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# A CLOSED EQUATION FOR THE JOINT PROBABILITY DENSITY FUNCTION OF THE MAGNITUDES OF FLUCTUATIONS OF A TURBULENT SCALAR REACTING FIELD AND ITS GRADIENT

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*We derived a closed system of equations for calculating the single-point joint probability density function (JPDF) of the magnitudes of fluctuations of a scalar reacting field and its gradient. The system of equations includes an equation for the JPDF and two equations for functions that describe the distribution of turbulent energy and of the reacting-scalar intensity over various length scales. The latter functions are necessary for calculation of the time-dependent coefficients in the equation for the JPDF.*

**1. Introduction.** Current approaches to turbulent combustion are associated with the study of flames that are far from the state of chemical equilibrium. The assumption of equilibrium chemistry, which provides the possibility of limiting oneself to the study of the statistics of a passive scalar field, turns out to be unsatisfactory. The development of theoretical models of turbulent combustion that take into account a large deviation from chemical equilibrium requires a deep knowledge of the statistical characteristics of the gradient of a turbulent scalar field.

In particular, it turned out that description of turbulent combustion in flows with nonpremixed reagents in a state close to local extinction requires a knowledge of the probability density of the magnitudes of the dissipation rates of the mixture coefficient fluctuations on a stoichiometric surface [1]. In order to calculate this function, it is necessary to derive and solve an equation for the joint probability density function (JPDF) of the magnitudes of the mixture coefficient and its gradient. So far, the problem has not been solved to an extent sufficient for practical application of such an equation, even though such attempts have been undertaken [2-6].

In [2] a closed equation was derived for the JPDF of a scalar and its gradient in an isotropic turbulent flow. It was used as a basis for analyzing the results of the action on the JPDF structure by the mechanisms of molecular mixing and chemical reaction and by the turbulent velocity field. The conclusion was drawn that a correlation between the field of the scalar and its gradient is induced by a chemical reaction and turbulent mixing. It was shown that the assumption of the statistical independence of a conservative scalar and its gradient in a turbulent flow becomes plausible only at large Reynolds numbers. Diffusion terms, which produce openness in the equation for the JPDF, were replaced by model expressions that describe relaxation of turbulent fluctuations of the scalar to its mean value. Because of the extreme simplification of diffusion effects, the solution of the equation for the JPDF closed in this manner incorrectly describes the evolution of the form of the sought function from a non-Gaussian initial condition.

In [3] another way of closing the equation for the JPDF of a scalar and its gradient was adopted. A mapping was established between the scalar field investigated and a multidimensional Gaussian standard field on each time interval, and thus the evolution of the statistical properties of the scalar field was found. As shown in [3], this amplitude closure is quite satisfactory for describing diffusion effects. However, the terms that describe turbulent stretching must be obtained on the basis of other considerations, for example, from results of direct numerical simulation of turbulent velocity and scalar fields.

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In [4, 5], to describe the JPDF of a scalar and its gradient, it is suggested that the Fokker–Planck equation based on a simple physical model of scalar transfer be used. This model gives results close to those obtained by numerical simulation of a nonpremixed system of certain formations (lamillas) with random dimensions. The evolution of marginal functions and the JPDF that was predicted on the basis of this model is in good qualitative agreement with results of numerical simulation.

In [6] certain properties of the JPDF of a scalar and its gradient have been studied. It is shown that the conditional probability density function of the scalar gradient values at a prescribed value of the scalar has a nearly Gaussian distribution. The conditional probabilities of the scalar derivatives were obtained in the form of Gramme–Charles series. The coefficients in these expansions were calculated using results of direct numerical simulation of a stationary turbulent scalar field.

We note once again that the JPDF of a scalar and its gradient is an important quantity for describing turbulent reacting flows and combustion and, as shown in [7], actually determines the chemical-reaction rate.

We made an attempt to derive a closed system of equations to describe the evolution of the JPDF of a reacting scalar and its gradient. The nonclosed equation given for this function in [8] was taken as the basis. This linear equation contains coefficients and conditional moments of various quantities that are to be calculated at fixed values of the scalar and its gradient. The closure of the equation for the JPDF is reduced to the calculation of these conditional moments. The closed equation for the JPDF contains time-dependent coefficients that can be calculated using any two-point functions. Spectral distributions of the energy of the turbulent velocity field and of the intensity of scalar fluctuations of the reacting fields and the corresponding closed equations for these functions are suitable for this purpose [9, 10]. It is also possible to resort to structural functions of the fields of the velocity $D_{LL}(r, t)$ and the scalar $D_{CC}(r, t)$. In the present work, in order to calculate the time-dependent coefficients in the equation for the JPDF, it is suggested that the functions $P_t(r) = -\partial D_{LL}(r, t)/\partial r$ and $P_t^{(c)}(r) = -\partial D_{CC}(r, t)/\partial r$ be used, closed equations for which are presented in [11]. These functions describe the distribution of the energy of turbulent fluctuations of the velocity and of the intensity of scalar fluctuations over various length scales. The closed system of equations obtained below for computing the JPDF of a scalar and its gradient will be used in what follows for deriving a closed equation for the conditional dissipation rate of the intensity of the mixture coefficient fluctuations.

**2. Nonclosed Equation for the JPDF of a Scalar and Its Gradient.** Equations that determine the dynamics of realizations of fluctuations of a scalar reacting field (and its gradient) have the form

$$\frac{\partial c}{\partial t} + u_\alpha \frac{\partial c}{\partial x_\alpha} = D \frac{\partial^2 c}{\partial x_\alpha \partial x_\alpha} = \dot{\omega}(c), \tag{1}$$

$$\frac{\partial z_i}{\partial t} + u_\alpha \frac{\partial z_i}{\partial x_\alpha} = \frac{\partial u_\alpha}{\partial x_i} z_\alpha + D \frac{\partial^2 z_i}{\partial x_\alpha \partial x_\alpha} + \frac{d\dot{\omega}}{dc} z_i, \quad i = 1, 2, 3. \tag{2}$$

In relations (1), (2) and below, the usual condition of summation over repeated indices from 1 to 3 is adopted; $D$ is the coefficient of kinematic diffusion; the variables $c$, $z_i$, and $u_\alpha$ denote fluctuations of the scalar reacting field, the components of its gradient, and the components of velocity fluctuations; the function $\dot{\omega}(c)$ describes fluctuations of the chemical-reaction rate. The variables $c$, $z_i$, and $u_\alpha$ are functions of the spatial variables $\vec{x}$ and the time $t$:

$$c \equiv c(\vec{x}, t); \quad z_i \equiv z_i(\vec{x}, t); \quad u_i \equiv u_i(\vec{x}, t); \quad i = 1, 2, 3. \tag{3}$$

The JPDF of a scalar and its gradient is defined by the formula

$$P_x(\vec{W}, \Gamma) = \left\langle \prod_{i=1}^{3} \delta(W_i - z_i)\, \delta(\Gamma - c) \right\rangle, \tag{4}$$

where $\langle\,\rangle$ denotes averaging over the ensemble of realizations; $x \equiv (\vec{x}, t)$; $W_i$ and $\Gamma$ are independent variables of the JPDF; $z_i$ and $c$ are functions that satisfy Eqs. (1) and (2).

In deriving an equation for the function $P_x(\vec{W}, \Gamma)$ the concept of the so-called fine-structure probability density is usually used (see p. 191 of [12]):

$$\mathscr{P} \equiv \prod_{i=1}^{3} \delta(W_i - z_i)\,\delta(\Gamma - c)\,. \tag{5}$$

Comparing Eqs. (4) and (5), we obtain that $P_x(\vec{W}, \Gamma) = \langle \mathscr{P} \rangle$.

An equation for the JPDF $P_x(\vec{W}, \Gamma)$ is derived by differentiation of expression (4) with respect to time, replacement of the derivatives $\partial c/\partial t$ and $\partial z_i/\partial t$ by their values from Eqs. (1) and (2), and subsequent averaging of each of the terms obtained. The nonclosed equation for the function $P_x(\vec{W}, \Gamma)$ is given in [8] (see formulas (305) and (306)). We will write it here as a matter of convenience, having changed somewhat the notation and restricting ourselves to the isotropic case. Here, all terms associated with spatial derivatives will be discarded:

$$\frac{\partial P_t(\vec{W}, \Gamma)}{\partial t} = -DW^2 \frac{\partial^2}{\partial \Gamma^2} P_t(\vec{W}, \Gamma) + \frac{\partial}{\partial W_\alpha}\left[W_\beta A_{\alpha\beta}(t \mid \vec{W}, \Gamma)\, P_t(\vec{W}, \Gamma)\right] -$$

$$- D \frac{\partial^2}{\partial W_\alpha \partial W_\beta}\left[N_{\alpha\beta}(t \mid \vec{W}, \Gamma)\, P_t(\vec{W}, \Gamma)\right] - 2D \frac{\partial^2}{\partial W_\alpha \partial \Gamma}\left[W_\beta X_{\alpha\beta}(\vec{W}, \Gamma)\, P_t(\vec{W}, \Gamma)\right] -$$

$$- \frac{\partial}{\partial \Gamma}\left[\dot{\omega}(\Gamma)\, P_t(\vec{W}, \Gamma)\right] - \frac{\partial}{\partial W_\alpha}\left[\frac{\partial \dot{\omega}}{\partial \Gamma} W_\alpha P_t(\vec{W}, \Gamma)\right]. \tag{6}$$

The first term on the right-hand side of Eq. (6) enters into the equation for the JPDF in closed form. It describes the effect of the process of diffusion in the space of scalar values. The second term of the equation contains the conditional mean tensor of the velocity gradient calculated at fixed values of the scalar $c = \Gamma$ and its gradient $\vec{z} = \vec{W}$:

$$A_{\alpha\beta}(t \mid \vec{W}, \Gamma) = \int d\vec{\vec{G}}\, G_{\alpha\beta} P_t(\vec{\vec{G}} \mid \vec{W}, \Gamma)\,. \tag{7}$$

Here $P_t(\vec{\vec{G}} \mid \vec{W}, \Gamma)$ is the conditional JPDF of the velocity gradient values; $\int d\vec{\vec{G}}$ denotes multidimensional integration over the values of the components of the velocity gradient tensor $G_{\alpha\beta}$. In contrast to the usual mean value of the velocity fluctuation gradient, equal to zero in a turbulent isotropic flow, the conditional mean components of the velocity gradient are not equal to zero. They tend to zero if there is no statistical dependence between the fluctuational field of the velocity gradient and the fields of the scalar and its gradient. By means of the second term on the right-hand side of Eq. (6), the effect of the gradient of turbulent velocity fluctuations on the joint statistics of the scalar reacting field and its gradient is described. The third term on the right-hand side of Eq. (6) involves the tensor of the conditional rate of dissipation of the dissipation calculated at fixed values of the scalar and its gradient:

$$N_{\alpha\beta}(t \mid \vec{W}, \Gamma) = \int d\vec{\vec{X}}_{\alpha i} X_{\beta i} P_t(\vec{\vec{X}} \mid \vec{W}, \Gamma)\,. \tag{8}$$

Here $P_t(\vec{\vec{X}} \mid \vec{W}, \Gamma)$ is the conditional JPDF of the values of the components of the tensor of the gradient of the gradient (i.e., of the second derivative) of the scalar; $\int d\vec{\vec{X}}$ denotes multidimensional integration over the values of the components of the tensor $X_{\alpha\beta}$. This term describes the effect of dissipation in the space of the scalar gradient on the joint statistics of the scalar reacting field and its gradient. The fourth term on the right-hand side of Eq. (6) involves the tensor of the mean conditional gradient of the scalar gradient, which must be calculated at fixed values of the scalar and its gradient. This term describes the effect of cross diffusion in the space of the scalar and the scalar gradient on the joint statistics of the reacting scalar and its gradient:

$$X_{\alpha\beta}(t \mid \vec{W}, \Gamma) = \int d\vec{\vec{X}} X_{\alpha\beta} P_t(\vec{\vec{X}} \mid \vec{W}, \Gamma). \tag{9}$$

Usual mean values of the second derivative of scalar fluctuations are equal to zero. But conditionally averaged components of this tensor are equal to zero only in the absence of a dependence between the second derivative of the scalar, its first derivative, and the scalar. The fifth and the sixth terms on the right-hand side of Eq. (6) describe the effect exerted on the JPDF by the chemical-reaction rate.

