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HEAT AND MASS TRANSFER IN TURBULENT FLOWS

LENGTH-SCALE DISTRIBUTIONS OF THE CONCENTRATION PULSATIONS OF A PASSIVE IMPURITY IN A HOMOGENEOUS TURBULENT FLOW

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A relation for calculating the probability density function $f_t^{\lambda}(\varphi)$ of the length scales of a passive concentration field in homogeneous turbulence has been obtained by consideration of the joint statistics of the concentration field and its gradient. The closed equation derived for $f_t^{\lambda}(\varphi)$ has been solved numerically using the data of direct numerical modeling of homogeneous turbulence for the mean characteristics involved in the equation as the coefficients. The results obtained for different values of the Schmidt number have been compared.

Introduction. Turbulence considerably intensifies the mixing and transfer of substances and heat in a flow. Many processes in the environment and in technical devices that are associated with flames, chemical reactions, and propagation of impurities would be completely impossible without efficient mixing. Although the history of study of turbulent mixing is rather long, its nature remains to be completely understood. We know of the equations using which one describes turbulent flows, but their numerical solution involves many difficulties.

Direct numerical modeling of combined turbulent flows, which develops in connection with the progress made in computer technologies, cannot be used for problems of practical significance [1]. Therefore, one continues to develop statistical approaches with one method of averaging or another. One of them is the method of the probability density function (PDF) of different hydro- and thermodynamic parameters [2], which has been fruitfully used in studying reacting media.

The advantages of the PDF method are primarily a simple and accurate representation of the influence of chemical sources on changes in the quantities sought and a lower consumption of computer time. Its main problem is that of modeling of the contribution of the process of fine-structure mixing of a scalar field of concentration (micromixing) to the general pattern of mixing. Micromixing is determined by the mechanism using which the scalar field brought to the state of "rough homogeneity" by the averaged flow and large vortices in the flow is broken by a statistically homogeneous turbulent velocity field down to the smallest turbulence scales due to the small-scale motion of the medium and next to the molecular level through molecular diffusion.

The presence of all kinds of values of the concentrations and the existence of the entire range of scales create constantly interacting categories of turbulent mixing: the evolution of the length-scale range leads to a constant change in the boundary conditions for the action of molecular diffusion, thus influencing the rate of change in the concentration pulsations. The structure of the pulsation field is dependent on the small scales directly influencing the rate of dissipation of concentration pulsations more strongly than on large scales.

Depending on the formulation of the problem, one selects the normalized temperature, the concentrations of the reactants or the inert impurity, the Schwab–Zel'dovich variables for turbulent flows with unmixed reactants, or the degree of development of the reaction for flows with premixed reactants as the quantities determining the state of a turbulent scalar field [2]. A single-point PDF of such random quantities is used to characterize diffusion processes.

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Unfortunately, the single-point statistics of scalar fields contains no information on the spatial structure of turbulence. Models operating with two-point and multipoint statistics [3] are much more difficult to realize; therefore, they are less common in computational practice. The spatial turbulence structure may be allowed for within the framework of single-point models by modeling the range of turbulent-pulsation-length scales.

Allowance for the existing range of characteristic length scales in turbulent mixing remains a necessary but nontrivial problem [4]. The PDF structure must be determined by all the details of the concentration field, not only by its mean characteristics, such as the mean scale and rate of dissipation of concentration pulsations [5]. A single-point concentration PDF demonstrating a substantially non-Gaussian two-mode form at intermediate mixing steps has been calculated in [6]. The function found by solution for a one-scale model has been averaged over the length-scale range using the prescribed form of the PDF of length scales.

An expression for the PDF of length scales has been obtained in [7] with allowance for the fractal character of the surfaces separating regions of different concentration in a turbulent flow. This form was used in obtaining analytical relations for the conditional rate of scalar dissipation and density of surfaces of equal concentration based on the hypothesis for typical realizations of a scalar turbulent concentration field at different steps of its evolution [7, 8].

The multiscale character of turbulent mixing is closely related to the distribution of time scales in turbulent flows. The distributions of characteristic time scales have been studied in [9] based on the data of direct numerical modeling in the problem of mixing of a scalar concentration field. As has been shown in [10], allowance for the time-scale distribution is important in studying diffusion flames with kinetic effects, whereas a prescribed form of the PDF of time scales is used in the model relation for the mean rate of a chemical reaction.

This work seeks to show the possibility of determining the length scales by consideration of the statistics of a passive concentration field and its gradient and to obtain a relationship between the PDF of concentration-length scales and the joint PDF of concentration and its gradient in the form of the integral relation and the transfer equation.

One usually obtains the scales of turbulence lengths and time from the joint statistics of velocity and velocity-gradient pulsations, which is not necessarily adequate in relation to the field of concentration pulsations, since the corresponding Schmidt numbers may noticeably be different from unity. Furthermore, of great interest for turbulent reacting flows are the distributions of length and time scales in a concentration space, since it is precisely they that determine the properties of a turbulent field in the zones of localization of the reaction. Therefore, we derive the equation for the PDF of length and time scales using the equation obtained earlier for the joint PDF of the concentration field and its gradient [11].

Determination of the Length and Time Scales of a Scalar Concentration Field. We consider the turbulent mixing of a dynamically passive scalar concentration field of reactants not mixed in advance. In such a process, neither the concentration transfer nor the chemical reactions in the flow exert an influence on the velocity field. This idealization assumes that the concentrations of the reacting components in the entire mixture are low; the reaction heat is considered to be negligible; hence, the reaction is isothermal; the density of the mixture and the kinematic viscosity are constant. Also, it is usually assumed that the coefficients of molecular diffusion of each component and the mixture are equal and constant [12]. Such a simplification is not necessarily acceptable in applications of practical importance. When there are large temperature gradients in the flow, a substantial inhomogeneity of the density field develops, which causes the scalar field to act on the dynamics of the flow. In the limit of a passive scalar, conversely, the change in the density is considered to be slight. Despite such a limitation, approaches used in modeling the mixing of passive scalars are called for in engineering developments [12].

The general approach in modeling unpremixed turbulent reacting flows is based on a study of the statistics of two quantities: a conservative scalar representing the coefficients of a mixture or the concentration of an inert impurity C and its gradient $|\Delta C|$ related to the rate of dissipation of scalar pulsations $c = C - \langle C \rangle$ in a turbulent flow [1]. In this case, a change in the scalar concentration field is described using the equation of convection and diffusion without the terms characterizing the influence of chemical reaction [2].

In considering the statistically homogeneous field of a conservative scalar with a constant mean $\langle C \rangle$ = const, the process of disappearance of inhomogeneities in the flow is determined by the dynamics of pulsations of the scalar c (in what follows simply the scalar);

$$\frac{\partial c}{\partial t}+\frac{\partial\,(u_i c)}{\partial x_i}=\frac{1}{\mathrm{Pe}}\frac{\partial^2 c}{\partial x_i^2}\,, \tag{1}$$

where u_i is the statistically homogeneous random velocity field considered to be known.

