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STATISTICAL COEFFICIENTS IN THE EQUATION FOR THE JOINT PROBABILITY DENSITY OF A SCALAR AND ITS GRADIENT

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The characteristic scales, dispersions, and dissipation rates of isotropic, degenerate, turbulent velocity and scalar fields as well as several third-order moments for these fields have been determined and compared to those obtained by direct numerical simulation. These quantities determined as a time function were used to close the equation for the joint probability density of a scalar and its gradient, obtained by the authors earlier. The coefficients of this equation calculated using two models developed by the authors are in good agreement with those determined by direct numerical simulation.

Introduction. In modeling processes of turbulent mixing and combustion it is necessary to calculate both the fields of average quantities (velocity, pressure, temperature, and reagent concentration) and the fields of their fluctuations. In the majority of cases, the rate of the chemical reaction attendant on these processes depends strongly and nonlinearly on the magnitude of these fluctuations and a large number of statistical moments should be determined. Therefore, the usual method of turbulence theory, consisting of gradient approximation of the unknown statistical moments, is not sufficiently adequate for calculating a turbulent scalar field in the case where a chemical reaction occurs.

In this case, a turbulent scalar field is frequently investigated with the use of models for the joint probability density function (JPDF) of quantities determining the rate of the chemical reaction. Knowledge of the joint probability densities of these quantities is equivalent to knowledge of all the statistical moments and makes it possible to cope with the high nonlinearity of the chemical reaction since its rate can be represented in a closed form in terms of the indicated joint probability densities.

Various nonclosed JPDF equations are described in [1]. They can be closed with the use of conditional Gaussian distribution functions as well as experimental data and data of direct numerical simulation. The numerical solution of JPDF equations is complicated by the multidimensionality of these distributions. For example, the joint probability density of the fluctuations of a three-dimensional field of velocity, temperature, and two independent scalars will be a function of six variables, not counting time. Because of this, the Monte Carlo method is widely used for numerical solution of various JPDF equations [2, 3].

One of the joint probability densities used for the description of turbulent flames, which are far from being chemically equilibrium, is the joint probability density of a scalar and its gradient [1]. Closed equations for this function have been constructed in [4–6]. Note that these models contain unknown coefficients, including the characteristic frequencies of turbulence of dynamic and scalar fields. They can be determined with the use of experimental data, data of direct numerical simulation, or additional coefficient models.

The aim of the present work is construction of models for determining the coefficients in the JPDF equation of [6] and testing these models by comparison of the data obtained with them to the data of direct numerical simulation.

Since the above-mentioned JPDF equations [4–6] are single-point from the viewpoint of the statistics used, their coefficients should account for the spatial structure of turbulence — the characteristic spatial and time scales of

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turbulence (characteristic frequencies) in the simplest case. More complex coefficients can be determined in the case where the distribution of the kinetic turbulent energy over the length scales or the frequency spectrum is known.

JPDF Equation for a Scalar and Its Gradient. The problem on coefficients of a JPDF equation is considered using the equation of [6] as an example. A closed JPDF equation has been constructed for $P_t(W, \Gamma)$. It has the form

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

$$-DN_t(\Gamma)\left[\frac{2}{W^2} - \frac{2}{W}\frac{\partial}{\partial W} + \frac{\partial^2}{\partial W^2}\right]P_t(W,\Gamma) - 2D\frac{\partial}{\partial\Gamma}\left\{X_t(\Gamma)\left[1+W\frac{\partial}{\partial W}\right]P_t(W,\Gamma)\right\} -$$

$$-\left[\dot{\omega}(\Gamma)\frac{\partial}{\partial\Gamma} + \frac{\partial\dot{\omega}(\Gamma)}{\partial\Gamma}\left(2+W\frac{\partial}{\partial W}\right)\right]P_t(W,\Gamma)\,. \tag{1}$$