From Eqs. (6)-(9) it is seen that the openness of the equation for the JPDF $P_t(\vec{W}, \Gamma)$ is due to the presence of the tensor coefficients $\vec{\vec{A}}$, $\vec{\vec{N}}$, and $\vec{\vec{X}}$ in Eq. (6). The components of these tensors are conditional moments of the fields of the velocity gradient and the gradient of the scalar-field gradient. These quantities must be calculated on the condition that the scalar field and its gradient take certain values: $c = \Gamma$, $\vec{z} = \vec{W}$. As is seen from equalities (7)-(9), in order to calculate the conditional quantities $\vec{\vec{A}}$, $\vec{\vec{N}}$, and $\vec{\vec{X}}$ it is necessary to have the conditional JPDFs $P_t(\vec{\vec{G}} \mid \vec{W}, \Gamma)$ and $P_t(\vec{\vec{X}} \mid \vec{W}, \Gamma)$. For approximate evaluation of the form of these functions, we can employ their formal definitions:

$$P_t(\vec{\vec{G}} \mid \vec{W}, \Gamma) = \frac{P_t(\vec{\vec{G}}, \vec{W}, \Gamma)}{P_t(\vec{W}, \Gamma)}, \quad P_t(\vec{\vec{X}} \mid \vec{W}, \Gamma) = \frac{P_t(\vec{\vec{X}}, \vec{W}, \Gamma)}{P_t(\vec{W}, \Gamma)}. \tag{10}$$

The right-hand sides of these formulas are expressed in terms of the usual (i.e., unconditional) quantities. Here $P_t(\vec{\vec{G}}, \vec{W}, \Gamma)$ is the JPDF of the fields of the velocity gradient, the scalar gradient, and the scalar; $P_t(\vec{\vec{X}}, \vec{W}, \Gamma)$ is the JPDF of the fields of the gradient of the scalar gradient, the scalar gradient, and the scalar; $P_t(\vec{W}, \Gamma)$ is the JPDF of the fields of the scalar gradient and the scalar, i.e., the very function for which we are trying to write a closed equation.

The tensor coefficients in Eqs. (7)-(9) can be expressed approximately in terms of the usual (unconditional) moments of the fields of the velocity gradient, the gradient of the scalar gradient, and the scalar and all cross moments of these fields. If we assume that all JPDFs on the right-hand sides of Eqs. (10) are Gaussian, then the expression for the conditional JPDFs will be determined by the second-order moments of the fields $\partial u_\alpha/\partial x_\beta$, $\partial z_\alpha/\partial x_\beta$, $z_\alpha$, and $c$. But if the Gaussian approximation turns out to be insufficient for calculating conditional quantities, then, to refine the corresponding JPDFs, one can use information on the higher-order moments of these fields. In the present case, expansion into a Gramme–Charles series may prove useful [13]. The problem of closure of Eq. (6) can be considered to be solved if one manages to obtain expressions for the conditional tensor coefficients $\vec{\vec{A}}$, $\vec{\vec{N}}$, $\vec{\vec{X}}$ in terms of the usual moments and to calculate these moments from closed equations. The entire remaining part of this paper is concerned with the calculation of the conditional tensor coefficients $\vec{\vec{A}}$, $\vec{\vec{N}}$, and $\vec{\vec{X}}$.

**3. Calculation of the Conditional JPDF $P_t(\vec{\vec{G}} \mid \vec{W}, \Gamma)$ in the Gaussian Approximation.** As seen from Eq. (10), in order to calculate the conditional JPDF of the velocity gradient tensor in the Gaussian approximation, it is necessary to calculate the functions $P_t(\vec{\vec{G}}, \vec{W}, \Gamma)$ and $P_t(\vec{W}, \Gamma)$ in this approximation. We will first write out the function $P_t(\vec{\vec{G}}, \vec{W}, \Gamma)$ in general form:

$$P_t(\vec{\vec{G}}, \vec{W}, \Gamma) = \frac{\exp\left\{-\frac{1}{2}\sum_{\alpha=1}^{12}\sum_{\beta=1}^{12} d_{\alpha\beta}\xi_\alpha\xi_\beta\right\}}{(2\pi)^6 D_1^{1/2}\sigma_1\sigma_2 \ldots \sigma_{12}}. \tag{11}$$

The symbols $\xi_i$, $i = 1, 2, \ldots, 12$, denote independent variables of the function $P_t(\vec{\vec{G}}, \vec{W}, \Gamma)$ that correspond to the components of the fields $\partial u_i/\partial x_j$, $z_\alpha$, and $c$. The correspondence between these components and the symbols

$\xi_i$ is prescribed by the following set of identities: $\partial u_1/\partial x_1 \Leftrightarrow \xi_1$, $\partial u_1/\partial x_2 \Leftrightarrow \xi_2$, $\partial u_1/\partial x_3 \Leftrightarrow \xi_3$, $\partial u_2/\partial x_1 \Leftrightarrow \xi_1$, $\partial u_2/\partial x_2 \Leftrightarrow \xi_5$, $\partial u_2/\partial x_3 \Leftrightarrow \xi_6$, $\partial u_3/\partial x_1 \Leftrightarrow \xi_7$, $\partial u_3/\partial x_2 \Leftrightarrow \xi_8$, $z_1 \Leftrightarrow \xi_9$, $z_2 \Leftrightarrow \xi_{10}$, $z_3 \Leftrightarrow \xi_{11}$, $c \Leftrightarrow \xi_{12}$. The acceleration component $\partial u_3/\partial x_3$ can be expressed in terms of $\partial u_1/\partial x_1$ and $\partial u_2/\partial x_2$ using the condition of incompressibility.

We will assume that all the variables $\xi_i$ are made dimensionlees by division by the corresponding dispersion: $\xi_i = \tilde{\xi}_i/\sigma_i$, $i = 1, 2, ..., 12$, where $\tilde{\xi}_i$ are the dimensional variables; $\sigma_i$ are the dispersions of the corresponding components; $D_1$ is the determinant of the correlation matrix $r_{ij}$; $d_{\alpha\beta}$ are elements of the matrix inverse to the correlation matrix, $d_{\alpha\beta} = r_{\alpha\beta}^{-1}$. The elements $r_{ik}$ are correlations between the quantities $\partial u_\alpha/dx_\beta$, $z_\alpha$, and $c$. In counting the number $n$ of correlations to be calculated, the symmetry of the matrix $r_{ik}$ is taken into account, as well as the fact that the diagonal elements of the correlation matrix are equal to unity: $n = [(12\cdot 12) - 12]/2 = 66$. The matrix elements that describe correlations between components of the velocity gradient field $r_{ik} = 1/(\sigma_i\sigma_k)\overline{(\partial u_j/\partial x_m)(\partial u_l/\partial x_n)}$ can be calculated by means of formula (13.53) of [14]:

$$r_{ik} = \frac{1}{2\sigma_i\sigma_k}\frac{\partial^2 D_{jl}(\vec{r})}{\partial r_m \partial r_n}\bigg|_{\vec{r}=0}. \tag{12}$$

Using the expression for the structural tensor $D_{jl}(\vec{r})$ in terms of the longitudinal structural function $D_{LL}(r, t)$:

$$D_{jl}(\vec{r}) = \left[\frac{r_j r_l}{r^2}\frac{r}{2}\frac{\partial}{\partial r} + \delta_{jl}\left(1 + \frac{r}{2}\frac{\partial}{\partial r}\right)\right] D_{LL}(r), \tag{13}$$

it is possible to express all the correlators of the form (12) in terms of local characteristics of the acceleration field (formula (13) is easily obtained from (13.69) and (13.87) of [14]).

Since the values of the structural function $D_{LL}(r, t)$ are required only for $r \to 0$, it is possible to avail ourselves of formulas (21.16) and (21.19′) of [14]:

$$D_{LL}(r) = Ar^2, \tag{14}$$

where $A = \varepsilon(t)/15\nu$, $\varepsilon(t)$ is the dissipation rate of the turbulent energy per unit mass of the liquid, and $\nu$ is the kinematic viscosity.

Using formulas (13) and (14), we obtain an expression for the single-point moments of the velocity gradient field:

$$\overline{\frac{\partial u_j}{\partial x_m}\frac{\partial u_l}{\partial x_n}} = \frac{A}{2}\left[4\delta_{jl}\delta_{mn} - \delta_{jn}\delta_{lm} - \delta_{ln}\delta_{jm}\right]. \tag{15}$$

With allowance for Eq. (15) we can easily calculate the magnitudes of the dispersions $\sigma_1, ..., \sigma_8$:

$$\sigma_1 = \sigma_5 = \sqrt{A}, \quad \sigma_2 = \sigma_3 = \sigma_4 = \sigma_6 = \sigma_7 = \sigma_8 = \sqrt{2A}. \tag{16}$$

Taking into account formulas (12) and (15), we obtain expressions for the elements of the correlation matrix $r_{ik}$ that are connected with the velocity gradient field. To calculate the remaining correlators of the matrix $r_{ik}$, it is necessary to consider expressions of the form

$$\overline{\frac{\partial c}{\partial x_i}\frac{\partial c}{\partial x_j}}, \quad \overline{c\frac{\partial c}{\partial x_j}}, \quad \overline{c^2}, \quad \overline{c\frac{\partial u_i}{\partial x_j}}, \quad \overline{\frac{\partial c}{\partial x_l}\frac{\partial u_i}{\partial x_j}}.$$

To calculate the correlators and dispersions connected with the scalar field gradient, we shall employ the formula for the two-point correlation tensor of the scalar field gradient (see (IV-5.3) of [15]) calculated for $r = 0$:

$$\overline{\frac{\partial c}{\partial x_i}\frac{\partial c}{\partial x_j'}} = \frac{1}{2}\left[\frac{rD''_{CC}(r) - D'_{CC}(r)}{r^3} r_i r_j + \frac{D'_{CC}(r)}{r}\delta_{ij}\right]. \tag{17}$$

Here $D_{CC}(r, t)$ is the structural function of the scalar field. In calculation of single-point correlators by means of Eq. (17) the value of the structural function $D_{CC}(r, t)$ can be taken at small values of $r$. As is known (see (21.86) of [14]),

$$\lim_{r \to 0} D_{CC}(r) = \chi(t)\, r^2/3D. \tag{18}$$

Using Eqs. (17) and (18) at $r = 0$, for the second-order single-point moments of the scalar-field gradient we obtain

$$\overline{\frac{\partial c}{\partial x_i}\frac{\partial c}{\partial x_j}} = \frac{\chi}{3D}\delta_{ij}. \tag{19}$$

The expression for the dispersions has the form

$$\sigma_i = \left(\overline{\left(\frac{\partial c}{\partial x_i}\right)^2}\right)^{1/2} = \sqrt{\left(\frac{\chi}{3D}\right)}^{1/2}, \quad i = 9, 10, 11. \tag{20}$$

The list of dispersions (16) and (20) should be supplemented with the obvious equality

$$\sigma_{12} = \sqrt{\left(\overline{c^2}\right)}. \tag{21}$$

For the correlators $r_{ii}$ at $i = 9$, 10, 11 we obtain

$$r_{9,9} = r_{10,10} = r_{11,11} = 1. \tag{22}$$

Taking into consideration the theorems on the correlations of random scalar and vector fields given in [15] (p. 148), we obtain that the correlation of the scalar field with the field of the scalar gradient and the velocity gradient is equal to zero in an isotropic flow. The same statement is also valid for the correlation of the scalar gradient and velocity gradient:

$$\overline{c\frac{\partial c}{\partial x_j}} = 0, \quad \overline{c\frac{\partial u_i}{\partial x_j}} = 0, \quad \overline{\frac{\partial c}{\partial x_l}\frac{\partial u_i}{\partial x_j}} = 0. \tag{23}$$

Finally, the correlation matrix $r_{\alpha\beta}$, where $\alpha, \beta = 1, \ldots, 12$, has the form

$r_{\alpha\beta} =$ (24)

| $\alpha \backslash \beta$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 0 | 0 | 0 | − 1/2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2 | 0 | 1 | 0 | − 1/4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | 0 | 0 | 1 | 0 | 0 | 0 | − 1/4 | 0 | 0 | 0 | 0 | 0 |
| 4 | 0 | − 1/4 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | − 1/2 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | − 1/4 | 0 | 0 | 0 | 0 |
| 7 | 0 | 0 | − 1/4 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 |
| 8 | 0 | 0 | 0 | 0 | 0 | − 1/4 | 0 | 1 | 0 | 0 | 0 | 0 |
| 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 |
| 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 |
| 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 |
| 12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |

To calculate $d_{\alpha\beta} = r_{\alpha\beta}^{-1}$, we can avail ourselves of the Gauss method [16] or the computer library MathCad. The result of the computation of the inverse matrix $d_{\alpha\beta}$ has the form

$$d_{\alpha\beta} = \left( \begin{array}{ccccccccccccc} \alpha \backslash \beta & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\ 1 & 4/3 & 0 & 0 & 0 & 2/3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 16/15 & 0 & 4/15 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & 16/15 & 0 & 0 & 0 & 4/15 & 0 & 0 & 0 & 0 & 0 \\ 4 & 0 & 4/5 & 0 & 16/15 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 5 & 2/3 & 0 & 0 & 0 & 4/3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 6 & 0 & 0 & 0 & 0 & 0 & 16/15 & 0 & 4/15 & 0 & 0 & 0 & 0 \\ 7 & 0 & 0 & 4/15 & 0 & 0 & 0 & 16/15 & 0 & 0 & 0 & 0 & 0 \\ 8 & 0 & 0 & 0 & 0 & 0 & 4/5 & 0 & 16/15 & 0 & 0 & 0 & 0 \\ 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 10 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 11 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 12 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array} \right) . \tag{25}$$