Equation (1) may be written in the form

$$\frac{\partial c^2}{\partial t}+\frac{\partial\,(u_i c^2)}{\partial x_i}=\frac{1}{\mathrm{Pe}}\frac{\partial^2 c^2}{\partial x_i^2}-2\chi_{ñ}\,. \tag{2}$$

Here the quantity $\chi_c = \frac{1}{\mathrm{Pe}}\frac{\partial c}{\partial x_i}\frac{\partial c}{\partial x_i} = \frac{1}{\mathrm{Pe}}\left|\nabla c\right|^2$ is the instantaneous rate of dissipation of the scalar. The averaging of Eq. (2) yields the relation for the variance of the scalar $\langle c^2\rangle(t)$ [1]. In the case of isotropic turbulent fields for large Reynolds numbers we obtain a relationship between $\langle c^2\rangle(t)$ and the mean rate of dissipation of the scalar $\chi(t) = \langle\chi_c\rangle$ in the form [1] $\partial\langle c^2\rangle(t)/\partial t = -2\chi(t)$.

The mean microscales of time $t_c(t)$ and lengths $l_c(t)$ of the scalar field are in essence the integral characteristics of its spectral state and are related as [1, 2] $t_c(t) = \frac{\langle c^2\rangle(t)}{2\chi(t)} = \frac{l_c^2(t)\mathrm{Pe}}{6}$. In its meaning, the length scale $l_c(t) = \sqrt{\frac{3}{\mathrm{Pe}}\frac{\langle c^2\rangle(t)}{\chi(t)}}$ is analogous to the length microscale of the turbulent velocity field $l_{\mathrm{t}}(t) = \sqrt{\frac{15}{\mathrm{Re}}\frac{u_{\mathrm{rms}}^2(t)}{\varepsilon(t)}}$.

Similarly, we introduce the determination for the local time scale of scattering of inhomogeneities due to molecular diffusion on the local length scale λ_c:

$$\tau_{\tilde{n}}=\frac{c^2}{2\chi_{\tilde{n}}}=\frac{\lambda_{\tilde{n}}^2\mathrm{Pe}}{6}\,, \tag{3}$$

where the length scale, on which a concentration pulsation (the scalar) is realized, is determined as

$$\lambda_{\tilde{n}}=\sqrt{\frac{3}{\mathrm{Pe}}\frac{c^2}{\chi_{\tilde{n}}}}=\sqrt{3}\,\left|c\right|/\left|\nabla c\right|\,. \tag{4}$$

Physically this length scale is the characteristic of the size of domains (thickness of diffusion layers) in the turbulent scalar field, which separate regions with different concentrations, and the PDF of such length scales shows the probability of existence of such domains.

It follows from relation (4) that λ_c is determined as the quotient of absolute values of the scalar and its gradient, i.e., by the joint statistics of c and $\left|\nabla c\right|$, which is expressed in terms of the corresponding PDF of the two quantities $P_{x_i,t}(\Gamma,\ W)$.

Analytical Relation for the PDF of Scalar-Length Scales. To obtain the form of the PDF of scalar-length scales we use data from general probability theory [13]. We consider a certain joint PDF of two random quantities (ϕ_1, ϕ_2) that is equal to $f_{x_i,t}(\psi_1,\ \psi_2)$. Let us assume that the domain of definition of the variables is $\phi_{\min} \le \phi_1 \le \phi_{\max}$ and $0 \le \phi_1 \le +\infty$; here, $\phi_{\min} < 0$. We write the PDF of the quotient $\lambda = \left|\phi_1\right|/\phi_2$. By definition, the distribution function of the random quantity λ has the form $F^2(\varphi) = \mathrm{Prob}\left\{\left|\phi_1\right|/\phi_2 \le \varphi\right\}$. Then the probability sought is equal to the probability of the point (ϕ_1, ϕ_2) arriving at the part of the domain of definition that satisfies the inequalities $-\varphi\phi_2 \le \phi_1 \le \varphi\phi_2$, i.e.,

$$F^{\lambda}(\varphi) = \int_0^{+\infty} d\psi_2 \left[\int_{\phi_{\min}}^{\phi_{\max}} f_{x_i,t}(\psi_1, \psi_2)\, d\psi_1 \right] -$$

$$- \int_0^{\phi_{\max}/\varphi} d\psi_2 \left[\int_{\varphi\psi_2}^{\phi_{\max}} f_{x_i,t}(\psi_1, \psi_2)\, d\psi_1 \right] - \int_0^{-\phi_{\min}/\varphi} d\psi_2 \left[\int_{\phi_{\min}}^{-\varphi\psi_2} f_{x_i,t}(\psi_1, \psi_2)\, d\psi_1 \right]. \tag{5}$$

Since the first integral is equal to unity according to the normalization condition for the PDF, from (5) we obtain

$$F^{\lambda}(\varphi) = 1 - \int_0^{\phi_{\max}/\varphi} \Phi_1(\psi_2, \varphi)\, d\psi_2 - \int_0^{-\phi_{\min}/\varphi} \Phi_2(\psi_2, \varphi)\, d\psi_2 = 1 - F_+ - F_-,$$

where $\Phi_1(\psi_2, \varphi) = \int_{\varphi\psi_2}^{\phi_{\max}} f_{x_i,t}(\psi_1, \psi_2) d\psi_1$ and $\Phi_2(\psi_2, \varphi) = \int_{\phi_{\max}}^{-\varphi\psi_2} f_{x_i,t}(\psi_1, \psi_2) d\psi_1$.

Differentiating the equality for $F^{\lambda}(\varphi)$ with respect to the variable φ, we find the PDF of the quotient. Using the formula of mathematical analysis for differentiation of the integrals dependent on the parameter

$$\frac{d}{d\varphi} \int_{\alpha(\varphi)}^{\beta(\varphi)} f(x, \varphi)\, dx = \int_{\alpha(\varphi)}^{\beta(\varphi)} \frac{\partial f(x, \varphi)}{\partial \varphi}\, dx + f(\beta(\varphi), \varphi) \frac{d\beta(\varphi)}{d\varphi} - f(\alpha(\varphi), \varphi) \frac{d\alpha(\varphi)}{d\varphi}, \tag{6}$$

we obtain

$$\frac{\partial F_+}{\partial \varphi} = \frac{\partial}{\partial \varphi} \left\{ \int_0^{\phi_{\max}/\varphi} \Phi_1(\psi_2, \varphi)\, d\psi_2 \right\} = \int_0^{\phi_{\max}/\varphi} \frac{\partial \Phi_1(\psi_2, \varphi)}{\partial \varphi}\, d\psi_2,$$

$$\frac{\partial F_-}{\partial \varphi} = \frac{\partial}{\partial \varphi} \left\{ \int_0^{-\phi_{\min}/\varphi} \Phi_2(\psi_2, \varphi)\, d\psi_2 \right\} = \int_0^{\phi_{\min}/\varphi} \frac{\partial \Phi_2(\psi_2, \varphi)}{\partial \varphi}\, d\psi_2.$$