The functions $X_t(\Gamma)$, $N_t(\Gamma)$, and $S_{UC}(t)$ in Eq. (1) are given by the formulas

$$N_t(\Gamma) = -\frac{1}{6}D_{CC}^{(\mathrm{IV})}(0,t)\left[5-3T^2(t)(1-\hat{\Gamma}^2)\right], \quad X_t(\Gamma) = -\frac{\chi(t)}{3D}\frac{\hat{\Gamma}}{\sqrt{\overline{c^2}}}, \quad \hat{\Gamma} = \Gamma/\sqrt{\overline{c^2}(t)}\,,$$

$$T^2(t) = \overline{\left(c\frac{\partial^2 c}{\partial x_1^2}\right)}^2 \Bigg/ \left(\overline{c^2}\,\overline{\left(\frac{\partial^2 c}{\partial x_1^2}\right)^2}\right), \quad S_{UC}(t) = \overline{\left(\frac{\partial u_1}{\partial x_1}\right)\left(\frac{\partial c}{\partial x_1}\right)^2} \Bigg/ \overline{\left(\frac{\partial u_1}{\partial x_1}\right)^2}^{1/2}\,\overline{\left(\frac{\partial c}{\partial x_1}\right)^2}\,. \tag{2}$$

Thus, to determine the coefficients of Eq. (1), it is necessary to know the following six time functions: $\overline{c^2}(t)$, $\chi(t)$, $\varepsilon(t)$, $S_{UC}(t)$, $T^2(t)$, and $D_{CC}^{(\mathrm{IV})}(0, t)$. They depend on the process and should not all be determined independently.

Expressions for Coefficients of the JPDF Equation in Terms of Distributions of the Intensity of Turbulent Fluctuations over the Length Scales. Let us consider relations between the above-mentioned coefficients, the JPDF, $P_t(W, \Gamma)$, $P_t(r)$, and $P_t^{(C)}(t)$. The latter two functions are related to the correlation ($B(r, t)$ and $B^{(C)}(r, t)$) and structural ($D_{LL}(r, t)$ and $D_{CC}(r, t)$) functions of the turbulent fluctuations of velocity and scalar by the following formulas [7]:

$$P_t(r) = -\frac{\partial B(r,t)}{\partial r} = \frac{1}{2}\frac{\partial D_{LL}(r,t)}{\partial r}\,, \tag{3}$$

$$P_t^{(C)}(t) = -\frac{\partial B^{(C)}(r,t)}{\partial r} = \frac{1}{2}\frac{\partial D_{CC}(r,t)}{\partial r}\,. \tag{4}$$

The first moments of the scalar field — its dispersion and dissipation rate — are expressed in terms of the JPDF function of the scalar and its gradient via the normalization relations

$$\overline{c^2}(t) = \int \Gamma^2 P_t(W,\Gamma)\,dWd\Gamma\,, \tag{5}$$

$$\chi(t) = \int W^2 P_t(W,\Gamma)\,dWd\Gamma\,. \tag{6}$$

The dispersions of the velocity and scalar fields and their dissipation rates can be calculated alternatively using the distribution functions $P_t(r)$ and $P_t^{(C)}(t)$. According to the definitions of $P_t(r)$ and $P_t^{(C)}(r)$, the following equalities are true for the dispersions:

$$\overline{c^2}(t) = \int_0^\infty P_t^{(C)}(r)\,dr\,, \quad \overline{q^2}(t) = \sum u_i^2 = 3\int_0^\infty P_t(r)\,dr\,. \tag{7}$$

Multiplier 3 appears in the expression for $\overline{q^2}(t)$ because the function $P_t(t)$ is written for one component of the velocity vector.

Expressions for the dissipation rates $\varepsilon(t)$ and $\chi(t)$ in terms of $P_t(r)$ and $P_t^{(C)}(r)$ will be given below after the formulation of equations for these functions.

$S_{UC}(t)$ can be expressed in terms of the third derivative of the third-order structural function of the velocity and scalar fields $D'''_{LCC}(0, t)$, the rate of dissipation of the intensity of the turbulent scalar fluctuations $\chi(t)$, and the rate of dissipation of the velocity fluctuations $\varepsilon(t)$:

$$S_{UC}(t) = \frac{\frac{1}{6} D'''_{LCC}(0, t)}{(\varepsilon(t)/15\nu)^{1/2}\,(\chi(t)/3D)}\,. \tag{8}$$

An expression for $S_{UC}(t)$ in terms of the function $D'''_{LCC}(0, t)$ can be obtained by comparison of formulas presented in [7]: (12.146) (p. 69) and $D_{LC,C}(r) = 4\,B_{LC,C}(r)$ (p. 367).