The determinant $D_1$ of the inverse matrix $d_{\alpha\beta}$ can easily be calculated:

$$D_1 = \| r_{ik} \| = \frac{3}{4} \left( \frac{15}{16} \right)^3 . \tag{26}$$

Formulas (26) for $D_1$, (16), (20), (21) for $\sigma_i$, and (25) for $d_{\alpha\beta}$ completely determine the 12-dimensional distribution density function (11) in Gaussian approximation. The JPDF $P_t(\vec{W}, \Gamma)$, which is necessary for calculating the conditional function (10), is prescribed in the Gaussian approximation by the formula

$$P_t(\vec{W}, \Gamma) = \frac{\exp\left\{ -\frac{1}{2} \sum_{\alpha=9}^{12} \sum_{\beta=9}^{12} d_{\alpha\beta} \xi_\alpha \xi_\beta \right\}}{(2\pi)^2 D_2^{1/2} \sigma_9 \sigma_{10} \sigma_{11} \sigma_{12}} . \tag{27}$$

The matrix $d_{\alpha\beta}$, $\alpha, \beta = 9, 10, 11, 12$, can be written in the form $d_{\alpha\beta} = \delta_{\alpha\beta}$. The determinant $D_2 = 1$. Substituting expressions (11) and (27) into (10), we obtain the JPDF $P_t(\vec{\vec{G}} | \vec{W}, \Gamma)$ in the Gaussian approximation:

$$P_t(\vec{\vec{G}} | \vec{W}, \Gamma) = \frac{\exp\left\{ -\frac{1}{2} \sum_{\alpha=1}^{8} \sum_{\beta=1}^{8} d_{\alpha\beta} \xi_\alpha \xi_\beta \right\}}{(2\pi)^4 D^{1/2} \sigma_1 \sigma_2 \dots \sigma_8} , \tag{28}$$

where $D = D_1/D_2 = (3/4)(15/16)^3$. The elements of the matrix $d_{\alpha\beta}$ are determined by the upper non-identity block in (25). Using the specific values of $d_{\alpha\beta}$, we shall write out the form of the function $P_t(\vec{\vec{G}} | \vec{W}, \Gamma) = P_t(\xi_1, \xi_2, \dots, \xi_8 | \xi_9, \xi_{10}, \xi_{11}, \xi_{12})$ in more detail:

$$P_t(\xi_1, \xi_2, \dots \xi_8 | \xi_9, \xi_{10}, \xi_{11}, \xi_{12}) = \frac{1}{(2\pi)^4 D \sigma_1 \sigma_2 \dots \sigma_8} \exp\left\{ -\frac{1}{2} Q \right\} \equiv f_{CG}\left( \{ \xi_\gamma \} \right) , \tag{29}$$

where

$$Q\left( \{ \xi \} \right) = \frac{4}{3} (\xi_1^2 + \xi_1 \xi_5 + \xi_5^2) + \frac{16}{15} (\xi_2^2 + \xi_3^2 + \xi_4^2 + \xi_6^2 + \xi_7^2 + \xi_8^2) +$$

$$+ \frac{8}{15} (\xi_2 \xi_4 + \xi_3 \xi_7 + \xi_6 \xi_8) .$$

Thus, the expression for JPDF in the Gaussian approximation is determined in terms of $\xi_i^2$. As is seen from Eq. (7), the expression for $A_{\alpha\beta}(t | \vec{W}, \Gamma)$ is an integral of the first degree of the independent variable multiplied by the distribution function. Therefore, in the Gaussian approximation all the components of the tensor $A_{\alpha\beta}(t|\vec{W}, \Gamma)$ are equal to zero. This circumstance compels one to use the JPDF $P_t(\vec{\vec{G}}|\vec{W}, \Gamma)$ for an approximate calculation of the tensor $A_{\alpha\beta}(t|\vec{W}, \Gamma)$, with asymmetry taken into account.

**4. Calculation of the Conditional JPDF $P_t(\vec{\vec{G}}|\vec{W}, \Gamma)$ with Account for Asymmetry.** From Eq. (29) it is seen that the JPDF $P_t(\vec{\vec{G}}|\vec{W}, \Gamma)$ in the Gaussian approximation is independent of the variables $\xi_9 - \xi_{12}$, which correspond to the fields $\vec{z}(\vec{x})$ and $c(\vec{x})$, i.e., in the Gaussian approximation the conditional JPDF (29) is described as independent of the fields $z_i(\vec{x})$ and $c(\vec{x})$. This is due to the fact that the second-order correlators between the velocity gradient field and the fields of the scalar and its gradient are equal to zero and in the Gaussian approximation the absence of correlation looks like independence.

Since there is dependence between these fields, it should be taken into account by means of the third-order moments, i.e., by resorting to the asymmetry in simulating the JPDF $P_t(\vec{\vec{G}}|\vec{W}, \Gamma)$. For this purpose we can employ the Gramme–Charles series [13]. In the multidimensional variant the first two terms of this series have the form

$$f\left(\{\xi_i\}\right) = f_G\left(\{\xi_i\}\right) + \frac{1}{3!} T_{\alpha\beta\gamma} \frac{\partial^3}{\partial\xi_\alpha\, \partial\xi_\beta\, \partial\xi_\gamma} f_G\left(\{\xi_i\}\right). \tag{30}$$

Here $f_G(\{\xi_i\})$ is the JPDF in the Gaussian approximation, $T_{\alpha\beta\gamma}$ are third-order moments made dimensionless by division by the corresponding dispersion.

Calculation of $P_t(\vec{\vec{G}}|\vec{W}, \Gamma)$ according to Eq. (30) yields

$$P(\vec{\vec{G}}, \vec{W}, \Gamma) = f_1\left(\{\xi_\gamma\}\right)\left[1 + \frac{1}{6}\tilde{T}_1\right], \tag{31}$$

where $f_1(\{\xi_\gamma\})$ is defined by expression (11), $\tilde{T}_1 = \sum_{\alpha=1}^{12}\sum_{\beta=1}^{12}\sum_{\gamma=1}^{12} T_{\alpha\beta\gamma}\Pi^{(1)}_{\alpha\beta\gamma}$, and

$$\Pi^{(1)}_{\alpha\beta\gamma} = -\sum_{i=1}^{12}\sum_{j=1}^{12}\sum_{k=1}^{12} d_{\alpha i}\, d_{\beta j}\, d_{\gamma k}\, \xi_i \xi_j \xi_k + \sum_{i=1}^{n}\left(d_{\alpha\beta}\, d_{\gamma i} + d_{\alpha\gamma}\, d_{\beta i} + d_{\beta\gamma}\, d_{\alpha i}\right)\xi_i,$$
$$\alpha, \beta, \gamma = 1, 2, \ldots, 12. \tag{32}$$

To calculate the conditional JPDF $P_t(\vec{\vec{G}}|\vec{W}, \Gamma)$ from formula (10), it is necessary to know the form of $P_t(\vec{W}, \Gamma)$. In the Gaussian approximation an expression for this function is prescribed by formula (27). With allowance for the third-order moments the function $P_t(\vec{W}, \Gamma)$ is written in the form

$$P_t(\vec{W}, \Gamma) = f_2\left(\{\xi_\gamma\}\right)\left[1 + \frac{1}{6}\tilde{T}_2\right]. \tag{33}$$

Here $f_2(\{\xi_\gamma\})$ is defined by expression (27), $\tilde{T}_2 = \sum_{\alpha=9}^{12}\sum_{\beta=9}^{12}\sum_{\gamma=9}^{12} T_{\alpha\beta\gamma}\Pi^{(2)}_{\alpha\beta\gamma}$, and

$$\Pi^{(2)}_{\alpha\beta\gamma} = -\sum_{i=9}^{12}\sum_{j=9}^{12}\sum_{k=9}^{12} d_{\alpha i}\, d_{\beta j}\, d_{\gamma k}\, \xi_i \xi_j \xi_k + \sum_{i=9}^{12}\left(d_{\alpha\beta}\, d_{\gamma i} + d_{\alpha\gamma}\, d_{\beta i} + d_{\beta\gamma}\, d_{\alpha i}\right)\xi_i,$$
$$\alpha, \beta, \gamma = 9, 10, 11, 12. \tag{34}$$

Now, we will calculate the conditional JPDF $P_t(\vec{\vec{G}}|\vec{W}, \Gamma)$ in accordance with Eq. (10), taking into account the third-order moments:

$$P_t(\vec{\vec{G}}|\vec{W}, \Gamma) = \left[f_1\left(\{\xi_\gamma\}\right) / f_2\left(\{\xi_\gamma\}\right)\right]\left(1 + \frac{1}{6}\tilde{T}_1\right) / \left(1 + \frac{1}{6}\tilde{T}_2\right) =$$

$$= f_{CG}\left(\left\{\xi_\gamma\right\}\right)\left(1+\frac{1}{6}\widetilde{T}_1\right)\Big/\left(1+\frac{1}{6}\widetilde{T}_2\right). \tag{35}$$

Here $f_{CG}(\{\xi_\gamma\})$ is the conditional JPDF defined in the Gaussian approximation by Eq. (29). It is seen from Eq. (35) that in order to calculate the JPDF $P_t(\vec{\vec{G}}\,|\,\vec{W},\Gamma)$ it is necessary to know the explicit form of the expressions for $\widetilde{T}_1$ and $\widetilde{T}_2$, which are represented by a convolution of the matrices $T_{\alpha\beta\gamma}$ and $\Pi^{(i)}_{\alpha\beta\gamma}$. In calculation of $\widetilde{T}_1$ and $\widetilde{T}_2$ it is convenient first to write out all the nonzero elements of the matrix $T_{\alpha\beta\gamma}$ and then to calculate only those elements of the matrix $\Pi^{(i)}_{\alpha\beta\gamma}$ that are needed to find $\widetilde{T}_i$.

The number of components $M$ of the tensor $T_{\alpha\beta\gamma}$ can be calculated as $M = (n-1+m)!/(n-1)!m!$ (see formula (14.17) of [17]). This formula gives the number of combinations of $n$ objects taken $m$ at a time. In the case considered $n = 12$ and $m = 3$, i.e., three subscripts for the tensor $T_{\alpha\beta\gamma}$, each of which can take on 12 values. As seen from the formula for $M$, the total number of components of the matrix $T_{\alpha\beta\gamma}$, i.e., the number of single-point third-order moments of the fields $\partial u_i/\partial x_j$, $z_\alpha$, and $c$, is rather large. It is necessary to take into account, in principle, the following moments:

$$\overline{\frac{\partial u_i}{\partial x_j}\frac{\partial u_k}{\partial x_l}\frac{\partial u_m}{\partial x_n}},\quad \overline{\frac{\partial u_i}{\partial x_i}\frac{\partial u_k}{\partial x_l}\frac{\partial c}{\partial x_m}},\quad \overline{\frac{\partial u_i}{\partial x_j}\frac{\partial c}{\partial x_k}\frac{\partial c}{\partial x_l}},\quad \overline{\frac{\partial c}{\partial x_i}\frac{\partial c}{\partial x_j}\frac{\partial c}{\partial x_k}},$$

$$\overline{\frac{\partial c}{\partial x_i}\frac{\partial c}{\partial x_j}c},\quad \overline{\frac{\partial c}{\partial x_i}c^2},\quad \overline{c^3},\quad \overline{\frac{\partial u_i}{\partial x_j}\frac{\partial u_k}{\partial x_l}c},\quad \overline{\frac{\partial u_i}{\partial x_j}c^2}. \tag{36}$$

Among all possible third-order moments there are ones that are equal to zero in the isotropic case. An indication of zero components is a change in their sign on rotation of the system 180° about any axis and mirror reflection relative to any plane. As a result of an analysis of all 364 moments, only nonzero ones were selected and among the latter the groups of moments having the same magnitude were determined. In all, the different groups of moments amounted to 18, among which 9 were connected with the velocity gradient, 3 with the velocity gradient and the scalar gradient, 4 with the velocity gradient and the scalar, 1 with the scalar gradient and the scalar, and 1 only with the scalar. Direct calculation shows that the groups of moments connected only with the velocity gradient, only with the scalar gradient, with the velocity gradient and the scalar, with the scalar gradient and the scalar, and only with the scalar make a zero contribution to the value of the conditional moments of the velocity gradient.