To the integrands in these relations we apply formula (6):

$$\frac{\partial \Phi_1(\psi_2, \varphi)}{\partial \varphi} = \frac{\partial}{\partial \varphi} \int_{\varphi\psi_2}^{\phi_{\max}} f_{x_i,t}(\psi_1, \psi_2)\, d\psi_1 = \int_{\varphi\psi_2}^{\phi_{\max}} \frac{\partial f_{x_i,t}(\psi_1, \psi_2)}{\partial \varphi}\, d\psi_1 +$$

$$+ \frac{\partial(\phi_{\max})}{\partial \varphi} f_{x_i,t}(\phi_{\max}, \psi_2) - \frac{\partial(\varphi\psi_2)}{\partial \varphi} f_{x_i,t}(\varphi\psi_2, \psi_2) = -\psi_2 f_{x_i,t}(\varphi\psi_2, \psi_2),$$

$$\frac{\partial \Phi_2(\psi_2, \varphi)}{\partial \varphi} = \frac{\partial}{\partial \varphi} \int_{\phi_{\min}}^{-\varphi\psi_2} f_{x_i,t}(\psi_1, \psi_2)\, d\psi_1 = \int_{\phi_{\min}}^{-\varphi\psi_2} \frac{\partial f_{x_i,t}(\psi_1, \psi_2)}{\partial \varphi}\, d\psi_1 +$$

$$+ \frac{\partial(-\varphi\psi_2)}{\partial \varphi} f_{x_i,t}(-\varphi\psi_2, \psi_2) - \frac{\partial(\phi_{\min})}{\partial \varphi} f_{x_i,t}(\phi_{\min}, \psi_2) = -\psi_2 f_{x_i,t}(-\varphi\psi_2, \psi_2),$$

whence it follows that the PDF sought is equal to

$$f^{\lambda}_{x_i,t}(\varphi) = \int_0^{\phi_{\max}/\varphi} \psi_2 f_{x_i,t}(\varphi\psi_2, \psi_2)\, d\psi_2 + \int_0^{-\phi_{\min}/\varphi} \psi_2 f_{x_i,t}(-\varphi\psi_2, \psi_2)\, d\psi_2 \,. \tag{7}$$

Now, introducing the variable ϕ_1 corresponding to the scalar c and the variable ϕ_2 corresponding to the value of its gradient $|\nabla c|$ with a joint PDF $P_{x_i,t}(\Gamma, W)$, for the PDF of scalar-length scales we obtain

$$f^{\lambda}_{x_i,t}(\varphi) = \int_0^{\sqrt{3}\Gamma_{\max}/\varphi} W P_{x_i,t}(\varphi W/\sqrt{3}, W)\, dW + \int_0^{-\sqrt{3}\Gamma_{\min}/\varphi} W P_{x_i,t}(-\varphi W/\sqrt{3}, W)\, dW = f_+(\varphi) + f_-(\varphi)\,. \tag{8}$$

Thus, if the form of the PDF of the scalar (concentration pulsation) and the value of its gradient or a closed equation for it are known, the PDF of scalar-length scales is calculated using (8) or by derivation and solution of the corresponding equation for the function sought. Knowledge of the latter makes it possible to determine the characteristic mean scales of scalar lengths and time:

$$\langle \lambda_{\tilde{n}} \rangle = \int_0^{+\infty} \varphi f^{\lambda}_{x_i,t}(\varphi)\, d\varphi\,, \quad \langle \tau_{\tilde{n}} \rangle = \frac{\mathrm{Pe}}{6} \int_0^{+\infty} \varphi^2 f^{\lambda}_{x_i,t}(\varphi)\, d\varphi\,.$$

It is noteworthy that formula (8) holds for arbitrary scalars not necessarily possessing the property of conservatism. For example, in the case of premixed mixtures such a scalar can be the degree of development of the reaction the equation for which contains source terms [1].

Equation for the PDF of Length Scales of a Conservative Scalar. To obtain an equation for the PDF of scalar-length scales we use the well-known closed equation for the joint PDF of a conservative scalar and the value of its gradient [11] (this equation has been derived under the assumption of homogeneous and isotropic turbulence):

$$\frac{\partial P_t(\Gamma, W)}{\partial t} = -\frac{W^2}{\mathrm{Pe}} \frac{\partial^2 P_t(\Gamma, W)}{\partial \Gamma^2} - \frac{S_{uc}(t)}{2} \sqrt{\frac{\varepsilon(t)\,\mathrm{Re}}{15}} \frac{\partial}{\partial W}\left[\left(1 - \frac{W^2}{\mathrm{Pe}\,\chi(t)}\right) W P_t(\Gamma, W)\right] -$$
$$- \frac{N_t(\Gamma)}{\mathrm{Pe}} \frac{\partial}{\partial W}\left[W^2 \frac{\partial}{\partial W}\left(\frac{P_t(\Gamma, W)}{W^2}\right)\right] - 2\frac{\partial}{\partial \Gamma}\left[\frac{X_t(\Gamma)}{\mathrm{Pe}} \frac{\partial (W P_t(\Gamma, W))}{\partial W}\right]. \tag{9}$$

This equation involves the joint asymmetry of the gradients of pulsations of the velocity and the scalar $S_{uc}(t) = \langle \partial u_1/\partial x_1 (\partial c/\partial x_1)^2 \rangle / [(\varepsilon(t)\mathrm{Re}/15)^{1/2} \chi(t)\mathrm{Pe}/3]$. The functions $N_t(\Gamma)$ and $X_t(\Gamma)$ in Eq. (9) are prescribed by the formulas

$$N_t(\Gamma) = -\frac{1}{6} D^{(\mathrm{IV})}_{\tilde{n}\tilde{n}}(0, t)\, [5 - 3T^2(t)(1 - \hat{\Gamma}^2)]\,, \quad X_t(\Gamma) = -\frac{\chi(t)\,\mathrm{Pe}}{3\sqrt{\langle c^2 \rangle (t)}} \hat{\Gamma}\,, \tag{10}$$

where $\hat{\Gamma} = \Gamma/\sqrt{\langle c^2 \rangle (t)}$, $T^2(t) = \langle c^2 (\partial^2 c/\partial x_1^2)^2 \rangle / (\langle c^2 \rangle \langle (\partial^2 c/\partial x_1^2)^2 \rangle)$ is the coefficient squared of correlation between the fields of the scalar and its second space derivative and the function $D^{(\mathrm{IV})}_{cc}(0, t)$ is the derivative of fourth order with respect to $D_{cc}(r, t)$ for the zero value of the variable r.

