamma)\frac{\partial F_t(\Gamma)}{\partial \Gamma}\right]$, $-\chi_t(\Gamma)\frac{\partial^2 \chi_t(\Gamma)}{\partial \Gamma^2}$, which formally look like terms with negative diffusion in the phase space of values of the scalar. This structure of the equations compels one to carry out the numerical calculation in the opposite direction in time. In the attempt to integrate the system of equations for $\chi_t(\Gamma)$ and $F_t(\Gamma)$ in the positive direction the numerical procedure turns out to be unstable, and the solution can be obtained only in a small interval of time ($\Delta t < 0.1$). Therefore all the results were obtained in numerical solution in the opposite direction in time from the "starting" distribution for the functions $\chi_t(\Gamma)$ and $F_t(\Gamma)$ to the initial one.

Here the method of straight lines was used in the form of a standard numerical procedure; as is known, this method reduces the solution of partial differential equations to a system of ordinary differential equations written for grid functions. The convenience of using this method for the given problem consists in the fact that the magnitude of the time step is automatically adapted within the numerical procedure, which makes it possible to cope with the problems of stability in domains of calculation in which the solution is close to singular, and, moreover, the integrals in auxiliary conditions (41) are found noniteratively at the next step.

The presence of "antidiffusion" terms makes the problem for Eqs. (30), (40) similar to classical inverse problems. There is an extensive literature devoted to the theory of solving inverse problems [17-20]. However, there are few felicitous examples of numerical calculation of inverse evolutional (or retrospective) problems for rather large time intervals without the existence of a critical dependence on a regularization parameter, which, incidentally, often cannot be selected small enough not to change the solution itself.

It is important to understand why Eqs. (39), (40) exhibit in "forward" solution the properties of an inverse problem, just like, by the way, all similar formulations based on the use of Eq. (27). Actually, we recover information about the evolution of the PDDF using as a basis certain model coefficients (functions of time) in Eq. (39). These lumped parameters result from many factors, including, of course, the distribution function itself. In our case the coefficients $A(t)$, $C(t)$, and $D(t)$ depend on $P_t^{(c)'}(0)$, $\overline{c^2(t)}$, and $P_t^{(c)'''}(0)$ and, by virtue of equalities (30) and (41), on the distributions $f_t(\Gamma)$ and $\chi_t(\Gamma)$. Thus, the "forward" solution of Eqs. (39), (40) is the problem of reconstructing the form of the evolution of the PDDF from its effects.

The solution of inverse problems by the method of "backward" computation is acceptable only when: a) the starting distribution is known; b) a definite form of the initial distribution is not given. Fortunately, in our case there is ample basis for the functions $\chi_t(\Gamma)$ and $F_t(\Gamma)$ to be indicated at the end of the process of mixing.

The selection of an analytical form for the "starting" values of the functions $\chi_t(\Gamma)$ and $F_t(\Gamma)$ was based on the following considerations. The single-point distribution function $f_t(\Gamma)$ has a Gaussian form at the end of the process of mixing. As is known, the approach of the single-point PDDF to a Gaussian form is associated with the fact that the CRSD becomes independent of the magnitude of the scalar [10]. Using this fact, it is possible to select a Gaussian form for the single-point PDDF and a form of the CRSD that is independent of the scalar-field magnitude as "starting" functions for the computation. Functions that satisfy these requirements are approximated by the following parametric dependences (starting values are denoted by the subscript s):

$$F_s(\Gamma) = \frac{\beta}{\alpha} \arctan \frac{\Gamma}{\alpha}, \quad \chi_t(\Gamma) = \frac{\chi(t_s)}{\pi} \arctan \frac{1-\Gamma}{\gamma}. \tag{42}$$

The parameters α and β control the form of the distribution; moreover, the first must satisfy the boundary condition $F_t|_{\Gamma=1} = 1/2$, which leads to the transcendental equation $\arctan(1/\alpha) - \alpha/(2\beta) = 0$, and the second is selected from the given value of the scalar dispersion c_s^2 with account for the fact that $\beta = (c_s^2 + \alpha^2)/2$. The small parameter γ ($\gamma = 0.01-0.001$) in the starting distribution for the CRSD controls the degree of rounding-off of the stepwise distribution. Here the magnitudes of the dispersion c_s^2 and the rate of dissipation $\chi(t_s)$ were found below by solving the direct problem ("forward") for the function $P_t^{(c)}$. For given c_s^2 and $\chi(t_s)$ relations (42) determine only the known form of the distributions.