To calculate the explicit form of the function $\widetilde{T}_j$, $j = 1, 2$, it is necessary to write out the values of the components of the tensors $\Pi^{(i)}_{\alpha\beta\gamma}$ whose indices coincide with the indices of the nonzero components of the tensor $T_{\alpha\beta\gamma}$. Each of the above-mentioned groups of tensor components involves components that have the same value. Therefore, it is reasonable to write out the corresponding sums of the components of the tensors $\Pi^{(i)}_{\alpha\beta\gamma}$, since these sums must be multiplied by the same value of the corresponding component of the tensor $T_{\alpha\beta\gamma}$ to calculate $\widetilde{T}_i$. We shall denote these sums by the symbol $\Pi_i$:

$$\Pi_i = \Sigma\ \Pi^{(j)}_{\alpha\beta\gamma}(i),\quad i = 1, 2, \ldots, 18, \tag{37}$$

where $\Pi^{(i)}_{\alpha\beta\gamma}(i)$ are the tensors $\Pi^{(j)}_{\alpha\beta\gamma}$ to which identical single-point third-order moments $T_{\alpha\beta\gamma} = a_i$ correspond. Thus, the expressions for $\widetilde{T}_1$ and $\widetilde{T}_2$ can be written in the form

$$\widetilde{T}_1 = \sum_{i=1}^{18} a_i\,\Pi_i,\quad \widetilde{T}_2 = \sum_{i=17}^{18} a_i\,\Pi_i. \tag{38}$$

We replace expression (35) for $P_t(\vec{\vec{G}}\,|\,\vec{W},\Gamma)$ by an approximate expression:

$$P_t(\vec{\vec{G}}\,|\,\vec{W},\Gamma) = f_{CG}\left(\left\{\xi_\gamma\right\}\right)\left(1+\widetilde{T}_1/6\right)\left(1+\widetilde{T}_2/6\right)^{-1} \approx f_{CG}\left(\left\{\xi_\gamma\right\}\right)\left(1+\widetilde{T}_1/6\right)\times$$

$$\times \left(1 - \widetilde{T}_2/6\right) \approx f_{CG} \left(\left\{ \xi_\gamma \right\}\right) \left[1 + (\widetilde{T}_1 - \widetilde{T}_2)/6\right] = f_{CG} \left[1 + \widetilde{T}(\xi)/6\right], \tag{39}$$

where $\widetilde{T}(\xi) = \widetilde{T}_1 - \widetilde{T}_2 = \sum_{j=1}^{16} a_i \Pi_i$. Here $a_i = a_i(t)$ are third-order single-point moments of the velocity gradient, the scalar gradient, and the scalar. Substituting the values of $\Pi_i$ into the expression for $\widetilde{T}(\xi)$, we obtain

$$\begin{aligned}\widetilde{T}(x) = {} & a_1 [0] + a_2 [0] + a_3 [0] + a_4 [0] + a_5 [0] + a_6 [0] + a_7 [0] + a_8 [0] + \\ & + a_9 [0] + a_{10} \left[\left(-\frac{4}{3}\xi_1 - \frac{2}{3}\xi_5\right)\xi_9^2 + \left(-\frac{2}{3}\xi_1 - \frac{4}{3}\xi_5\right)\xi_{10}^2 + 2(\xi_1 + \xi_5)\right] + \\ & + a_{11} \left[\left(-\frac{2}{3}\xi_1 - \frac{4}{3}\xi_5\right)\xi_9^2 + \left(-\frac{4}{3}\xi_1 - \frac{2}{3}\xi_5\right)\xi_{10}^2 + (-2\xi_1 - 2\xi_5)\xi_{11}^2 + 4(\xi_1 + \xi_5)\right] + \\ & + a_{12} \left[-\frac{4}{3}(\xi_2 + \xi_4)\xi_9\xi_{10} - \frac{4}{3}(\xi_3 + \xi_7)\xi_9\xi_{11} - \frac{4}{3}(\xi_6 + \xi_8)\xi_{10}\xi_{11}\right] + \\ & + a_{13} [0] + a_{14} [0] + a_{15} [0] + a_{16} [0].\end{aligned} \tag{40}$$

Thus, formulas (39), (40), and (29) prescribe the conditional probability density function of the velocity gradient with allowance for asymmetry.

**5. Calculation of the Components of the Tensor of the Mean Conditional Velocity Gradient.** The tensor of the mean conditional velocity gradient is defined by formula (7). We write it in a form more convenient for further use:

$$A_{\alpha\beta}(t \mid \vec{W}, \Gamma) = \left\langle \frac{\partial u_\alpha}{\partial x_\beta} \mid \vec{W}, \Gamma \right\rangle = \sqrt{A} \int \ldots \int d\xi_1 \ldots d\xi_8 \xi_i P_t(\xi_1, \ldots, \xi_8 \mid \xi_9, \xi_{10}, \xi_{11}, d\xi_{12}). \tag{41}$$

We rewrite Eq. (41) explicating the form of the JPDF by means of (39) and (29):

$$A_{\alpha\beta}(t \mid \vec{W}, \Gamma) = \frac{\sqrt{A}}{(2\pi)^4 D^{1/2}} \int \ldots \int d\xi_1 \ldots d\xi_8 \exp\left\{-\frac{1}{2}Q(\xi)\right\} \xi_i \left[1 + \frac{1}{6}\widetilde{T}(\xi)\right], \quad i = 1, 2, \ldots, 8. \tag{42}$$

The quadratic form $Q(\xi)$ is determined by formula (29) and the expression for $\widetilde{T}(\xi)$ is determined by Eq. (40).

To calculate the components of the tensor $A_{11}(t \mid \vec{W}, \Gamma)$, we assume that $\xi_i \to \xi_1$ on the right-hand side of Eq. (42). In calculation of the 8-dimensional integral in Eq. (42) it is convenient to go over to integration variables in which the quadratic form $Q(\{\xi_\alpha\})$ would acquire the canonical form of a sum of squares. The matrix $S_{\alpha\beta}$ of the linear transformation of $\hat{S}$ that reduces $Q(\{\xi_\alpha\})$ to the canonical expression $\hat{S}Q(\{\xi_\alpha\}) = \widetilde{Q}(\eta_\alpha) \equiv \sum_{i=1}^{8} \eta_i^2$ has the form

$S_{\alpha\beta}$ = (43)

| $\alpha \backslash \beta$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| 1 | 1/2 | 0 | 0 | 0 | $\sqrt{3}/2$ | 0 | 0 | 0 |
| 2 | 0 | $\sqrt{3/8}$ | 0 | $\sqrt{5/8}$ | 0 | 0 | 0 | 0 |
| 3 | 0 | 0 | $\sqrt{3/8}$ | 0 | 0 | 0 | $\sqrt{5/8}$ | 0 |
| 4 | 0 | $\sqrt{3/8}$ | 0 | $-\sqrt{5/8}$ | 0 | 0 | 0 | 0 |
| 5 | 1/2 | 0 | 0 | 0 | $-\sqrt{3}/2$ | 0 | 0 | 0 |
| 6 | 0 | 0 | 0 | 0 | 0 | $\sqrt{3/8}$ | 0 | $\sqrt{5/8}$ |
| 7 | 0 | 0 | $\sqrt{3/8}$ | 0 | 0 | 0 | $-\sqrt{5/8}$ | 0 |
| 8 | 0 | 0 | 0 | 0 | 0 | $\sqrt{3/8}$ | 0 | $-\sqrt{5/8}$ |

The Jacobian of transformation (43) is equal to the determinant of the matrix $S_{\alpha\beta}$:

$$J_s = \| S_{\alpha\beta} \| = 45 \sqrt{5}/128 \,. \tag{44}$$

After the transformation of the integration variables and substitution of the values of $J_s$ and $D^{1/2}$ into the expression for $A_{11}(t/\vec{W}, \Gamma)$ we obtain

$$A_{11}(t \mid \vec{W}, \Gamma) = \frac{\sqrt{A}}{6(2\pi)^4} \int \dots \int d\eta_1 \dots d\eta_8 \exp\left\{-\frac{1}{2}\sum_{k=1}^{8} \eta_k^2\right\} \widetilde{T}_1\left(\{\eta_\beta\}\right), \tag{45}$$

where $\widetilde{T}_1(\{\eta_\beta\})$ is the expression $\xi_1 \widetilde{T}(\{\xi\})$ transformed to the variables $\{\eta_\beta\}$:

$$\widetilde{T}_1(\{\eta\}) = -a_{10}\left[\frac{1}{2}(\eta_1^2 + \eta_5^2)\xi_9^2 + \frac{1}{2}(\eta_1^2 - \eta_5^2)\xi_{10}^2 - \eta_1^2\right] -$$

$$- a_{11}\left[\frac{1}{2}(\eta_1^2 - \eta_5^2)\xi_9^2 + \frac{1}{2}(\eta_1^2 + \eta_5^2)\xi_{10}^2 + \eta_1^2\xi_{11}^2 - 2\eta_1^2\right] + a_{12}\,[0]\,. \tag{46}$$

Using the integrals

$$I_0 = \int_{-\infty}^{+\infty} \exp\left(-\frac{\eta^2}{2}\right) d\eta = \sqrt{2\pi}\,, \quad I_1 = \int_{-\infty}^{+\infty} \eta^2 \exp\left(-\frac{\eta^2}{2}\right) d\eta = \sqrt{2\pi}\,,$$

$$I_2 = \int_{-\infty}^{+\infty} \eta^4 \exp\left(-\frac{\eta^2}{2}\right) d\eta = 3\sqrt{2\pi}\,, \tag{47}$$

we obtain an expression for the component $A_{11}(t/\vec{W}, \Gamma)$ in the form

$$A_{11}(t \mid \vec{W}, \Gamma) = A_t(W) = -\frac{\sqrt{A}}{6}\, 2a_{10}\,[(\xi_9^2 + \xi_{10}^2 + \xi_{11}^2) - 3]\,. \tag{48}$$

In writing expression (48) we adopted the hypothetical equality of the moments $a_{10}$ and $a_{11}$.

A similar calculation leads to the result

$$A_{22}(t \mid \vec{W}, \Gamma) = A_{11}(t \mid \vec{W}, \Gamma) = A_t(W)\,. \tag{49}$$

From considerations of symmetry we obtain that

$$A_{33}(t \mid \vec{W}, \Gamma) = A_t(W)\,. \tag{50}$$

Calculation by means of formula (42) shows that all the off-diagonal elements of the tensor $A_{\alpha\beta}(t \mid \vec{W}, \Gamma)$ are equal to zero. Thus, we obtain

$$A_{\alpha\beta}(t \mid \vec{W}, \Gamma) = \delta_{\alpha\beta}\sqrt{A}\, A_t(W)\,, \tag{51}$$

where

$$A_t(W) = B(t) - \frac{3D}{\chi(t)}\, C(t)\, W^2\,, \tag{52}$$

$$B(t) = \frac{a_{10}}{2}\,, \quad C(t) = \frac{a_{10}}{6}\,. \tag{53}$$

The dimensionless third-order single-point mixed moment of the velocity gradient and the scalar gradient $a_{10}(t)$ must be prescribed as a function of time. It can be measured or calculated using results of direct numerical simulation of turbulent fields:

$$a_{10} = \frac{\overline{(\partial u_1/\partial x_1)(\partial c/\partial x_1)^2}}{\overline{(\partial u_1/\partial x_1)^2}^{1/2}\ \overline{(\partial c/\partial x_1)^2}}. \tag{54}$$

Taking into consideration the physical meaning of the moment $a_{10}(t)$, we write the formulas for $B(t)$ and $C(t)$ in the form

$$B(t) = \frac{S_{UC}(t)}{2},\quad C(t) = \frac{S_{UC}(t)}{6}. \tag{55}$$

where $S_{UC}(t)$ is the asymmetry of the joint probability density function of the magnitudes of the velocity and scalar gradients. The function $S_{UC}(t)$ can be expressed in terms of the third derivative of the third-order structural function of the velocity and scalar fields $D_{LCC}(r, t)$, the dissipation rate of the intensity of turbulent scalar fluctuations $\chi(t)$, and the dissipation rate $\varepsilon(t)$:

$$S_{UC} = \frac{\frac{1}{6} D'''_{LCC}(0, t)}{(\chi(t)/3D)(\varepsilon(t)/15\nu)^{1/2}}. \tag{56}$$

An expression for the mixed moment $\overline{(\partial u_1/\partial x_1)(\partial c/\partial x_1)^2}$ in terms of $D'''_{LCC}(0, t)$ can be obtained by comparing formulas (12.146) on p. 69 of [14] with the formula $D'''_{LCC}(r) = 4B_{LC,C}(r)$ on p. 367 of [14].

With allowance for what has been said above concerning the tensor of the conditional velocity gradient, we write the final result in the form

$$A_{\alpha\beta}(t\,|\,\vec{W}, \Gamma) = \ = \delta_{\alpha\beta}\left(\frac{\varepsilon(t)}{15\nu}\right)^{1/2} A_t(W), \tag{57}$$

where

$$A_t\, W = \frac{S_{UC}(t)}{2}\left[1 - \frac{DW^2}{\chi(t)}\right]. \tag{58}$$

Note that averaging of the conditional velocity gradient over all values of the scalar gradient must give the usual mean value of this quantity, which is equal to zero in an isotropic flow. It is not difficult to note that formula (58) satisfies this condition.

All the functions needed to calculate $A_{\alpha\beta}(t\,|\,\vec{W}, \Gamma)$ can be obtained from a closed system of equations for two-point or spectral functions that describe the distribution of turbulent energy and of the intensity of scalar fluctuations over the spectrum of length scales or over the spectrum of wave numbers.