For convenience of further transformations, we write (9) in terms of the function $f = WP_t$:

$$\frac{\partial f}{\partial t} = -\frac{W^2}{\mathrm{Pe}} \frac{\partial^2 f}{\partial \Gamma^2} - \frac{S_{u\tilde{n}}(t)}{2} \sqrt{\frac{\varepsilon(t)\,\mathrm{Re}}{15}}\, W \frac{\partial}{\partial W}\left[\left(1 - \frac{W^2}{\mathrm{Pe}\,\chi(t)}\right) f\right] -$$

$$-\frac{N_t(\Gamma)}{\mathrm{Pe}}\left(\frac{6}{W^2}-\frac{4}{W}\frac{\partial}{\partial W}+\frac{\partial^2}{\partial W^2}\right)f-2\frac{\partial}{\partial\Gamma}\left[\frac{X_t(\Gamma)}{\mathrm{Pe}}W\frac{\partial f}{\partial W}\right]. \tag{11}$$

We write an equation for the term $f_+(\varphi)$ from (8) as follows. Assuming that $\Gamma = \varphi W^*/\sqrt{3}$ and $W = W^*$, we use the following formulas of transition from some variables to others:

$$\frac{\partial}{\partial\Gamma}=\frac{\sqrt{3}}{W^*}\frac{\partial}{\partial\varphi},\quad \frac{\partial}{\partial W}=\frac{\partial}{\partial W^*}-\frac{\varphi}{W^*}\frac{\partial}{\partial\varphi},\quad \frac{\partial^2}{\partial\Gamma^2}=\frac{3}{{W^*}^2}\frac{\partial^2}{\partial\varphi^2},$$

$$\frac{\partial^2}{\partial W^2}=\left(\frac{\partial}{\partial W^*}-\frac{\varphi}{W^*}\frac{\partial}{\partial\varphi}\right)\left(\frac{\partial}{\partial W^*}-\frac{\varphi}{W^*}\frac{\partial}{\partial\varphi}\right)=\frac{\partial^2}{\partial {W^*}^2}-2\frac{\varphi}{W^*}\frac{\partial^2}{\partial W^*\partial\varphi}+2\frac{\varphi}{{W^*}^2}\frac{\partial}{\partial\varphi}+\left(\frac{\varphi}{W^*}\right)^2\frac{\partial^2}{\partial\varphi^2}.$$

Applying the latter transformations, we rewrite Eq. (11) for the function $f(\varphi W^*/\sqrt{3},\ W^*)$. Integrating it over the corresponding interval with allowance for the boundary conditions and formula (6), we obtain the equation for $f_+(\varphi)$ of the form

$$\frac{\partial f_+(\varphi)}{\partial t}=-\frac{3}{\mathrm{Re}}\frac{\partial^2 f_+(\varphi)}{\partial\varphi^2}+\frac{S_{uc}(t)}{2}\sqrt{\frac{\varepsilon(t)\mathrm{Re}}{15}}\frac{\partial}{\partial\varphi}\left[\varphi\left(1-\frac{1}{\mathrm{Pe}\,\chi(t)}\underbrace{\int_0^{\sqrt{3}\Gamma_{\max}/\varphi}W^3 f_t(W\,|\,\varphi)dW}_{I_+^3}\right)f_+(\varphi)\right]-$$

$$-\frac{\partial^2}{\partial\varphi^2}=\left(B(t)\varphi^4 f_+(\varphi)+A(t)\varphi^2 f_+(\varphi)\underbrace{\int_0^{\sqrt{3}\Gamma_{\max}/\varphi}W^{-1}f_t(W\,|\,\varphi)dW}_{I_+^{-1}}\right)-\frac{3}{2}\frac{\chi(t)}{\left\langle c^2\right\rangle(t)}\frac{\partial}{\partial\varphi}\left[\varphi\frac{\partial}{\partial\varphi}(\varphi f_+(\varphi))\right].$$

Here we have dropped the asterisks of the variable W and have taken into account the well-known property for the conditional distribution functions $f(\phi\,|\,\varphi) = f(\phi, \varphi)f(\varphi)$ [13] and the specific form of expressions (10), where

$$A(t)=-\frac{1}{6}\frac{D^{(\mathrm{IV})}_{\tilde n\tilde n}(0,t)}{\mathrm{Pe}}[5-3T^2(t)]\,;\quad B(t)=-\frac{1}{6}\frac{D^{(\mathrm{IV})}_{\tilde n\tilde n}(0,t)}{\mathrm{Pe}}[T^2(t)/\langle c^2\rangle(t)]\,.$$

Acting analogously for the pair of variables $\Gamma = -\varphi W^*/\sqrt{3}$ and $W = W^*$, we impart nearly the same form to the equation for the function $f_-(\varphi)$. The difference is that, instead of the integrals I_+^3 and I_+^{-1}, we will accordingly have the integrals $I_-^3 = \int_0^{-\sqrt{3}\Gamma_{\min}/\varphi} W^3 f_t(W\,|\,\varphi)dW$ and $I_-^{-1} = \int_0^{-\sqrt{3}\Gamma_{\min}/\varphi} W^{-1} f_t(W\,|\,\varphi)dW$. Then the equation sought for the length-scale PDF $f_t^\lambda(\varphi)$ is written as

$$\frac{\partial f_t^\lambda(\varphi)}{\partial t}=-\frac{3}{\mathrm{Pe}}\frac{\partial^2 f_t^\lambda(\varphi)}{\partial\varphi^2}+\frac{S_{uc}(t)}{2}\sqrt{\frac{\varepsilon(t)\,\mathrm{Re}}{15}}\frac{\partial}{\partial\varphi}\left[\varphi\left(1-\frac{1}{\mathrm{Pe}\,\chi(t)}(I_+^3+I_-^3)\right)f_t^\lambda(\varphi)\right]-$$

$$-\frac{\partial^2}{\partial\varphi^2}\left(B(t)\,\varphi^4 f_t^\lambda(\varphi)+A(t)\,\varphi^2(I_+^{-1}+I_-^{-1})f_t^\lambda(\varphi)\right)-\frac{2}{3}\frac{\chi(t)}{\langle c^2\rangle(t)}\frac{\partial}{\partial\varphi}\left[\varphi\frac{\partial}{\partial\varphi}(\varphi f_t^\lambda(\varphi))\right]. \tag{12}$$

Equation (12) is open due to the indeterminacy of integral-type quantities involved in it. To approximate them we use an assumption of the form of χ^2, i.e., the distribution of the modulus of a three-dimensional vector for the conditional distribution function $f_t(W|\varphi) = \sqrt{\frac{2}{\pi}}\frac{1}{\sigma^3}W^2\exp\left(-\frac{W^2}{2\sigma^2}\right)$, where $\sigma = (\chi(t)\ \mathrm{Pe}/3)^{1/2}$ is the variance of the scalar gradient. Then allowance for the corresponding limits of integration and equalities

$$\int W^3\sqrt{\frac{2}{\pi}}\frac{1}{\sigma^3}W^2\exp\left(-\frac{W^2}{2\sigma^2}\right)dW = -4\sqrt{\frac{2}{\pi}}\sigma^3\exp\left(-\frac{W^2}{2\sigma^2}\right)\left(\left[\frac{W^2}{2\sigma^2}+1\right]^2+1\right),$$

$$\int W^{-1}\sqrt{\frac{2}{\pi}}\frac{1}{\sigma^3}W^2\exp\left(-\frac{W^2}{2\sigma^2}\right)dW = -\sqrt{\frac{2}{\pi}}\frac{1}{\sigma}\exp\left(-\frac{W^2}{2\sigma^2}\right)$$

makes it possible to calculate the unknown sums in Eq. (12) and to close it.