6. Numerical Solution of the Problem for the Distributions over Length Scales. The equations that describe the evolution of the distributions of the kinetic energy of turbulence $P_t(\rho)$ and the intensity of scalar fluctuations $P_t^{(c)}(\rho)$ over the length scales r (33), (34) with initial and boundary conditions (37), (38) are solved by means of a Newton-type linearization procedure using an algorithm of matrix fitting for solving linear problems. These problems are well posed and are solved "forward," i.e., in the normal direction of time. The two problems are similar, and therefore we will describe only the procedure for solving one of them for $P_t^{(c)}(\rho)$. First, we reduce Eq. (34) to a system of first-order equations. It is integrated once with respect to ρ. As a result, we obtain an equation for the integral distribution function $S_t^{(c)} = \int_0^\rho P_t^{(c)} d\rho$:

$$\frac{\partial S_t^{(c)}}{\partial t} = F_t^{(c)} \left(\frac{\partial P_t^{(c)}}{\partial \rho} + \frac{2}{\rho} P_t^{(c)} \right) - \frac{6}{\mathrm{Pe}_0} \frac{\partial P_t^{(c)}}{\partial \rho} \Bigg|_{\rho=0}, \tag{43}$$

where $F_t^{(c)} = 2/\mathrm{Pe} + 2\beta \int_0^\rho \sqrt{\rho P_t} d\rho$. The squared dispersion of the scalar $\overline{c^2}$ is expressed in terms of the integral distribution function as $\overline{c^2} = \int_0^\infty P_t^{(c)} d\rho = S_t^{(c)}|_{\rho=\infty}$. Integrating (34) with an infinite upper limit, we obtain an equation for $\overline{c^2}$:

$$\frac{d\overline{c^2}}{dt} = -\frac{6}{\mathrm{Pe}_0} \frac{\partial P_t^{(c)}}{\partial \rho} \Bigg|_{\rho=0}$$

The equation for the normalized integral distribution $S^{(c)} = S_t^{(c)}/\overline{c^2}$ has the form

$$\mathrm{Pe}_0 \frac{\partial S^{(c)}}{\partial t} = F_t^{(c)} \mathrm{Pe}_0 \left(\frac{\partial P_t^{(c)}}{\partial \rho} + \frac{2P_t^{(c)}}{\rho} \right) - 6 \frac{\partial P_t^{(c)}}{\partial \rho} \Bigg|_{\rho=0} (1 - S^{(c)}).$$

Introducing the variable $\varphi^{(c)} = P_t^{(c)} / \left(\rho \frac{\partial P_t^{(c)}}{\partial \rho}|_{\rho=0} \right)$, we write a boundary-value problem for the functions $\varphi^{(c)}(t, \rho)$, $S^{(c)}(t, \rho)$, $F^{(c)}(t, \rho) = F_t^{(c)}\mathrm{Pe}$, and $f_0^{(c)}(t) = \frac{\partial P_t^{(c)}}{\partial \rho}|_{\rho=0}$:

$$F^{(c)} \left(\frac{\partial (\rho \varphi^{(c)})}{\partial \rho} + 2\varphi^{(c)} \right) - 6(1 - S^{(c)}) - \frac{\mathrm{Pe}}{f_0^{(c)}} \frac{\partial S^{(c)}}{\partial t} = 0,$$