**6. Calculation of the Conditional JPDF $P_t(\vec{\vec{X}}\,|\,\vec{W}, \Gamma)$.** As is seen from Eq. (10), in order to calculate the conditional JPDF of the magnitude of the components of the tensor of the gradient of the scalar gradient in the Gaussian approximation it is necessary to calculate the functions $P_t(\vec{\vec{X}}, \vec{W}, \Gamma)$ and $P_t(\vec{W}, \Gamma)$ in this approximation, with the second function being prescribed by formula (27). The general form of the function $P_t(\vec{\vec{X}}, \vec{W}, \Gamma)$ in the Gaussian approximation has the form

$$P_t(\vec{\vec{X}}, \vec{W}, \Gamma) = \frac{\exp\left\{-\frac{1}{2}\sum_{\alpha=1}^{10}\sum_{\beta=1}^{10} d_{\alpha\beta}^{(3)}\xi_\alpha\xi_\beta\right\}}{(2\pi)^5 D_3^{1/2}\sigma_1^{(3)}\sigma_2^{(3)}\ldots\sigma_{10}^{(3)}}. \tag{59}$$

The symbols $\xi_i$, $i = 1, 2, ..., 10$, denote the independent (made dimensionless by division by their dispersions) variable functions $P_t(\vec{\vec{X}}, \vec{W}, \Gamma)$ corresponding to the components of the fields $\partial z_\alpha/\partial x_\beta$, $z_i$, and $c$. The correspondence between these components and the symbols $\xi_i$ is prescribed by the following relationships: $\partial z_1/\partial x_1 \leftrightarrow \xi_1$, $\partial z_1/\partial x_2 \leftrightarrow \xi_2$, $\partial z_1/\partial x_3 \leftrightarrow \xi_3$, $\partial z_2/\partial x_2 \leftrightarrow \xi_4$, $\partial z_2/\partial x_3 \leftrightarrow \xi_5$, $\partial z_3/\partial x_3 \leftrightarrow \xi_6$, $z_1 \leftrightarrow \xi_7$, $z_2 \rightarrow \xi_8$, $z_3 \leftrightarrow \xi_9$, $c \leftrightarrow \xi_{10}$. The variables $\partial z_2/\partial x_1$, $\partial z_3/\partial x_1$, $\partial z_3/\partial x_2$ are expressed in terms of other variables: $\partial z_2/\partial x_1 = \partial z_1/\partial x_2$, $\partial z_3/\partial x_1 = \partial z_1/\partial x_3$, $\partial z_3/\partial x_2 = \partial z_2/\partial x_3$.

The dispersions $\sigma_i^{(3)}$, $i = 1, 2, ..., 10$, are interpreted by the formulas

$$\sigma_i^{(3)} = \left(\overline{(\partial z_\alpha/\partial x_\beta)^2}\right)^{1/2}, \quad i = 1, 2, ..., 6, \quad \sigma_j^{(3)} = \left(\overline{z_\alpha^2}\right)^{1/2},$$
$$j = 7, 8, 9, \quad \sigma_{10}^{(3)} = \left(\overline{c^2}\right)^{1/2}. \tag{60}$$

The inverse matrix is

$$d_{\alpha\beta}^{(3)} = r_{\alpha\beta}^{(3)^{-1}}, \tag{61}$$

$$\xi_\alpha = \tilde{\xi}_\alpha/\sigma_\alpha, \quad \alpha = 1, 2, ..., 10, \tag{62}$$

where $\tilde{\xi}_\alpha$ are the dimensional variables.

The total of the correlations to be calculated in the matrix $r_{\alpha\beta}$ is $n = [(10\cdot 10) - 10]/2 = 45$. The symmetry of the matrix and the unitariness of its diagonal elements are taken into account in the count. To fill in the matrix $r_{ik}$ it is necessary to calculate correlation moments of the form $\overline{c^2}$, $\overline{cz_i}$, $\overline{c(\partial z_i/\partial x_j)}$, $\overline{z_i z_j}$, $\overline{z_\alpha(\partial z_i/\partial x_j)}$, $\overline{(\partial z_\alpha/\partial x_\beta)(\partial z_i/\partial x_j)}$ and to make dimensionless each of the correlators by division by the corresponding dispersion. The correlator $r_{10,10}$ is defined by the formula

$$r_{10,10} = 1. \tag{63}$$

The correlators of the form $\overline{cz_i} = c(\partial c/\partial x_i) = 0$, $i = 1, 2, 3$ (see (23)). The correlation moments $\overline{z_i z_j}$ are expressed by means of Eq. (19):

$$\overline{z_i z_j} = \frac{\chi}{3D}\delta_{ij}. \tag{64}$$

For the dispersions $\sigma_i^{(3)}$, $i = 7, 8, 9$, we have

$$\sigma_i^{(3)} = \sqrt{\chi/3D}. \tag{65}$$

According to Eqs. (64) and (65) the correlators $r_{7,7}^{(3)} = r_{8,8}^{(3)} = r_{9,9}^{(3)} = 1$, and the correlators $r_{7,8}^{(3)} = r_{7,9}^{(3)} = r_{8,9}^{(3)} = 0$. The correlators of the form $\overline{c(\partial z_i/\partial x_j)}$ in the isotropic case are expressed in terms of the correlators $\overline{z_j z_i}$:

$$\overline{c\frac{\partial z_i}{\partial x_j}} = -\overline{z_j z_i} = -(\chi/3D)\,\delta_{ij}. \tag{66}$$

This equality, with allowance for the formula $\sigma_{10}^{(3)} = \sqrt{\overline{c^2}}$, yields

$$r_{i,10}^{(3)} = \frac{\overline{c\,(\partial z_k/\partial x_k)}}{\sigma_{10}^{(3)}\sigma_i^{(3)}} = -\frac{\chi}{3D\left(\overline{c^2}\right)^{1/2}\sigma_i^{(3)}}\,, \quad i = 1, 4, 6\,. \tag{67}$$

To calculate the correlation moments of the form $\overline{(\partial z_i/\partial x_j)(\partial z_k/\partial x_l)}$, we employ the formula for the two-point correlation tensor of the scalar-field gradient (17). Let us differentiate Eq. (17) with respect to $x_j'$ and $x_l$ and assume $\vec{r} = 0$. As a result, we obtain a formula for calculating the single-point moments $\overline{(\partial z_i/\partial x_j)(\partial z_k/\partial x_l)}$:

$$\overline{\frac{\partial z_i(\vec{x})}{\partial x_j}\frac{\partial z_k(\vec{x})}{\partial x_l}} = -\frac{1}{6}D_{CC}^{(IV)}(0)\,(\delta_{il}\delta_{kj} + \delta_{kl}\delta_{ij} + \delta_{ik}\delta_{lj})\,. \tag{68}$$

Here $D_{CC}^{(IV)}$ is the fourth derivative of the structural function of the scalar field. As is known [14], this quantity is always negative. In the equation for the mean square of the gradient of scalar-field fluctuations this function describes its decrease due to molecular diffusion (see formula (15.13) of [14]).

Let us introduce the notation

$$-D_{CC}^{(IV)}(0, t)/2 = \omega\,. \tag{69}$$

Using Eq. (68), we calculate the dispersions:

$$\sigma_i^{(3)} = \sqrt{\omega}\,, \quad i = 1, 4, 6\,; \quad \sigma_j^{(3)} = \sqrt{\omega/3}\,, \quad j = 2, 3, 5\,. \tag{70}$$

Using Eq. (68), we can find the elements of the correlation matrix that describe the correlations of the gradient of the scalar-field gradient:

$$r_{14}^{(3)} = r_{16}^{(3)} = r_{46}^{(3)} = 1/3\,, \tag{71}$$

$$r_{12}^{(3)} = r_{13}^{(3)} = r_{15}^{(3)} = r_{23}^{(3)} = r_{24}^{(3)} = r_{25}^{(3)} = r_{26}^{(3)} = r_{34}^{(3)} = r_{35}^{(3)} = r_{36}^{(3)} = r_{45}^{(3)} = r_{56}^{(3)} = 0\,. \tag{72}$$

Differentiating Eq. (17) once with respect to $x_j$, we will obtain a formula for calculating the correlation moments of the scalar gradient and the gradient of the scalar gradient:

$$\overline{\frac{\partial z_i(\vec{x})}{\partial x_j}\, z_k(\vec{x}\,')} = 0\,. \tag{73}$$

As a result,

$$r_{i7}^{(3)} = r_{i8}^{(3)} = r_{i9}^{(3)} = 0\,, \quad i = 1, 2, \ldots, 6\,. \tag{74}$$

Using formulas (67) and (70) for $i = 1, 4, 6$, for the correlators $r_{i,10}^{(3)}$ we obtain

$$r_{i,10}^{(3)} = -\frac{\chi/3D}{\left(\overline{c^2}\,\omega\right)^{1/2}} \equiv -T\,, \quad i = 1, 4, 6\,. \tag{75}$$

Having used the expressions starting from formula (63), we fill in all the cells of the correlation matrix $r_{\alpha\beta}^{(3)}$:

$$
r_{\alpha\beta}^{(3)} = \left(\begin{array}{c|cccccccccc}
 & \frac{\partial z_1}{\partial x_1} & \frac{\partial z_1}{\partial x_2} & \frac{\partial z_1}{\partial x_3} & \frac{\partial z_2}{\partial x_2} & \frac{\partial z_2}{\partial x_3} & \frac{\partial z_3}{\partial x_3} & z_1 & z_2 & z_3 & c \\
\frac{\partial z_1}{\partial x_1} & 1 & 0 & 0 & 1/3 & 0 & 1/3 & 0 & 0 & 0 & -T \\
\frac{\partial z_1}{\partial x_2} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{\partial z_1}{\partial x_3} & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{\partial z_2}{\partial x_2} & 1/3 & 0 & 0 & 1 & 0 & 1/3 & 0 & 0 & 0 & -T \\
\frac{\partial z_2}{\partial x_3} & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
\frac{\partial z_3}{\partial x_3} & 1/3 & 0 & 0 & 1/3 & 0 & 1 & 0 & 0 & 0 & -T \\
z_1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
z_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
z_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
c & -T & 0 & 0 & -T & 0 & -T & 0 & 0 & 0 & 1
\end{array}\right). \tag{76}
$$

The inverse matrix $d_{\alpha\beta}^{(3)}$ can be calculated by the Gauss method [16] or using the computer library MathCad. The result for $d_{\alpha\beta}^{(3)}$ has the form

$$
d_{\alpha\beta}^{(3)} = \left(\begin{array}{c|cccccccccc}
 & \frac{\partial z_1}{\partial x_1} & \frac{\partial z_1}{\partial x_2} & \frac{\partial z_1}{\partial x_3} & \frac{\partial z_2}{\partial x_2} & \frac{\partial z_2}{\partial x_3} & \frac{\partial z_3}{\partial x_3} & z_1 & z_2 & z_3 & c \\
\frac{\partial z_1}{\partial x_1} & \frac{6-9T^2}{5\Delta} & 0 & 0 & \frac{-3+9T^2}{10\Delta} & 0 & -\frac{3+9T^2}{10\Delta} & 0 & 0 & 0 & \frac{3T}{5\Delta} \\
\frac{\partial z_1}{\partial x_2} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{\partial z_1}{\partial x_3} & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{\partial z_2}{\partial x_2} & \frac{-3+9T^2}{10\Delta} & 0 & 0 & \frac{6-9T^2}{5\Delta} & 0 & \frac{-3+9T^2}{10\Delta} & 0 & 0 & 0 & \frac{3T}{5\Delta} \\
\frac{\partial z_2}{\partial x_3} & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
\frac{\partial z_3}{\partial x_3} & \frac{-3+9T^2}{10\Delta} & 0 & 0 & \frac{-3+9T^2}{10\Delta} & 0 & \frac{6-9T^2}{5\Delta} & 0 & 0 & 0 & \frac{3T}{5\Delta} \\
z_1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
z_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
z_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
c & \frac{3T}{5\Delta} & 0 & 0 & \frac{3T}{5\Delta} & 0 & \frac{3T}{5\Delta} & 0 & 0 & 0 & 1/\Delta
\end{array}\right). \tag{77}
$$

Here the notation $\Delta = 1 - 9T^2/5$ was used. The determinant of this matrix is equal to

$$D_3 = 20\,(1 - 9T^2/5)/27\,. \tag{78}$$

Expressions for $P_t(\vec{\vec{X}}, \vec{W}, \Gamma)$ are prescribed by formulas (59), (65), (70), (77), and (78). The function $P_t(\vec{W}, \Gamma)$ is expressed by formulas (27), which with allowance for the other numbering of the variables have the form

$$P_t(\vec{W}, \Gamma) = \frac{\exp\left\{-\frac{1}{2} \sum\limits_{\alpha=7}^{10} \sum\limits_{\beta=8}^{10} d^{(3)}_{\alpha\beta}\, \xi_\alpha\, \xi_\beta\right\}}{(2\pi)^2\, D_2^{1/2}\, \sigma_7 \sigma_8 \sigma_9 \sigma_{10}}, \tag{79}$$

$$d^{(3)}_{\alpha\beta} = \delta_{\alpha\beta}\,, \quad \alpha, \beta = 7, 8, 10\,, \quad D_2 = 1\,. \tag{80}$$

Let us substitute into Eq. (10) the expressions for $P_t(\vec{\vec{X}}, \vec{W}, \Gamma)$ and $P_t(\vec{W}, \Gamma)$. As a result we have

$$P_t(\vec{\vec{X}} \mid \vec{W}, \Gamma) = \frac{\exp\left\{-\frac{1}{2} \sum\limits_{\alpha=1}^{10} \sum\limits_{\beta=1}^{10} \tilde{d}^{(3)}_{\alpha\beta}\, \xi_\alpha\, \xi_\beta\right\}}{(2\pi)^3\, \tilde{D}_2^{1/2}\, \sigma_1^{(3)} \sigma_2^{(3)} \sigma_3^{(3)} \sigma_4^{(3)} \sigma_5^{(3)} \sigma_6^{(3)}}. \tag{81}$$