Method of Solution of the Equation for the PDF of Scalar-Length Scales. For convenience of numerical solution we write Eq. (12) in terms of the cumulative distribution function $F_t^\lambda(\varphi) = \int_0^\varphi f_t^\lambda(\varphi')d\varphi'$:

$$\frac{\partial F_t^\lambda(\varphi)}{\partial t} = -\frac{3}{\mathrm{Pe}}\frac{\partial^2 F_t^\lambda(\varphi)}{\partial\varphi^2} + \frac{S_{u\tilde{n}}(t)}{2}\sqrt{\frac{\varepsilon(t)\,\mathrm{Re}}{15}}\left(1-\frac{1}{\mathrm{Pe}\,\chi(t)}(I_+^3+I_-^3)\right)\varphi\frac{\partial F_t^\lambda(\varphi)}{\partial\varphi} -$$

$$-\frac{\partial}{\partial\varphi}\left[(B(t)\,\varphi^4 + A(t)\,\varphi^2\,(I_+^{-1}+I_-^{-1}))\frac{\partial F_t^\lambda(\varphi)}{\partial\varphi}\right] - \frac{2}{3}\frac{\chi(t)}{\langle c^2\rangle(t)}\varphi\frac{\partial}{\partial\varphi}\left(\varphi\frac{\partial F_t^\lambda(\varphi)}{\partial\varphi}\right). \tag{13}$$

Boundary conditions are set from the properties of this function, i.e.,

$$F_t^\lambda(\varphi)\big|_{\varphi=0} = 0\,,\quad F_t^\lambda(\varphi)\big|_{\varphi=\infty} = 1\,. \tag{14}$$

It is noteworthy that Eqs. (12) and (13) inherit such a property of Eq. (9) as its inversely parabolic form [14], which makes the problem ill posed [15]. Therefore, to overcome numerical instability we consider (13) in the opposite direction with time (retrospectively). For this purpose, we set a certain "starting" condition at the instant of time $t = T$ for a fairly long T and realize the numerical solution from this value to $t = 0$. The possibility of using such an approach is discussed in [16]. Using this approach, Sosinovich et al. found the solution of a system of equations for the conditional rate of scalar dissipation in a homogeneous turbulent flow in [17].

At $t = T$, we represent the PDF of scalar-length scales in the form $f_t^\lambda\big|_{t=T} = 2\varphi/L^2\exp\{-\varphi^2/L^2\}$, which corresponds to the approximation of the probability distribution function

$$F_t^\lambda\big|_{t=T} = 1-\exp\left\{-\varphi^2/L^2\right\}, \tag{15}$$

where the coefficient L is related to the medium scale of scalar lengths at $t = T$.

Since (13) has the form of the equation of convection and diffusion for the opposite time direction, in numerical solution we use a monotone difference scheme for general parabolic equations of second order of approximation [18, p. 401]. The unknown coefficients involved in Eq. (13) can be selected the results of direct numerical modeling or from those of calculation according to the model relations [19]. Since the function $D_{cc}^{(\mathrm{IV})}(0, t)$ is expressed by the variance $\langle c^2\rangle(t)$, the mean rate of dissipation of the scalar $\chi(t)$, and the joint asymmetry of the gradients of velocity pulsations and the scalar $S_{uc}(t)$ [19], the external parameters for finding the evolution of the forms of $f_t^\lambda(\varphi)$ are the last three quantities of those mentioned and the kinetic energy of the velocity field $K_t(t)$ and the rate of its dissipation $\varepsilon(t)$.

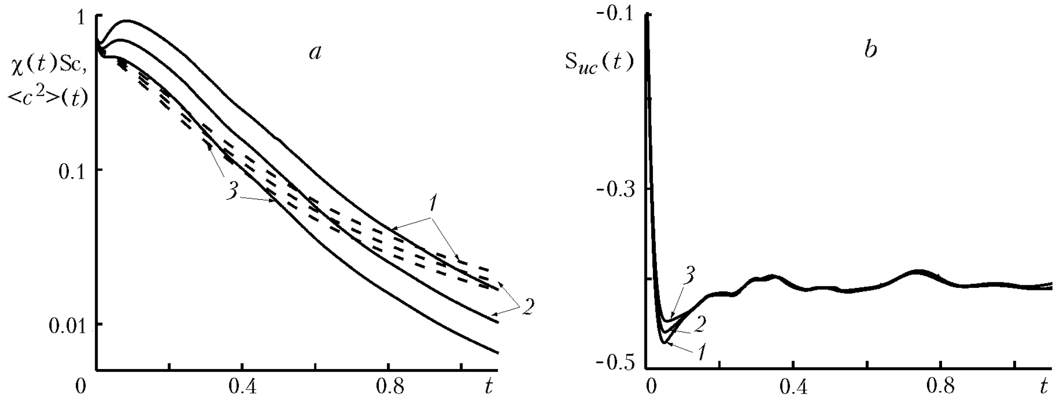

Fig. 1. Data of direct numerical modeling [19] for different Schmidt numbers [1) Sc = 1, 2) 0.7, and 3) 0.5]: a) variance $\langle c^2\rangle(t)$ (dashed curves) and mean rate of dissipation of the scalar $\chi(t)$ multiplied by Sc (solid curves); b) joint asymmetry of the velocity-pulsation and scalar gradients $S_{uc}(t)$.

These coefficients as functions of time for different Schmidt numbers have been obtained using direct numerical modeling [19] within the framework of the same series of numerical experiments. The direct numerical modeling was carried out for a homogeneous isotropic turbulent flow of an incompressible medium in the computational domain in the shape of a cube of size $(2\pi)^3$ with the number of nodes 128^3. For this purpose, we used a pseudospectral code of solution of Navier–Stokes equations and those of scalar transfer [20]. Both the velocity field and the scalar field evolved without the external pumping of energy and were damping. The scalar field presented by the concentration of a passive impurity was chemically inert with a constant mean $\langle C\rangle = 0.7$. The maximum dimensionless wave number was equal to $k = 383$. The initial field consisted of large-scale pulsations, which corresponded to sharp peaks for low k values in the distributions of the turbulent energy $E(k, t)$ and the intensity of concentration pulsations (scalar) $E_c(k, t)$ over the spectrum of wave numbers ([19, Fig. 1]).

The initial state is determined by the following dimensionless parameters coincident with the conditions of the direct numerical modeling [19]: the Reynolds number Re = 736.7, the Schmidt number Sc = 0.5, 0.7, and 1, the turbulent Reynolds number $\mathrm{Re}_{\mathrm{turb}}(0) = 56.45$, the kinetic energy $K_t(0) = 1.5$, the dissipation of the velocity field $\varepsilon(0) = 3.46$, the variance of the scalar field $\langle c^2\rangle(0) = 0.62$, and the dissipation of the scalar field $\chi(0)\,\mathrm{Sc} = 0.73$; the left-hand limit of the scalar is $\Gamma_{\min} = -\sqrt{7/3}$, the right-hand limit of the scalar is $\Gamma_{\max} = \sqrt{3/7}$, and the computational domain is $L_0^3 = (2\pi)^3$.