$$\frac{\partial F^{(c)}}{\partial \rho} = 2\beta \, \mathrm{Pe} \, \rho \sqrt{f_0 \varphi q_t}, \quad \frac{\partial S^{(c)}}{\partial \rho} = \rho \varphi^{(c)} f_0^{(c)}, \quad \frac{d\overline{c^2}}{dt} = -6 \frac{f_0^{(c)}}{\mathrm{Pe}} \overline{c^2},$$

$$\varphi^{(c)}|_{\rho=0} = 1, \quad F^{(c)}|_{\rho=0} = 2, \quad S^{(c)}|_{\rho=0} = 0, \quad S^{(c)}|_{\rho=\infty} = 1. \tag{44}$$

Here the functions $f_0 = (\partial P/\partial \rho)|_{\rho=0}$ and $\varphi = P/\left(\rho \frac{\partial P}{\partial \rho}\right)$, where $P = P_t / \int_0^\infty P_t d\rho$, are determined from a similar problem, solved preliminarily, for the distribution of the kinetic energy over the length scales $P_t(\rho)$.

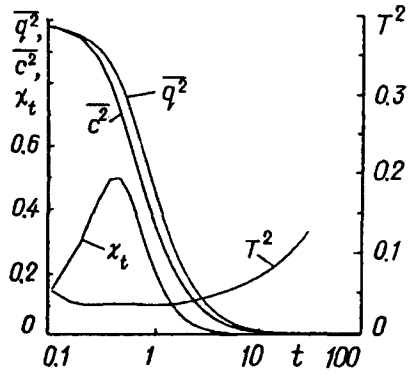
The meaning of the introduction of the function $\varphi^{(c)}$ consists in the fact that in contrast to $P^{(c)}$ it is monotonic over the entire range of values of ρ and smoother, which facilitates numerical solution of the system of equations. The quantity $P_{31}^{(c)} = \frac{\partial^3 P^{(c)}}{\partial \rho^3}|_{\rho=0} \Big/ \frac{\partial P^{(c)}}{\partial \rho}|_{\rho=0}$ is found by solving problem (44) as

$$P_{31}^{(c)} = 3\varphi^{(c)'}|_{\rho=0}. \tag{45}$$

The rate of dissipation of fluctuations of the scalar χ is related to the quantity $f_0^{(c)}$ as

$$\chi = \frac{3}{\mathrm{Pe}} \frac{\partial P^{(c)}}{\partial \rho} \Bigg|_{\rho=0} = \frac{3}{\mathrm{Pe}} f_0^{(c)}. \tag{46}$$

The formulated problem (44) and a similar hydrodynamic problem were approximated according to purely implicit schemes in time. The boundary-value problems in ρ were solved at each time step. Usually, two-three



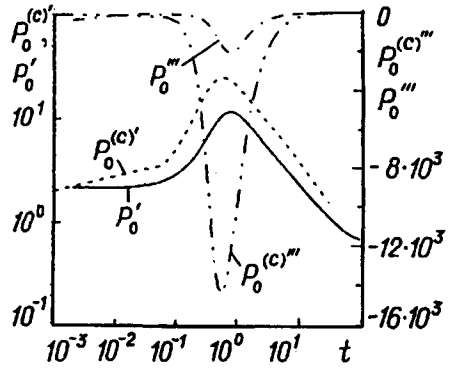


Fig. 1. Results of calculation of the system of equations (33)-(34): on the left, the evolution of the kinetic energy of turbulence q^2, the intensity of fluctuations of the scalar c^2, and the rate of dissipation of the scalar χ_t; on the right, the evolution of the correlator $T^2(t)$.

Fig. 2. Results of calculation of the system of equations (33)-(34): on the left, the evolution of the functions $P_0'(t)$, $P_0^{(c)'}(t)$; on the right, of the functions $P_0'''(t)$ and $P_0^{(c)'''}(t)$.