Here $\tilde{D}_3 = D_3/D_2 = 20\Delta/27$. The matrix $\tilde{d}^{(3)}_{\alpha\beta}$ has the form

$$\tilde{d}^{(3)}_{\alpha\beta} = \left(\begin{array}{c|ccccccc}
 & \frac{\partial z_1}{\partial x_1} & \frac{\partial z_1}{\partial x_2} & \frac{\partial z_1}{\partial x_3} & \frac{\partial z_2}{\partial x_2} & \frac{\partial z_2}{\partial x_3} & \frac{\partial z_3}{\partial x_3} & c \\
\frac{\partial z_1}{\partial x_1} & \frac{6 - 9T^2}{5\Delta} & 0 & 0 & \frac{-3 + 9T^2}{10\Delta} & 0 & \frac{-3 + 9T^2}{10\Delta} & \frac{3T}{5\Delta} \\
\frac{\partial z_1}{\partial x_2} & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
\frac{\partial z_1}{\partial x_3} & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
\frac{\partial z_2}{\partial x_2} & \frac{-3 + 9T^2}{10\Delta} & 0 & 0 & \frac{6 - 9T^2}{5\Delta} & 0 & \frac{-3 + 9T^2}{10\Delta} & \frac{3T}{5\Delta} \\
\frac{\partial z_2}{\partial x_3} & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
\frac{\partial z_3}{\partial x_3} & \frac{-3 + 9T^2}{10\Delta} & 0 & 0 & \frac{-3 + 9T^2}{10\Delta} & 0 & \frac{6 - 9T^2}{5\Delta} & \frac{3T}{5\Delta} \\
c & \frac{3T}{5\Delta} & 0 & 0 & \frac{3T}{5\Delta} & 0 & \frac{3T}{5\Delta} & (1/\Delta) - 1
\end{array}\right). \tag{82}$$

The magnitudes of the dispersions $\sigma_i^{(3)}$, $i = 1, 2, \ldots, 6$, are prescribed by formulas (70). Thus, formulas (81), (82), and (70) completely prescribe the form of the conditional JPDF of the magnitudes of the components of the tensor of the gradient of the scalar gradient in the Gaussian approximation.

**7. Calculation of the Components of the Tensor $N_{\alpha\beta}(t \mid \vec{W}, \Gamma)$.** According to Eq. (8), this calculation presumes averaging of the tensor expression $X_{\alpha i} X_{\beta i}$ by the conditional distribution function $P_t(\vec{\vec{X}} \mid \vec{W}, \Gamma)$ whose form in the Gaussian approximation is written out in the previous section. As seen from Eq. (8), each component of the tensor $X_{\alpha i} X_{\beta i}$ is a sum of products of derivatives of scalar gradient components. Since $P_t(\vec{\vec{X}} \mid \vec{W}, \Gamma)$ depends only on six dimensionless variables corresponding to six components of the derivatives, it is worthwhile to write the tensor $X_{\alpha i}X_{\beta i}$ componentwise in terms of these dimensionless variables:

$$X_{\alpha i}\, X_{\beta i} = \frac{1}{3}\,\omega \times$$

$$\times \begin{vmatrix} 3\xi_1^2 + \xi_2^2 + \xi_3^2 & \sqrt{3}\,\xi_1\xi_2 + \sqrt{3}\,\xi_2\xi_4 + \xi_3\xi_5 & \sqrt{3}\,\xi_1\xi_3 + \xi_2\xi_5 + \sqrt{3}\,\xi_5\xi_6 \\ \sqrt{3}\,\xi_1\xi_2 + \sqrt{3}\,\xi_2\xi_4 + \xi_3\xi_5 & \xi_2^2 + 3\xi_4^2 + \xi_5^2 & \xi_2\xi_3 + \sqrt{3}\,\xi_4\xi_5 + \sqrt{3}\,\xi_5\xi_6 \\ \sqrt{3}\,\xi_1\xi_3 + \xi_2\xi_5 + \sqrt{3}\xi_3\xi_6 & \xi_3\xi_2 + \sqrt{3}\,\xi_4\xi_5 + \sqrt{3}\,\xi_5\xi_6 & \xi_3^2 + \xi_5^2 + 3\xi_6^2 \end{vmatrix}. \tag{83}$$

Comparing the expressions for the components of the tensor $X_{\alpha i}X_{\beta i}$ with matrix (82) for the elements $\tilde{d}^{(3)}_{\alpha\beta}$ in the exponent of the conditional JPDF, we come to the conclusion that all the off-diagonal elements of matrix (83) will make a zero contribution to $N_{\alpha\beta}(t\,|\,\vec{W},\Gamma)$ after averaging, i.e., we obtain

$$N_{\alpha\beta} = (t\,|\,\vec{W},\Gamma) = \delta_{\alpha\beta} N_\alpha\,(t\,|\,\vec{W},\Gamma) \tag{84}$$

(summation is not taken over the subscript $\alpha$). Here

$$N_\alpha\,(t\,|\,\vec{W},\Gamma) = \frac{\omega}{3}\int d\vec{\vec{X}}\,\tilde{N}_\alpha\,(\xi)\,P_t\,(\vec{\vec{X}}\,|\,\vec{W},\Gamma)\,,\quad \tilde{N}_\alpha\,(\xi) = \begin{vmatrix} 3\xi_1^2 + \xi_2^2 + \xi_3^2 \\ \xi_2^2 + 3\xi_4^2 + \xi_5^2 \\ \xi_3^2 + \xi_5^2 + 3\xi_6^2 \end{vmatrix}.$$

Using Eq. (81) for $P_t(\vec{\vec{X}}\,|\,\vec{W},\Gamma)$, we write down an expression for $N_\alpha(t\,|\,\vec{W},\Gamma)$ in the form

$$N_\alpha\,(t\,|\,\vec{W},\Gamma) = \frac{\omega}{3\,(2\pi)^3\tilde{D}_3^{1/2}}\int\ldots\int d\xi_1\ldots d\xi_6\,\tilde{N}_\alpha\,(\xi)\exp\left\{-\frac{1}{2}\sum_{\alpha=1}^{7}\sum_{\beta=1}^{7}\tilde{d}^{(3)}_{\alpha\beta}\,\xi_\alpha\xi_\beta\right\}. \tag{85}$$

We will find the transformation of the integration variables $\xi_1, \xi_2, \ldots, \xi_6$ that brings the quadratic expression $Q(\xi) = \tilde{d}^{(3)}_{\alpha\beta}\xi_\alpha\xi_\beta$ to a canonical form. The form of this transformation can be found by calculating the main directions of the $(6 \times 6)$ fragment of matrix (82) connected with the variables $\xi_1, \xi_2, \ldots, \xi_6$:

$$\xi_1 = \frac{\sqrt{5\Delta}\,\eta_1}{3} - \frac{2\eta_4}{3}\,,\quad \xi_2 = \eta_2\,,\quad \xi_3 = \eta_3\,,\quad \xi_4 = \frac{\sqrt{5\Delta}\,\eta_1}{3} + \frac{\eta_4}{3} + \frac{\eta_6}{\sqrt{3}}\,,$$

$$\xi_5 = \eta_5\,,\quad \xi_6 = \frac{\sqrt{5\Delta}\,\eta_1}{3} + \frac{\eta_4}{3} + \frac{\eta_6}{\sqrt{3}}\,. \tag{86}$$

In the variables $\eta_i$ the quadratic form is

$$Q\left(\left\{\eta_i\right\}\right) = \sum_{i=1}^{6}\eta_i^2 + \frac{3T}{5\Delta}\eta_1\hat{\Gamma} + \left(\frac{1}{\Delta} - 1\right)\hat{\Gamma}^2. \tag{87}$$

Here $\hat{\Gamma} = \Gamma/(\overline{c^2})^{1/2}$. The matrix $\tilde{N}_\alpha(\xi)$ transformed to the new variables acquires the form

$$N_\alpha\left(\left\{\eta_i\right\}\right) = \begin{vmatrix} 5\Delta\eta_1^2/3 + 4\eta_4^2/3 + \eta_2^2 + \eta_3^2 \\ 5\Delta\eta_1^2/3 + \eta_4^2/3 + \eta_6^2 + \eta_2^2 + \eta_5^2 \\ 5\Delta\eta_1^2/3 + \eta_4^2/3 + \eta_6^2 + \eta_3^2 + \eta_5^2 \end{vmatrix}. \tag{88}$$

In writing (88) we omit cross terms that make a zero contribution in integration. The Jacobian of transformation (86) is

$$J = 2\sqrt{5\Delta}/3\sqrt{3}\,. \tag{89}$$

With allowance for Eqs. (87)-(89) the expression for $N_\alpha(t|\vec{W},\Gamma)$ can be written in the form

$$N_\alpha(t|\vec{W},\Gamma) = \frac{\omega}{3}\exp\left\{-\frac{1}{2}\left(\frac{1}{\Delta}-1\right)\hat{\Gamma}^2\right\} I_\alpha(\Gamma)\,,\quad \alpha = 1, 2, 3\,, \tag{90}$$

where

$$I_\alpha = \frac{1}{(2\pi)^3}\int\ldots\int d\eta_1\ldots d\eta_6\, N_\alpha\left(\{\eta_j\}\right)\exp\left\{-\frac{1}{2}\sum_{i=1}^{6}\eta_i^2 - \frac{3T\hat{\Gamma}}{2\sqrt{5\Delta}}\eta_1\right\}.$$

Calculation of the integrals leads to the result

$$N_\alpha(t|\vec{W},\Gamma) = N_t(\Gamma) = -\frac{1}{6}D_{CC}^{(IV)}(0,t)\left[5 - 3T^2(t)\left(1-\frac{\hat{\Gamma}^2}{4}\right)\right]\exp\left\{-\frac{\hat{\Gamma}^2}{8}\frac{27T^2(t)}{5-9T^2(t)}\right\}. \tag{91}$$

As is seen from Eq. (91), the tensor of the conditional rate of dissipation of the dissipation of scalar fluctuations depends not on the magnitude of the gradient, but only on the magnitude of the scalar. The fourth derivative of the two-point structural function of the scalar turbulent field over the spatial variable $r$ at its zero value enters the definition of the function $N_t(\Gamma)$ in two ways: $D_{CC}^{(IV)}(0,t)$ enters the expression for the function $N_t(\Gamma)$ and the definition of the correlation function $T(t)$, which, with allowance for formulas (75) and (69), can be written in the form

$$T(t) = \frac{\sqrt{2}\,\chi(t)}{3D\left(-\overline{c^2}(t)\,D_{CC}^{(IV)}(0,t)\right)^{1/2}}. \tag{92}$$

Here $\chi(t)$ is the dissipation rate of scalar fluctuations, $\overline{c^2}(t)$ is the mean-square value of the intensity of scalar fluctuations.

For complete determination of the function $N_t(\Gamma)$ it is necessary to prescribe the quantities $D_{CC}^{(IV)}(0,t)$, $\overline{c^2}(t)$, and $\chi(t)$. This can be done by solving a closed system of equations for the structural function.