The quantities are made dimensionless using the characteristic scales of length $L_0 = 2\pi$, equal to the size of the rib of the computational domain, velocity $U_0 = u_{\mathrm{rms}}(0) = 1.407$, where $u_{\mathrm{rms}}(0)$ is the root-mean-square pulsation of the velocity field at $t = 0$, time $t_0 = L_0/U_0$, and kinematic viscosity $\nu = 0.012$, related to the diffusion coefficient D by the Schmidt number Sc. The variance of a totally separated scalar field $c_0 = \langle c^2\rangle_s = \sqrt{\langle C\rangle(1-\langle C\rangle)} = \sqrt{0.21}$ is selected as the characteristic parameter of scalar quantities. This value for such a scalar field is obtained from the assumption of the form of the single-point PDF of the scalar in the form of two δ functions for $\Gamma = \Gamma_{\min}$ and $\Gamma = \Gamma_{\max}$.

The dimensionless variance of the scalar $\langle c^2\rangle(t)$ is the characteristic of the level of intensity of the separation of the scalar field, i.e., the measure of the concentration difference between neighboring small volumes of the medium. At $t = 0$, it is determined by the conditions of introduction of a random concentration field into the flow and is computed from the initial distribution of concentration-pulsation intensity by wave numbers. At this instant, we have $\langle c^2\rangle(0) = \int_0^\infty E_c(k, 0)dk = 0.62$, which points to a fairly high degree of separation of the initial concentration field. Were there no process of molecular diffusion in the flow but the size of the concentration field were only reduced by a statistically homogeneous velocity field, the quantity $\langle c^2\rangle(t)$ would remain constant. The variance acts as the indicator of small-scale diffusion transfer; when the variance decreases down to zero, we may say that the system is completely mixed. The rate for which such a state is attained is determined by the mean rate of dissipation of the scalar

$$\chi(t) = \frac{1}{\mathrm{ScRe}} \int_0^{\infty} k^2 E_c(k, t) dk.$$

Since the initial spectral distribution $E_c(k, 0)$ and the ratio of the Taylor time microscales of the velocity field and the scalar-field for all the Schmidt numbers Sc in direct numerical modeling [19] are selected the same, variation of Sc leads to different values of dissipative length scales l_{turb}/l_c. What this means is that the scalar field has different structures at the initial instant of time, since the velocity field was the same for all Sc. Therefore, the initial levels of the mean rate of scalar dissipation $\chi(0)$ differ by a factor equal to Sc.

Analysis of the Data of Direct Numerical Modeling That Are Used in Finding the PDF of Scalar-Length Scales. The mean characteristics of the scalar field as functions of time for different Schmidt numbers are shown in Fig. 1. These coefficients were obtained using direct numerical modeling [19] in the same series of computational experiments, but the data of the direct numerical modeling for different Schmidt numbers were not included in [19].

Figure 1a gives the evolution of the variance and mean rate of scalar dissipation. Since there are no sources of development of the turbulent energy of an isotropic scalar field, it degenerates for all Sc values and the variance $\langle c^2 \rangle(t)$ decreases with time. An increase in the Schmidt number causes the degeneration of the scalar field to delay, since the intensity of turbulent transfer is attenuated.

The rate of dissipation of the scalar $\chi(t)$ changes with time nonmonotonically (Fig. 1a). On the initial portion, $\chi(t)$ is reduced for all Sc, which is attributed to the "breaking" of the scalar field substantially separated at $t = 0$ ($\langle c^2 \rangle(0) = 0.62$) by the turbulent velocity field. This leads to an increase in the mean dimension of diffusion layers and to a shift of the peak of the distribution of concentration-pulsation intensity $E_c(k, t)$ toward smaller k. Such a shift is accompanied by the decrease in the rate of dissipation of the scalar $\chi(t)$. Next, the turbulent field continues to "grind" the inhomogeneities of the scalar field, which is characterized by the thinning of diffusion layers; an active stage of the dissipative process with a close interaction of mechanical turbulent motions and molecular diffusion begins. The peak of the distribution $E_c(k, t)$ shifts toward larger wave numbers k and we have an increase in the dissipation, which is related to the increase in the vorticity of the scalar field. A considerable number of small-scale domains of a mixed medium appears in the flow (these domains separate regions with substantially different concentrations); the peaking of the scalar gradients occurs.

When $\langle c^2 \rangle(t) = 0.5$ the rapid stage of mixing is completed and the rate of dissipation of the scalar attains its local maximum $\chi(t)$ (Fig. 1a). In further evolution, determining is the mechanism of molecular diffusion. The latter ensures molecular motion across the boundaries of the domains of an unmixed medium, which reflects on the decrease in the variance $\langle c^2 \rangle(t)$ and the increase in the characteristic dimension of diffusion layers. The rate of scalar diffusion $\chi(t)$ for all Sc values also drops due to the considerable reduction in the level of variance. However, turbulence participates, as previously, in the reduction of the concentration field in size, thus creating new boundary conditions for the action of molecular diffusion.

Figure 1b shows the change in the joint asymmetry of the velocity-pulsation and scalar gradients $S_{uc}(t)$ with time. This function represents a correlation between the small-scale turbulent deformations of the velocity field and the scalar gradients existent in the flow. It shows the intensity of the action of the hydrodynamic field on the field of scalar inhomogeneities. As is clear from Fig. 1b, with the exception of the initial domain, the function $S_{uc}(t)$ is independent of the values of the Schmidt numbers in question and takes on values similar to an asymptotic value of –0.4. The analysis given in [21] has shown that such an asymptotic behavior of $S_{uc}(t)$ holds in a wide range of Sc numbers (from 0.04 to 144).

Results of Calculation of the PDF of Scalar-Length Scales and Its Statistical Moments. We consider the evolution of the forms of the scalar-length-scale PDF $f_t^{\lambda}(\varphi)$ in the form of the dependence of the level of variance of the scalar $\langle c^2 \rangle(t)$. The change in the length-scale PDF for the Schmidt number Sc = 0.7 is plotted in Fig. 2. The dynamics of change in this function for other Sc values is analogous.