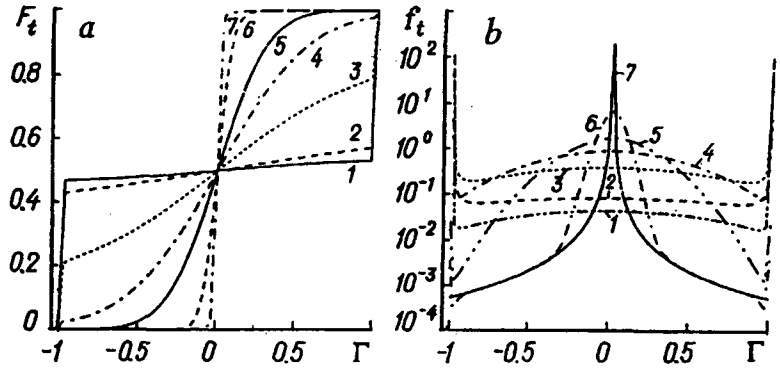


Fig. 3. Results of solution of the system of equations (39)-(40). The change in the form of the integral distribution function (a) and the probability distribution density function (b): 1) $t = 0$, 2) 0.2, 3) 1, 4) 2.5, 5) 5, 6) 15, 7) 25.

iterations of Newton's method are required at each step. The algebraic problem for the grid equations was solved by the matrix-sweep method [21, 22].

Over the segment of dimensionless time (0, 30) the initial kinetic energy of turbulence and the energy of fluctuations of the scalar field decreased by about three orders of magnitude. Here the maximum possible step of integration over t was of the order of 10^{-3} at $t = 0$ and of the order of 0.2 at $t = 30$.

7. Results of Numerical Solution of the System of Equations for the CRSD and the PDDF. The evolution of the kinetic energy $q^2(t)$ calculated from the distribution $P_t(\varphi)$ is shown in Fig. 1 (the problem for $P_t(\varphi)$ is similar in form to (44)). According to this figure, strong dissipation of energy begins at the instant $t = 0.5$. As is known, the dimensionless time $t = 1$ corresponds to one revolution of an energy-containing vortex. The dissipation of the intensity of scalar fluctuations, calculated by means of $P_t^{(c)}$, is also presented in Fig. 1. The intensity of scalar fluctuations decreases more rapidly than $q^2(t)$. This is explained in the main by the fact that the constant β in the equation for $P_t(\varphi)$ is smaller ($\beta = 0.24$) than the constant γ in the equation for $P_t^{(c)}(\varphi)$ ($\gamma = 1.08$). Dissipation of $c^2(t)$ begins when $t \sim 0.5$. At this instant the mean dissipation of scalar fluctuations $\overline{\chi_t}$, associated with the function $P_t^{(c)'}(0)$, attains a maximum. Later the dissipation rate decreases gradually. The behavior of the function $\overline{\chi_t}$ is determined by the initial splitting of turbulent vortices and their subsequent dissipation. Figure 1 also shows the

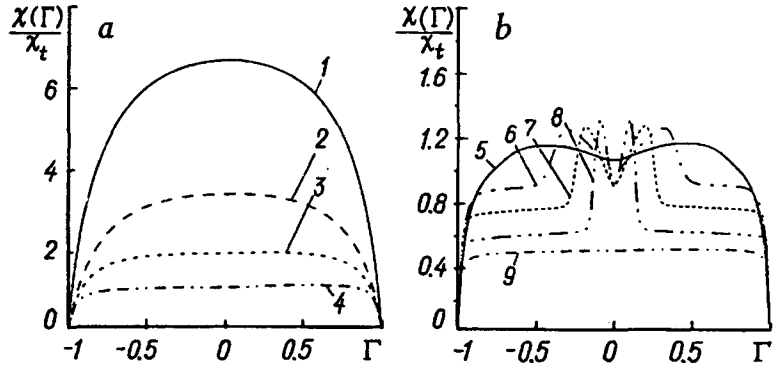


Fig. 4. Evolution of the form of the conventional rate of dissipation at the initial (a) and intermediate and final (b) stages of mixing: 1) $t = 0$, 2) 0.5, 3) 1, 4) 2.5, 5) 5, 6) 10, 7) 15, 8) 20, 9) > 25 (asymptotic state).

evolution of the correlation function $T^2(t)$, which determines the dissipation of the dissipation in the equation for $\chi_t(\Gamma)$. This function attains a minimum when the rate of dissipation is maximum.