**8. Calculation of the Components of the Tensor $X_{\alpha\beta}(t|\vec{W},\Gamma)$.** The calculation of the components of the mean conditional tensor $X_{\alpha\beta}(t|\vec{W},\Gamma)$ according to (9) presupposes first-degree averaging of the tensor $X_{\alpha\beta}$ by the conditional distribution function $P_t(\vec{\vec{X}}|\vec{W},\Gamma)$. The form of this function in the Gaussian approximation is given in Sec. 6. We write out the components of the tensor $X_{\alpha\beta}$ in terms of the dimensionless variables:

$$X_{\alpha\beta} = \sqrt{\omega}\begin{vmatrix} \xi_1 & \xi_2/\sqrt{3} & \xi_3/\sqrt{3} \\ \xi_2/\sqrt{3} & \xi_4 & \xi_5/\sqrt{3} \\ \xi_3/\sqrt{3} & \xi_5/\sqrt{3} & \xi_6 \end{vmatrix}. \tag{93}$$

Comparing the expressions for the components of the tensor $X_{\alpha\beta}$ with matrix (82) for the elements $\tilde{d}_{\alpha\beta}^{(3)}$ in the exponent of the conditional JPDF, we come to the conclusion that all off-diagonal elements of matrix (93) will make a zero contribution to the conditional tensor $X_{\alpha\beta}(t|\vec{W},\Gamma)$ after averaging. The nonzero contribution is provided by the presence of the nonzero components $\tilde{d}_{\alpha,7}^{(3)}$ in the matrix $d_{\alpha p}^{(3)}$. Thus

$$X_{\alpha\beta}(t|\vec{W},\Gamma) = \delta_{\alpha\beta}X_\alpha(t|\vec{W},\Gamma) \tag{94}$$

(there is no summation over the subscript $\alpha$). Here

$$X_\alpha(t|\vec{W},\Gamma) = \sqrt{\omega}\int d\vec{\vec{X}}\,\tilde{X}_\alpha(\xi)\,P_t(\vec{\vec{X}}\,|\vec{W},\Gamma)\,,\quad \tilde{X}_\alpha(\xi) = \begin{pmatrix}\xi_1\\ \xi_4\\ \xi_6\end{pmatrix}.$$

Using Eq. (81) for $P_t(\vec{\vec{X}}|\vec{W},\Gamma)$, we write the expression for $X_\alpha(t|\vec{W},\Gamma)$ in the form

$$X_\alpha(t|\vec{W},\Gamma) = \frac{\sqrt{\omega}}{(2\pi)^3\,\tilde{D}_3^{1/2}}\int\ldots\int d\xi_1\ldots d\xi_6\,\tilde{X}_\alpha(\xi)\exp\left\{-\frac{1}{2}\sum_{\alpha=1}^{7}\sum_{\beta=1}^{7}\tilde{d}_{\alpha\beta}^{(3)}\,\xi_\alpha\xi_\beta\right\}. \tag{95}$$

The transformation that brings the quadratic expression $\tilde{d}_{\alpha\beta}^{(3)}\xi_\alpha\xi_\beta$ to a canonical form was found in Sec. 7 and is represented by formula (86). The quadratic form is prescribed by Eq. (87). The transformation of the matrix $\tilde{X}_\alpha(\xi)$ to the variables $\{\eta\}$ has the form

$$\tilde{X}_\alpha[\xi(\eta)] = X_\alpha(\eta) = \begin{vmatrix}\sqrt{5\Delta}\,\eta_1/3 - 2\eta_4/3\\ \sqrt{5\Delta}\,\eta_1/3 + \eta_4/3 + \eta_6/3\\ \sqrt{5\Delta}\,\eta_1/3 + \eta_4/3 - \eta_6/3\end{vmatrix}. \tag{96}$$

The terms proportional to $\eta_4$, $\eta_6$ give zero in integration. Therefore

$$X_\alpha(\eta) = X(\eta) = \sqrt{5\Delta}\,\eta_1/3\,,\quad \alpha = 1, 2, 3\,. \tag{97}$$

The Jacobian of the transformation from the variables $\{\xi\}$ to the variables $\{\eta\}$ is prescribed by Eq. (89). With account for Eqs. (97) and (89), Eq. (95) takes the form

$$X_\alpha(t|\vec{W},\Gamma) = X_t(\Gamma) = \frac{\sqrt{\omega}\,\sqrt{5\Delta}}{3}\exp\left\{-\left(\frac{1}{\Delta}-1\right)\frac{\hat{\Gamma}^2}{2}\right\}\int\ldots\int d\eta_1\ldots d\eta_6\eta_1\,\times$$
$$\times\exp\left\{-\frac{1}{2}\sum_{i=1}^{6}\eta_i^2 - \frac{3T}{2\sqrt{5\Delta}}\frac{\Gamma}{(\overline{c^2})^{1/2}}\eta_1\right\}. \tag{98}$$

After calculation of the six-dimensional integral we obtain

$$X_t(\Gamma) = K_t(\Gamma)\exp\left\{-\alpha(T)\,\hat{\Gamma}^2\right\}. \tag{99}$$

Here we use the notation

$$K_t(\Gamma) = -\frac{\chi(t)}{6D(\overline{c^2})^{1/2}}\hat{\Gamma}\,, \tag{100}$$

$$\alpha(T) = \frac{27T^2}{8\,[5-9T^2]}. \tag{101}$$

With allowance for Eqs. (94), (98), and (99) we write

$$X_{\alpha\beta}(t|\vec{W},\Gamma) = \delta_{\alpha\beta}\,X_t(\Gamma)\,. \tag{102}$$

For complete determination of the tensor of the conditional second derivative $X_\alpha(t|\vec{W},\Gamma)$ it is necessary to prescribe the quantities $D_{CC}^{(IV)}(0,t)$, $\overline{c^2}(t)$, and $\chi(t)$. All these functions can be calculated by solving the system of equations for the functions $P_t^{(c)}(\rho)$ and $P_t(\rho)$.

Let us give critical consideration to the result of calculation of the mean conditional gradient of the scalar field fixed in Eqs. (99)-(102). The mean conditional value of the second derivative of the scalar turns out to be negative with respect to the value of the scalar field Γ at all admissible values of the correlation function $T(t)$. As is seen from Eq. (66), the negative sign of the mean correlation between the scalar field and the components of its second derivative is a general result. The reason for such behavior of this correlation is evident when a sinusoid is a typical realization of the turbulent scalar field. In this case the second derivative is a sinusoid with the opposite sign. At any level of the scalar field $c(\vec{x}, t) = \Gamma$ this situation is preserved. This ensures a negative sign for the function $K_t(\hat{\Gamma})$, although in deriving the expression for the conditional mean value of the second derivative the assumption of a Gaussian JPDF of the scalar and its derivatives was used. Note that this assumption may turn out to be incorrect, as well as Eq. (100) for $K_t(\Gamma)$.

We clarify the foregoing statement using another typical realization of the scalar field. We assume that this realization is represented by a function of the form

$$c(x, t) = a(t)\left(\sin\frac{x}{\lambda}\right)^{2n+1}, \qquad (103)$$

where $n$ is a certain parameter, an integer. When $n > 0$, the function $c(x, t)$ changes its form so that a segment with a positive second derivative appears in it. But the segment with a negative second derivative is kept so large that a negative mean correlation is ensured between the scalar field and its second derivative for a period. This turns out to be valid at any value of $n > 0$. Despite of the negativity of the period-average correlation between the fields $c$ and $c''_{xx}$, the value of the second derivative at certain values of the scalar field $c(\vec{x}, t) = \Gamma$ may turn out to be positive, i.e., the presence of typical realizations (103) in a turbulent flow may lead to a form of the expression for $K_t(\Gamma)$ for which the conditional second derivative of the scalar field will be positive at certain values of the scalar field.

Note that expression (100) for $K_t(\Gamma)$ is valid only for the initial stage of mixing, when the scalar field consists mainly of diffusion layers that separate regions with constant values of the scalar and therefore are close to sinusoidal. At a later stage of mixing the character of realization acquires a more pointed shape typical of realizations with a large excess (see Fig. 64 in [18]).

It is possible in principle to take into account the excess in the JPDF of the scalar and its derivatives by means of a Gramme–Charles series (see Sec. 5). But this approach is complicated substantially by the absence of information on the fourth-order cumulants of the fields of the scalar and its derivatives. In the present work an attempt is made to calculate the function $K_t(\Gamma)$ on the basis of the form of a typical realization of the scalar field (103) and thus to take into account somewhat the excess of the scalar field and its derivatives.

It is possible to obtain statistical information on the evolution of the parameters of the typical realization $a(t)$, $\lambda(t)$, $n(t)$ by using the solution of an auxiliary system of equations for $P_t^{(c)}(\rho)$ and $P_t(\rho)$. Simple calculations allow one to connect the parameter $a(t)$ with the dispersion $\overline{c^2}(t)$:

$$a(t) = \left(\overline{c^2}(t)\, N(n)\right)^{1/2}, \qquad (104)$$

where

$$N(n) = \frac{\sqrt{\pi}\,\Gamma(2n+1)}{\Gamma(2n+3/2)}, \qquad (105)$$

$\Gamma(x)$ is the gamma-function.

For the correlator of the scalar and its second derivative, which is defined by the formula $T(t) = \overline{c(x, t)c''_{xx}(x, t)}/(\overline{c^2(x, t)})^{1/2}(\overline{c''^2_{xx}(x, t)})^{1/2}$, on the basis of realization (103) it is possible to obtain the expression

$$T(t) = -\frac{(2n+1)}{(4n-1)}\sqrt{\left(\frac{|16n^2-1|}{|12n^2+4n-1|}\right)}. \qquad (106)$$

Since the statistical quantities $\overline{c^2(t)}$ and $T(t)$ are to be calculated from an auxiliary system of equations, then using Eqs. (104) and (106) it is possible to evaluate the parameters $a(t)$ and $n(t)$ at any instant of time. The parameter $\lambda(t)$ is related to the dissipation rate of the intensity of scalar fluctuations by the formula $\lambda^2(t) = 6D\overline{c^2}/\chi(t)$. Since $\chi(t)$ is calculated from an auxiliary system of equations, the parameter $\lambda(t)$ must be calculated as a function of time.

Using Eq. (103), we write in explicit form a relation for the conditional probability density of the values of the second derivative of the scalar:

$$P(\kappa\,|\,\hat{\Gamma}) = \delta\,[\kappa - c''(\hat{\Gamma})] =$$

$$= \delta\left\{\kappa - \left(\frac{(\overline{c^2})^{1/2}}{\lambda^2} N(n)\,(2n+1)\,(\hat{\Gamma}/N(n))^{\frac{2n-1}{2n+1}}\right)\Big/\lambda^2\left[2n - (2n+1)\,(\hat{\Gamma}/N(n))^{\frac{2}{2n+1}}\right]\right\}. \tag{107}$$

Using Eq. (107), it is possible to calculate the mean conditional magnitude of the second derivative:

$$K_t(\hat{\Gamma}) = \int \kappa P(\kappa\,|\,\hat{\Gamma})\,d\kappa = \chi(t)\,\kappa(\hat{\Gamma})/6D\,(\overline{c^2})^{1/2}, \tag{108}$$

where

$$\kappa(\hat{\Gamma}) = N(n)\,(2n+1)\,(\hat{\Gamma}/N(n))^{\frac{2n-1}{2n+1}}\left[2n - (2n+1)\,(\hat{\Gamma}/N(n))^{\frac{2}{2n+1}}\right]. \tag{109}$$

Note that $\kappa(\hat{\Gamma})$ at $n = 0$ takes the form $\kappa(\Gamma) = -\Gamma$, and Eq. (108) becomes identical to Eq. (100). Thus, Eq. (108) for $K_t(\hat{\Gamma})$ can be considered as a generalization of Eq. (100) that to a certain extent takes account of the excess in the probability distribution of the values of the scalar and its second derivative. The importance of the proposed generalization will be revealed in solution of the equation for the JPDF and a system of equations for the conditional dissipation rate (CDR) and the single-point probability density of scalar fluctuations.

**9. Equation for the JPDF with Account for the Results Obtained for the Tensors $\vec{\vec{A}}, \vec{\vec{N}}, \vec{\vec{X}}$.** Using the results of calculations of the tensors $A_{\alpha\beta}(t|\vec{W},\Gamma)$, $N_{\alpha\beta}(t|\vec{W},\Gamma)$ and $X(t|\vec{W},\Gamma)$ given in Secs. 5, 7, and 8, we write Eq. (6) for the JPDF of a reacting scalar and its gradient in a closed form, having represented it preliminarily in the symbolic form

$$\frac{\partial P_t(\vec{W},\Gamma)}{\partial t} = (1) + (2) + (3) + (4) + (5) + (6), \tag{110}$$

and we explicate the specific form of each term on the right-hand side of this equation with account for the obtained results of calculation of the tensors $\vec{\vec{A}}, \vec{\vec{N}}, \vec{\vec{X}}$. The first term on the right-hand side of Eq. (110) remains unchanged:

$$(1) = -DW^2\frac{\partial^2}{\partial\Gamma^2}P_t(\vec{W},\Gamma). \tag{111}$$

Using formula (57) for $A_{\alpha\beta}(t|\vec{W},\Gamma)$, we obtain the following equation for the second term:

$$(2) = \left(\frac{\varepsilon(t)}{15\nu}\right)^{1/2}\frac{\partial}{\partial W_\alpha}[W_\beta\,\delta_{\alpha\beta}\,A_t(W)\,P_t(\vec{W},\Gamma)] = \left(\frac{\varepsilon(t)}{15\nu}\right)^{1/2}\frac{\partial}{\partial W_\alpha}\times$$

$$\times[W_\alpha A_t(W)\,P_t(\vec{W},\Gamma)] = \left(\frac{\varepsilon(t)}{15\nu}\right)^{1/2}\left(3 + W\frac{\partial}{\partial W}\right)A_t(W)\,P_t(\vec{W},\Gamma).$$

Taking into account Eq. (58), we find

$$(2) = \left(\frac{\varepsilon(t)}{15\nu}\right)^{1/2} \left(3 + W\frac{\partial}{\partial W}\right) \left\{\left[B(t) - \frac{3D}{\chi(t)} C(t) W^2\right] P_t(\vec{W}, \Gamma)\right\}. \tag{112}$$

Taking account of formulas (84) and (91), we write an expression for the third term on the right-hand side of Eq. (110) in the form

$$(3) = -D\frac{\partial^2}{\partial W_\alpha \partial W_\beta}[\delta_{\alpha\beta} N_t(\Gamma) P_t(\vec{W}, \Gamma)] = -DN_t(\Gamma)\frac{\partial^2}{\partial W_\alpha}\frac{P_t(\vec{W}, \Gamma)}{\partial W_\alpha} =$$

$$= -DN_t(\Gamma)\left[\frac{\partial^2 P_t(\vec{W}, \Gamma)}{\partial W^2} + \frac{\partial P_t(\vec{W}, \Gamma)}{\partial W}\left[3W - \frac{W_\alpha \cdot W_\alpha}{W}\right] \Big/ W^2\right].$$

Thus

$$(3) = -DN_t(\Gamma)\left[\frac{2}{W}\frac{\partial}{\partial W} + \frac{\partial^2}{\partial W^2}\right] P_t(\vec{W}, \Gamma). \tag{113}$$

The function $N_t(\Gamma)$ is defined by formula (91).