To relate the quantity $D'''_{LCC}(0, t)$ to the distributions $P_t(r)$ and $P_t^{(C)}(t)$, we will use the Yaglom equation [7]

$$D_{LCC}(r, t) - 2D\frac{\partial D_{CC}(r, t)}{\partial r} = -\frac{4}{3}\chi(t)\,r\,. \tag{9}$$

Differentiating it three times with respect to the variable r and taking into account formula (4), we obtain

$$D'''_{LCC}(0, t) = 4DP_t^{(C)'''}\,. \tag{10}$$

To determine the relation between the distribution of the velocity fluctuations and the quantity $\varepsilon(t)$, we will use the Kolmogorov equation (formula (22.2) in [7]):

$$D_{LLL}(r) - 6\nu\frac{\partial D_{LL}(r)}{\partial r} = -\frac{4}{5}\varepsilon(t)\,r\,. \tag{11}$$

Since at small values of r the third-order structural function of the velocity field is a third-order infinitesimal, we obtain that

$$D_{LL}(r) = \frac{1}{15}\frac{\varepsilon(t)}{\nu}r^2 \tag{12}$$

at $r < \eta$. Differentiating relation (12) two times with respect to r and taking into account (3), we find

$$\varepsilon(t) = 15\nu P'_t(0)\,. \tag{13}$$

Since at small r the function $D_{LCC}(r, t)$ in the Yaglom equation (9) is a third-order infinitesimal with respect to r, we have

$$\chi(t) = 3DP_t^{(C)'}(0)\,. \tag{14}$$

Taking into account formulas (13), (14), and (10), we write the expression for $S_{UC}(t)$:

$$S_{UC}(t) = \frac{\frac{2}{3} D P_t^{(C)'''}(0)}{[P_t'(0)]^{1/2}\,[P_t^{(C)'}(0)]} \,. \tag{15}$$

For the correlator $T(t)$ in [6] we have obtained the formula

$$T(t) = \frac{\sqrt{2}\,\chi(t)}{3D\,[-\overline{c^2}(t)\,D_{CC}^{(\mathrm{IV})}(0, t)]^{1/2}} \,. \tag{16}$$

In view of the definition of the second-order structural function of the scalar field $D_{CC} = \overline{(c(x, t) - c(x + r, t))^2}$, the fourth derivative of it with respect to r (at $r = 0$) $D_{CC}^{(IV)}(t) \equiv D_{CC}^{(IV)}(0, t)$ can be related to the distribution of the intensity of the scalar fluctuations over various length scales in the following way:

$$D_{CC}^{(\mathrm{IV})}(0, t) = 2P_t^{(C)'''}(0) \,. \tag{17}$$

Thus, all six auxiliary functions in the JPDF equation for $P_t(W, \Gamma)$ can be expressed in terms of the distributions $P_t(r)$ and $P_t^{(C)}(r)$. In actuality, only the higher moments $S_{UC}(t)$, $T^2(t)$, and $D_{CC}^{(IV)}(t)$ in Eq. (1) are unknowns, and their definitions in terms of JPDF (5) and (6) can be used for calculating the square of the dispersion of the scalar field and its dissipation rate. The latter circumstance can be used for selection of the parameters and testing the coefficient model. In order that the information on the behavior of the higher moments can be used, it is necessary that the values of the dispersion and dissipation $\overline{c^2}(t)$ and $\chi(t)$ calculated by the coefficient model correspond to the normalizations of the JPDF (5) and (6).