A more complex evolution is demonstrated by the function $P_t^{(c)'''}(0) = P_0^{(c)'''}$. Figure 2 shows that this function is nonmonotonic and remains negative during evolution because of the proportionality of the function $P_0^{(c)'''}$ to the third derivative of the third-order two-point structural function $D_{LCC}'''(0, t)$ with respect to the variable ρ at $\rho = 0$. This function with a negative sign in the equation for the mean square of the scalar gradient describes the enhancement of the scalar gradient due to inertial approach of liquid volumes with different scalar content [23]. The enhancement increases the mean square of the scalar gradient, and therefore the function must always be negative.

Figure 2 also presents the evolution of the functions P_0' and $P_0^{(c)'}$, which are directly associated with the rates of dissipation of turbulent fluctuations of the velocity and the scalar. We note that the main changes in the functions P_0', $P_0^{(c)'}$, and $P_0^{(c)'''}$ are virtually synchronized in time.

Figure 3a shows the evolution of the integral PDDF, which is calculated directly from the solution of the system of equations (39)-(40). The evolution of the single-point PDDF is presented in Fig. 3b, from which it is seen that the initial form of the single-point PDDF (curve 1) looks like a sum of two δ-functions: at $\Gamma = 1$ and at $\Gamma = -1$. This form of the PDDF reflects the state of complete nonmixing of the scalar field typical of the start of the process of mixing. The flat nonzero portion between the points $\Gamma = \pm 1$ reflects the presence of a certain small portion of mixed liquid. This fraction increases with increase in the time of mixing (curve 2). However, the form of the single-point PDDF remains the same and reminiscent of the distribution of probabilities typical of sinusoidal realization of a scalar field. As pointed out in [12], this form of the PDDF is associated with the presence of diffusion layers in the turbulent flow at the initial stage. The PDDF in the form of curves 3 and 4 demonstrates the appearance of a greater portion of mixed liquid in the flow. Along with the peaks of the function at $\Gamma = \pm 1$, a noticeable maximum appears at $\Gamma = 0$ due to an increase in the fraction of mixed mixture in the flow. The corresponding dependences of the integral function $F_t(\Gamma)$ demonstrate this process by an increase in the inclination in the middle portion of the curve. On curves 5, 6 (Fig. 3b) this maximum is more pronounced, and the peaks of the function at $\Gamma = \pm 1$ remain quite appreciable, i.e., the curves of the PDDF have a two-mode form at intermediate stages of mixing, which reflects the simultaneous presence of a mixture mixed to the molecular level and unmixed fragments of liquid in the flow.

At a later stage the PDDF acquires a single-mode form with a maximum at $\Gamma = 0$, which corresponds to a state close to complete mixing. It is not possible to carry out a calculation in the case of a still more peaked form of the PDDF because of the presence of extremely large gradients of this function (see also the shape of the corresponding curves of the integral function in Fig. 3a).

The main feature of the result obtained in calculation of the single-point PDDF of a scalar is the manifestation of a two-mode form at intermediate stages of mixing by this function. The presence of maxima at $\Gamma = \pm 1$ and $\Gamma = 0$ corresponds to the simultaneous presence of unmixed scalar and mixture mixed to the molecular

level in the flow. This feature of the PDDF cannot be reconstructed by means of direct numerical simulation (DNS), evidently because of the very small Reynolds and Peclet numbers at which DNS of turbulent velocity and scalar fields is realized. This property also cannot be reconstructed by the majority of the proposed models on the use of averaged characteristics of turbulence.