Using formula (102) for the tensor $X_{\alpha\beta}(t \mid \vec{W}, \Gamma)$, we transform the fourth term on the right-hand side of Eq. (110):

$$(4) = -2D\frac{\partial^2}{\partial W_\alpha \partial \Gamma}[W_\alpha \delta_{\alpha\beta} X_t(\Gamma) P_t(\vec{W}, \Gamma)] =$$

$$= -2D\frac{\partial}{\partial \Gamma}\left\{X_t(\Gamma)\left[3P_t(\vec{W}, \Gamma) + W\frac{\partial}{\partial W} P_t(\vec{W}, \Gamma)\right]\right\}.$$

Thus

$$(4) = -2D\frac{\partial}{\partial \Gamma}\left\{X_t(\Gamma)\left[3 + W\frac{\partial}{\partial W} P_t(\vec{W}, \Gamma)\right]\right\}. \tag{114}$$

Differentiating with respect to the variable $\Gamma$ the fifth term on the right-hand side of Eq. (6), we obtain

$$(5) = -\left[\frac{\partial \dot{\omega}(\Gamma)}{\partial \Gamma} + \dot{\omega}(\Gamma)\frac{\partial}{\partial \Gamma}\right] P_t(\vec{W}, \Gamma). \tag{115}$$

The sixth term takes the form

$$(6) = -\frac{\partial \dot{\omega}(\Gamma)}{\partial \Gamma}\left[3 + W\frac{\partial}{\partial W}\right] P_t(\vec{W}, \Gamma). \tag{116}$$

We note that in none of the terms on the right-hand side of the equation for the JPDF is there a dependence on the direction of the vector $\vec{W}$. Therefore we can assume that the equation obtained serves for finding $P_t(W, \Gamma)$, i.e., the joint probability density of the scalar and the magnitude of its gradient. Allowing for this remark and formulas (111)-(116), we can write a closed equation for the JPDF $P_t(\vec{W}, \Gamma)$ in the final form:

$$\frac{\partial P_t(W, \Gamma)}{\partial t} = -DW^2\frac{\partial^2 P_t(W, \Gamma)}{\partial \Gamma^2} + \left(\frac{\varepsilon(t)}{15\nu}\right)^{1/2}\left(3 + W\frac{\partial}{\partial W}\right) \times$$

$$\times \left\{ \left[ \frac{S_{UC}(t)}{2} \left( 1 - \frac{DW^2}{\chi(t)} \right) \right] P_t(W, \Gamma) \right\} - DN_t(\Gamma) \left[ \frac{2}{W} \frac{\partial}{\partial W} + \frac{\partial^2}{\partial W^2} \right] P_t(W, \Gamma) -$$

$$- 2D \frac{\partial}{\partial \Gamma} \left\{ X_t(\Gamma) \left[ 3 + W \frac{\partial}{\partial W} \right] P_t(W, \Gamma) \right\} -$$

$$- \left[ 4 \frac{\partial \dot{\omega}(\Gamma)}{\partial \Gamma} + \dot{\omega}(\Gamma) \frac{\partial}{\partial \Gamma} + \frac{\partial \dot{\omega}(\Gamma)}{\partial \Gamma} W \frac{\partial}{\partial W} \right] P_t(W, \Gamma) . \tag{117}$$

It must be solved under the following initial and boundary conditions:

$$P_t(W, \Gamma)|_{t=0} = P_0(W, \Gamma) , \tag{118}$$

$$P_t(W, \Gamma)|_{W=\infty} = 0 , \quad P_t(W, \Gamma)|_{|\Gamma|=\Gamma_{max}} = 0 . \tag{119}$$

Here $P_0(W, \Gamma)$ is the initial form of the JPDF; $\Gamma_{max}$ is the maximum value of the scalar fluctuation, which is determined by the initial condition.

In Eq. (117) the function $S_{UC}(t)$ is determined by formula (56), $N_t(\Gamma)$ by (91), (92), $X_t(\Gamma)$ by (99), (108), (109), and $\omega(\Gamma)$ is prescribed in selecting a specific mechanism of the chemical reaction.

**10. Calculation of Auxiliary Functions.** As is seen from the formulas that determine the functions $S_{UC}(t)$, $N_t(\Gamma)$, and $X_t(\Gamma)$, for their calculation it is necessary to know the time evoluation of the following single-point functions:

1) $\varepsilon(t)$, the dissipation rate of the turbulent energy of the velocity field;

2) $\chi(t)$, the dissipation rate of the intensity of turbulent fluctuations of the reacting scalar;

3) $\overline{c^2(t)}$, the dispersion of the turbulent scalar field;

4) $D_{LCC}(r, t)$, the third-order structural two-point function of the turbulent fields of the velocity and the scalar;

5) $D_{CC}^{(IV)}(0, t)$, the fourth derivative at $r = 0$ over the distance $r$ between two points from the second-order structural two-point function of the turbulent scalar field.

The evolution of these functions can be calculated, having related them to the corresponding spectral functions or the functions $P_t(r)$ and $P_t^{(c)}(t)$ that describe the distributions of turbulent energy and of the intensity of scalar fluctuations over various length scales. These functions are related to the correlation, structural, and spectral functions by the following equalities:

$$P_t(r) = - \frac{\partial B(r, t)}{\partial r} = \frac{1}{2} \frac{\partial D(r, t)}{\partial r} =$$

$$= 2 \int_0^\infty \left\{ \left[ \frac{3}{(kr)^4} - \frac{1}{(kr)^2} \right] \sin(kr) - \frac{3}{(kr)^3} \cos(kr) \right\} kE(k, t)\, dk , \tag{120}$$

$$P_t^{(c)}(r) = - \frac{\partial}{\partial r} B^c(r, t) = \frac{1}{2} \frac{\partial}{\partial r} D_{CC}(r, t) = \int_0^\infty \left[ \frac{\sin(kr)}{(kr)^2} - \frac{\cos(kr)}{kr} \right] kE^c(k, t)\, dk . \tag{121}$$

The closed system of equations for calculating these functions has the form

$$\frac{\partial P_t(r)}{\partial t} = \frac{\partial}{\partial r} \left[ 2\nu + 2\gamma \int_0^r \sqrt{\tilde{r} P_t(\tilde{r})}\, d\tilde{r} \right] \left( \frac{\partial}{\partial r} + \frac{4}{r} \right) P_t(r) , \tag{122}$$

$$\frac{\partial P_t^{(c)}(r)}{\partial t} = \frac{\partial}{\partial r}\left[2D + 2\beta \int_0^r \sqrt{\tilde{r} P_t(\tilde{r})}\, d\tilde{r}\right]\left(\frac{\partial}{\partial r} + \frac{2}{r}\right) P_t^{(c)}(r) - 2\frac{\partial}{\partial r} B(r, t), \tag{123}$$

$$\gamma = 0.24, \quad \beta = 1.08, \tag{124}$$

$$B(r, t) = \langle \dot{\omega}\, [c(\vec{x}, t)\, c(\vec{x} + \vec{r}, t)] \rangle . \tag{125}$$

The system of equations (122)-(123) must be solved under the following initial and boundary conditions:

$$P_t(r)|_{r=0} = P_t(r)|_{r=\infty} = 0, \quad P_t(r)|_{t=0} = P_0(r). \tag{126}$$

There are similar conditions for the function $P_t^{(c)}(r)$. The last term in Eq. (123) describes the effect of the chemical source on the distribution of the intensity of scalar-field fluctuations.

The system of equations (122)-(123) is closed on the basis of a hypothesis similar to Heisenberg's hypothesis for turbulent-energy transfer over the spectrum of wave numbers. The constants of the equations are calculated in solving the obtained system for the passive scalar in inertial and inertial-convective intervals of the length scales.

The function $B(r, t)$ presents still another problem of closure, which will be solved upon specific assignment of the form of the chemical source term. In solving problems of combustion within the framework of the flamelet conceptualization, closure of this term is possible by means of values of $c(x, t)$ on a stoichiometric surface. The functions needed to calculate the coefficients $S_{UC}(t)$, $N_t(\Gamma)$, and $X_t(\Gamma)$ are related to the functions $P_t(r)$ and $P_t^{(c)}(r)$ by the following formulas:

$$D_{CC}^{(IV)}(0, t) = 2P_t^{(c)'''}(0) \tag{127}$$

$$\varepsilon(t) = 15\nu P_t'(0), \tag{128}$$

$$\chi(t) = 3DP_t^{(c)'}(0), \tag{129}$$

$$\overline{c^2}(t) = \int_0^\infty P_t^{(c)}(r)\, dr. \tag{130}$$

Knowing $P_t^{(c)}(r)$, it is possible to calculate the function $D_{LCC}(r, t)$ using an exact relation, namely, the nonclosed equation for $P_t^{(c)}(r)$:

$$D_{LCC}(r, t) = \frac{2}{5}\frac{r^2}{L^2}\chi(t)\, r + 4DP_t^{(c)}(r) - \frac{2}{r^2}\frac{\partial}{\partial t}\int_0^r \tilde{r}^{-2}\int_0^{\tilde{r}} P_t^{(c)}(r')\, dr' . \tag{131}$$

From formulas (127)-(131) it is seen that the auxiliary system of equations for the two-point functions $P_t(r)$ and $P_t^{(c)}(r)$ allows one to solve the problem of calculation of the time-dependent coefficients in the equation for the JPDF $P_t(W, \Gamma)$.

**Conclusion.** In this work we derived a closed equation for the joint probability density function (JPDF) of a reacting scalar and its gradient. The basic idea that made it possible to close the equation for the JPDF consists in the use of approximate expressions for the joint conditional distributions of the probabilities of the tensor components of the velocity gradient and the tensor components of the gradient of the scalar gradient.

The conditional JPDF of the tensor components of the velocity gradient is calculated in a quasi-Gaussian approximation with allowance for single-point mixed moments of the fields of the velocity gradient and the scalar gradient. Here the hypothesis of the equality of the third-order single-point mixed moments to the mixed moment $a_{10}(t) = (\partial u_1/\partial x_1)(\partial c/\partial x_1)^2/\overline{(\partial u_1/\partial x_1)^2}^{1/2}\,\overline{(\partial c/\partial x_1)^2}$ was adopted.

The evolution of the moment $a_{10}(t)$ can be related to the evolution of the third-order derivative at $r = 0$ of the third-order two-point structural function $D'''_{LCC}(0, t)$ over the distance. The evolution of the latter can be related to the evolution of the function $P_t^{(c)}(r)$ that describes the distribution of the intensity of turbulent scalar fluctuations over various length scales. For the functions $P_t(r)$ and $P_t^{(c)}(r)$ we suggested a simple system of equations that is closed on the level of Heisenberg's hypothesis on turbulent-energy transfer over the spectrum of length scales.

The coefficient $S_{UC}(t)$ in the equation for $P_t(W, \Gamma)$ turns out to be expressed in terms of the function $D'''_{LCC}(0, t)$ and in terms of the energy dissipation rate of turbulent fluctuations $\varepsilon(t)$ and the intensity dissipation rate of scalar turbulent fluctuations $\chi(t)$. The functions $\varepsilon(t)$ and $\chi(t)$ are expressed in terms of derivatives of the functions $P_t(r)$ and $P_t^{(c)}(r)$ at $r = 0$.

The coefficients $N_t(\Gamma)$ and $X_t(\Gamma)$ are expressed in terms of the fourth derivative at zero of the two-point structural function of the turbulent scalar field $D_{CC}^{(IV)}(0, t)$, the dispersion $\overline{c^2}(t)$, and the dissipation rate $\chi(t)$ over the spatial variable. The evolution of the functions $D_{CC}^{(IV)}(0, t)$ and $\overline{c^2}(t)$ is related to the evolution of the function $P_t^{(c)}(r)$.

Thus, all the functions needed to calculate the coefficients $S_{UC}(t)$, $N_t(\Gamma)$, and $X_t(\Gamma)$ can be related to the evolution of the functions $P_t(r)$ and $P_t^{(c)}(r)$.

It should be emphasized once again that the information needed to calculate the functions $S_{UC}(t)$, $N_t(\Gamma)$, and $X_t(\Gamma)$ can also be obtained in terms of the corresponding spectral functions, for which a whole series of model closed equations of various degrees of complexity were suggested [9, 10], or from experiment.

The results obtained in the present work can be considered as a closed system of equations for the JPDF of a scalar and its gradient in a reacting turbulent isotropic flow. This system can be solved numerically, and the evolution of the function $P_t(W, \Gamma)$ can be obtained. As yet, this problem has not been solved. In further work the closed equation for the JPDF $P_t(W, \Gamma)$ will be used for derivation and numerical solution of a system of equations for the conditional rate of dissipation and the single-point probability density of scalar fluctuations.

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