When $\langle c^2 \rangle(t) = 0.62$ the form $f_t^{\lambda}(\varphi)$ retrospectively obtained by solution of (13)–(15) has the form of a smooth function with the existence of a wide range of scalar scales in the flow (Fig. 2a, curve 1). Next, the function shifts toward higher values of φ. The fraction of such scales increases (Fig. 2a, curves 2 and 3). For a variance of the scalar of the order of $\langle c^2 \rangle(t) = 0.58$ (here $\chi(t)$ attains its local minimum), the reverse motion of the peak of the

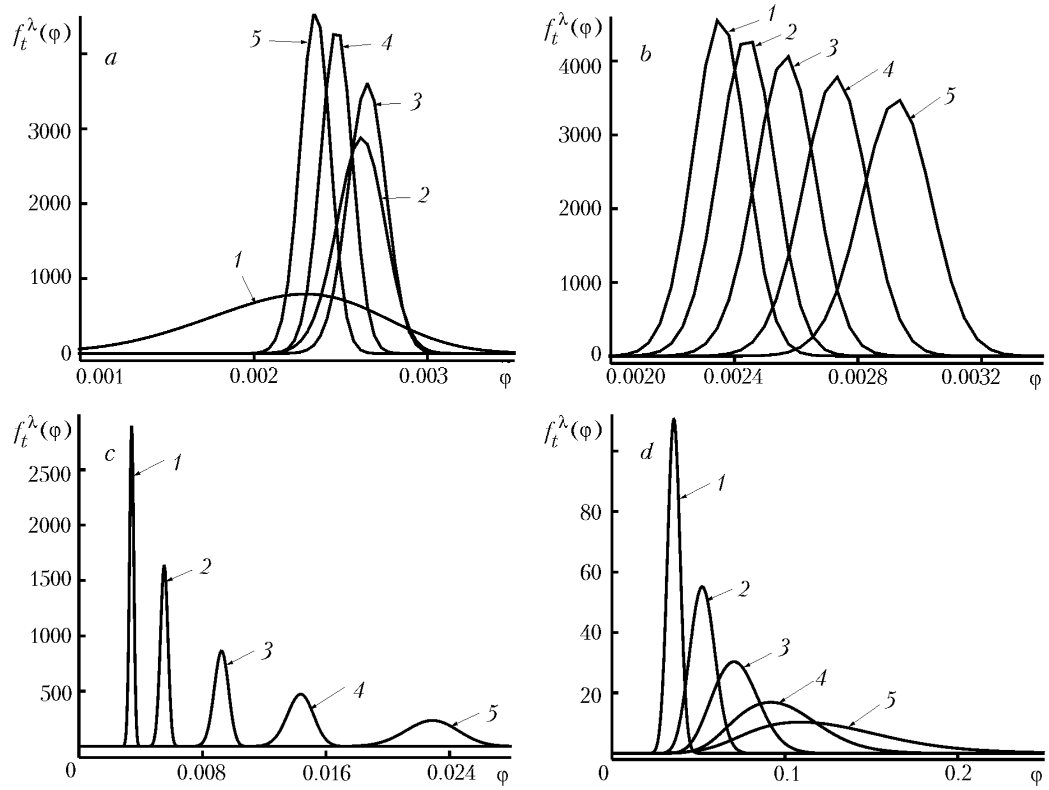

Fig. 2. Scalar-length-scale PDF for Sc = 0.7 at different levels of variance of the scalar: a) 1) $\langle c^2\rangle(t)$ = 0.62; 2) 0.6; 3) 0.58; 4) 0.55; 5) 0.5; b) 1) $\langle c^2\rangle(t)$ = 0.5; 2) 0.45; 3) 0.4; 4) 0.37; 5) 0.34; c) 1) $\langle c^2\rangle(t)$ = 0.3; 2) 0.2; 3) 0.12; 4) 0.09; 5) 0.06; d) 1) $\langle c^2\rangle(t)$ = 0.05; 2) 0.04; 3) 0.03; 4) 0.025; 5) 0.02.

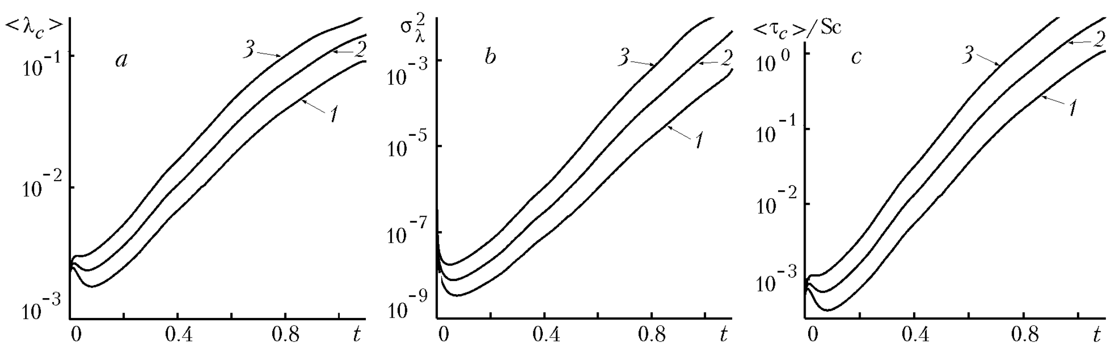

Fig. 3. Mean length scale $\langle\lambda_c\rangle$ (a); variance of length scales $\sigma_\lambda^2 = \langle\lambda_c^2\rangle - \langle\lambda_c\rangle^2$ (b); mean time scale $\langle\tau_c\rangle$ divided by Sc (c) vs. values of the Schmidt number Sc. Notation 1–3 is the same as in Fig. 1.

$f_t^\lambda(\varphi)$ distribution begins with its further growth (Fig. 2a, curves 3–5). Once the level of variance $\langle c^2\rangle(t) = 0.5$ has been attained and the rate of scalar dissipation has overcome its maximum, a slow evolution of $f_t^\lambda(\varphi)$ (Fig. 2, b–d) in the direction of high φ values begins. The probability of existence of a wide range of values of the scalar-length scales is reduced. We can explain such a behavior of the PDF of length scales, considering the statistical moments of this function: the mean length and time scales and the variance of length scales (Fig. 3).

During the initial time interval, the disturbed scalar field is broken and deformed by the velocity field to the characteristic minimum scales of turbulence; the action of molecular diffusion is slight. An increase in the area of diffusion layers due to this reflects on the increase in the mean scale of scalar lengths (Fig. 3a). Next, an active phase of action of the mechanism of molecular diffusion, which smooths out the boundaries between domains of different