The two-mode character of the PDDF was noted in the experimental work [24] and the theoretical works [25, 26], with [25] being based on simulation of turbulent mixing by a simplified velocity field and [26] being associated with account for the multiscale character of turbulent mixing.

As is seen from the results obtained, the present model, which uses the evolution of the CRSD to calculate the single-point PDDF, evidently also takes into account the multiscale character of turbulent mixing.

Curves for the conventional rate of scalar dissipation at different stages of turbulent mixing are shown in Fig. 4. A parabola with a maximum at $\Gamma = 0$ figures as the initial form of the CRSD (curve 1). This form of the CRSD corresponds to sinusoidal realizations of the turbulent scalar field, whose presence in the flow is associated with the presence of diffusion layers there that separate regions with a homogeneous content of the scalar.

At subsequent stages of mixing, when $5 < t < 15$ (curves 3, 4) the CRSD becomes nearly flat in its middle portion between the points $\Gamma = \pm 1$. This is possibly due to the fact that typical realizations of a scalar turbulent field acquire an almost sawtoothed shape, so that most of the time the fields of the scalar and its gradient remain almost uncorrelated.

At a later stage of turbulent mixing, when $t > 15$ (Fig. 4b), the curve of the CRSD becomes similar in its middle portion to a parabola with a minimum at $\Gamma = 0$. It is possible to assume that this form of the CRSD is due to enhancement of typical realizations of the scalar field in such a manner that the maximum of the gradient is observed at large values of the scalar field and, as a result, leads to a strong correlation of the scalar and its gradient. Further evolution of the process of mixing imparts an almost flat shape to the CRSD curve at intermediate values of Γ (curve 9). This form of the CRSD can be attributed to loss of marked correlation of the scalar field and its gradient at almost all the values of Γ. At this stage the form of the single-point PDDF starts to resemble a Gaussian one. Probably, this is due precisely to the fact that the CRSD in Eq. (27) for $f_t(\Gamma)$ becomes independent of the magnitude of the field Γ.

Note that the obtained sequence of forms of the CRSD is in satisfactory qualitative agreement with results of its calculation on the basis of DNS in [12] and with data of the experimental works [13-15].

Conclusion. A closed system of equations for the CRSD and the single-point PDDF of the values of scalar fluctuations is derived on the basis of the closed equation for the JPDF of the magnitudes of the scalar and its gradient obtained by the authors.

In the derivation we used the hypothesis of equality of the mean square of the CRSD to the squared mean value of the CRSD. All the time-dependent coefficients $A(t)$, $B(t)$, $C(t)$, $D(t)$, and $T(t)$ that enter the equation for the CRSD are expressed in terms of the functions $P_t(\rho)$ and $P_t^{(c)}(\rho)$, for which a closed system of equations is written.

Numerical solution of the system of equations for $\chi_t(\Gamma)$ and $f_t(\Gamma)$ is realized in the reverse direction in time starting from the final "starting" values of these functions to the initial ones, which made it possible to overcome serious problems associated with the presence of terms with "negative diffusion" in the equations for $\chi_t(\Gamma)$ and $f_t(\Gamma)$. The solution of the system of equations for the functions $P_t(\rho)$ and $P_t^{(c)}(\rho)$ is realized in the forward direction in time starting from their initial values.

The evolution of the single-point PDDF $f_t(\Gamma)$ obtained as a result of the solution manifests a two-mode form at the intermediate stage of the process of turbulent mixing, which is in qualitative agreement with experiment and is obtained theoretically for the first time.

The sequence of forms of the function $\chi_t(\Gamma)$ obtained in the numerical solution is in satisfactory agreement with results of DNS of a turbulent scalar field and with data of existing experiments.

The closed model suggested for calculating the functions $\chi_t(\Gamma)$ and $f_T(\Gamma)$ can be used in the calculation of chemical reactions in turbulent flows and processes of turbulent combustion within the framework of the flamelet approach.

The work was carried out with support from the Fund for Fundamental Research of the Republic of Belarus, project T95-181.

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