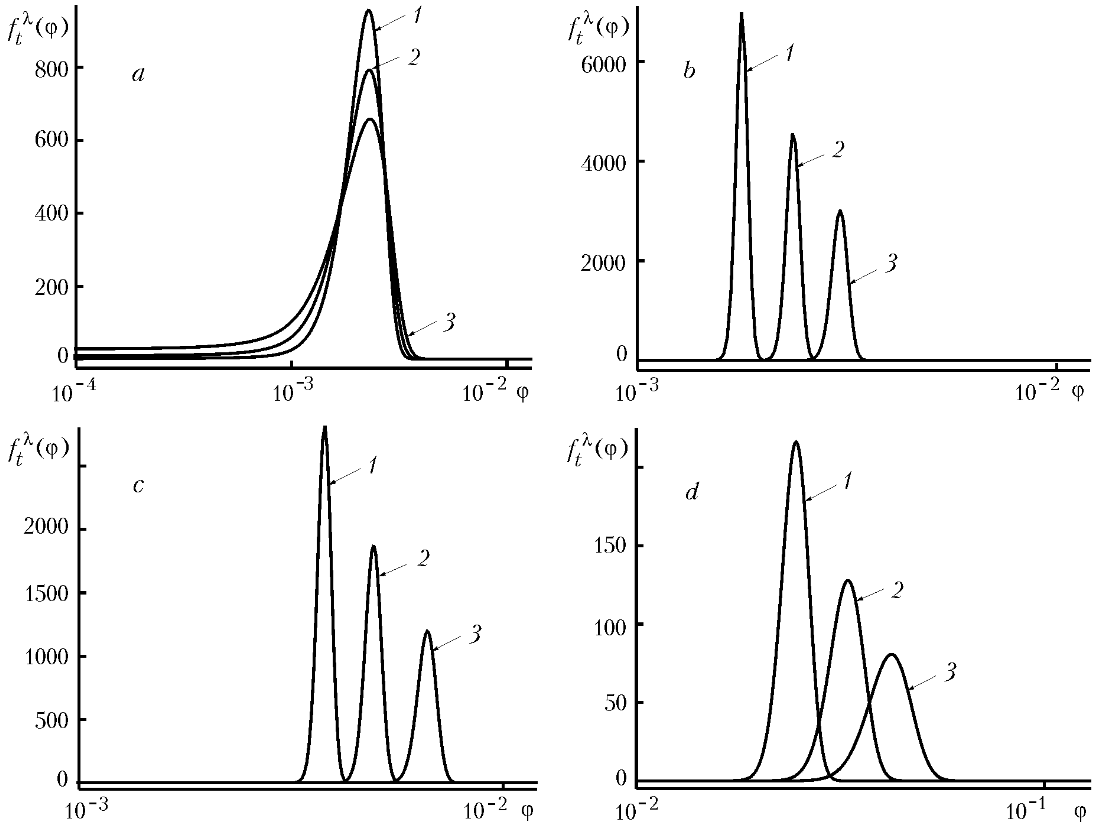

Fig. 4. Scalar-length-scale PDF for different values of the Schmidt number for $\langle c^2\rangle(t)$ = 0.62 (a), $\langle c^2\rangle(t)$ = 0.5 (b), $\langle c^2\rangle(t)$ = 0.2 (c), and $\langle c^2\rangle(t)$ = 0.05 (d). Notation 1–3 is the same as in Fig. 1.

concentration, begins against the background of the decrease in the inertia of the turbulent velocity field. A large number of thin diffusion layers separating such domains appears. Therefore, the mean length scale and the variance of the scales decrease (Fig. 3a and b). The subsequent formation of large volumes of a mixed medium in the flow as a result of the action of molecular diffusion leads to an increase in the relative weight of large diffusion-layer scales. This manifests itself as a growth in the mean length scale (Fig. 3a). At the same time, the decrease in the variance of the length scale (Fig. 3b) makes it impossible to speak of the disappearance of small scales, which is clear from the form of $f_t^\lambda(\varphi)$ as smooth functions in a wide range of the domain of definition (Fig. 2c and d).

Figure 3 also gives the mean scales of scalar lengths and time as functions of the Schmidt number. For all Sc, the change in these scales is linked with the dynamics of dissipative processes occurring in the flow: with the degeneration of the intensity of separation of the scalar field $\langle c^2\rangle(t)$ with a rate determined by the rate of scalar dissipation $\chi(t)$. A relatively weak inertia of the turbulent scalar field for smaller Schmidt numbers Sc leads to its more rapid degeneration. Such a circumstance brings about a difference in the forms of the PDF of scalar-length scales, which have been taken for different Sc at the same level of variance of the scalar (Fig. 4).

Conclusions. Based on the joint statistics of a passive scalar concentration field and its gradient, we have considered the process of fine-structure mixing (micromixing) in homogeneous turbulence. Such an approach made it possible to obtain the integral expression of the PDF of scalar-length scales in terms of the joint PDF of the scalar and its gradient. The closed equation derived for the PDF of scalar-length scales has been solved numerically. A significant difference in the evolution of the forms of the function sought and the mean length and time scale as a function of the Schmidt number has been shown.

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NOTATION

C, concentration; c, concentration pulsation (scalar); $\langle C \rangle$, mean value of the concentration; $|\nabla C|$, concentration gradient; $|\nabla c|$, scalar gradient; $\langle c^2 \rangle(t)$, variance of the scalar; D, diffusion coefficient, m^2/sec; $D_{cc}(r, t)$, structural function of second order of the scalar field; $E(k, t)$, turbulent-energy distribution over the spectrum of wave numbers k; $E_c(k, t)$, scalar-intensity distribution over the spectrum of wave numbers; $f_t^{\lambda}(\varphi)$, PDF of length scales; F_t^{λ}, distribution function; k, wave number; $K_{\text{turb}}(t)$, kinetic turbulence energy; L_0, t_0, U_0, and c_0, characteristic scales of length, time, velocity, and scalar; $l_c(t)$ and $t_c(t)$, mean microscales of scalar lengths and time; $l_{\text{turb}}(t)$, length microscale of the turbulent velocity field; $P_{x_i,t}(\Gamma, W)$, joint PDF of the scalar and its gradient; $\text{Pe} = U_0L_0/D$, Péclet number; $\text{Re} = U_0L_0/\nu$, Reynolds number; $\text{Re}_{\text{turb}} = u_{\text{rms}}l_{\text{turb}}/\nu$, turbulent Reynolds number; $\text{Sc} = \nu/D$, Schmidt number; $S_{uc}(t)$, joint asymmetry of the velocity-pulsation and scalar gradients; T, final instant of the time t; t, time variable; u_i, components of the velocity vector; $u_{\text{rms}}(t) = \sqrt{2K_{\text{turb}}(t)/3}$, root-mean-square velocity pulsation; W, probability variable of the scalar gradient $|\nabla c|$; α and β, limits of integration; Γ, probability variable of the scalar c; $\Gamma_{\max}$ and $\Gamma_{\min}$, maximum and minimum values of the change in the scalar; $\chi(t)$, mean rate of scalar dissipation; χ_c, instantaneous rate of scalar dissipation; ψ, random quantity; $\varepsilon(t)$, dissipation of velocity pulsations; ϕ_1, ϕ_2, and λ, arbitrary random quantities; $\phi_{\min}$ and $\phi_{\max}$, limits of variation in random quantities; φ, probability variable of the scale λ_c; λ_c and τ_c, local length and time scales of the scalar; $\langle \lambda_c \rangle$ and $\langle \tau_c \rangle$, mean length and time scales of the scalar; ν, kinematic viscosity, m^2/sec; σ, variance of the scalar gradient. Subscripts: i and j, components of vector quantities; max and min, maximum and minimum values; 0, parameters of making quantities dimensionless; rms, root-mean-square; s, totally separated field; turb, turbulence; t and x_i, dependence of the functions on the time and space variables.

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