Introducing the scales of the velocity field $U_0 = 2\sqrt{\overline{q_0^2}/3}$, the scalar field $s_0 = \sqrt{\overline{c_0^2}}$, the Reynolds number Re $= LU_0/\nu$, and the Peclet number Pe $= LU_0/D$, we write the formulas for calculating the desired coefficients in dimensionless form. Since below we will use only the dimensionless functions, the same designations will be left for the dimensionless variables

$$\overline{q^2}(t) = 3\int_0^\infty P_t(r)\,dr \,, \quad \overline{c^2}(t) = \int_0^\infty P_t^{(C)}(r)\,dr \,, \quad \varepsilon(t) = \frac{15}{\mathrm{Re}} P_t'(0) \,, \quad \chi(t) = \frac{3}{\mathrm{Pe}} P_t^{(C)'}(0) \,, \tag{18}$$

$$S_{UC}(t) = \frac{2P_t^{(C)'''}(0)}{3\mathrm{Pe}\,P_t'(0)^{1/2}\,P_t^{(C)'}(0)} \,, \quad D_{CC}^{(\mathrm{IV})}(0, t) = 2P_t^{(C)'''}(0) \,, \quad T^2(t) = -\frac{(P_t^{(C)'}(0))^2}{\overline{c^2}(t)\,P_t^{(C)'''}(0)} \,. \tag{19}$$

Reviewing this section, we note that the quantities on the left-hand side of equality (18) can be obtained from the normalization relations (5) and (6), and the required higher moments in (19) can be expressed in terms of the function $P_t^{(C)'''}(0)$ representing the third derivative of the distribution of the intensity of the scalar fluctuations over the length scales r at a zero value of r, because at r equal to zero the first derivatives $P_t'(0)$ and $P_t^{(C)'}(0)$ are related to the dispersions and the dissipation rates via (18).

Closed Model for the Distributions $P_t(r)$ and $P_t^{(C)}(r)$. Let us formulate models for determining the functions $P_t(r)$ and $P_t^{(C)}(r)$. At first we derive an equation for the distribution of the scalar fluctuations of a reagent over various length scales and then repeat the same derivation procedure for the distribution of the velocity fluctuations.

As the initial point, we will use the Corrsin equation for the correlation function of the reagent $B_{CC} = \overline{c(x)c(x + r)}$ in the dimensional form (formula (14.72) in [7])

$$\frac{\partial B_{CC}(r,t)}{\partial t} = 2\left(\frac{\partial}{\partial r} + \frac{2}{r}\right)\left[B_{LC,C}(r) + D\,\frac{\partial B_{CC}(r,t)}{\partial r}\right] - 2B_{\varphi l}(r,t)\,. \tag{20}$$

Here $B_{LC,C}(r) = \overline{u(x)c(x)c(x+r)}$ is the third-order, two-point moment of the velocity field and the fluctuating scalar field and $B_{\varphi l}(r) = \overline{\Phi[C(\mathbf{x})]c(\mathbf{x} + \mathbf{r})}$ is the correlation function of the chemical-reaction rate $\Phi(C)$ and the reagent-concentration fluctuations. Since $\overline{C} = \overline{C}(t)$ (i.e., the average concentration of the reagent depends on time), to make a complete description it is also necessary to use the equation for the average quantity $\overline{C}(t)$:

$$\frac{\partial \overline{C}(t)}{\partial t} = \Phi\,[\overline{C}(t) + c]\,. \tag{21}$$

Let us take a derivative of the left and right sides of Eq. (20) with respect to r. Then, for the function describing the distribution of the intensity of the reagent fluctuations we obtain

$$\frac{\partial P_t^{(C)}(r)}{\partial t} = -2\,\frac{\partial}{\partial r}\left(\frac{\partial}{\partial r} + \frac{2}{r}\right)\left[B_{LC,C}(r) - DP_t^{(C)}(r)\right] + 2W_t(r)\,. \tag{22}$$

The function $W_t(r)$ is produced by the chemical source term in the initial equation, i.e.,

$$W_t(r) = \frac{\partial}{\partial r}\langle \Phi(C)\,c\,(x+r)\rangle\,. \tag{23}$$

The nonclosedness of Eq. (22) is due to the presence of the functions $B_{LC,C}(r)$ and $W_t(r)$ in it. An expression for the function $B_{LC,C}(r)$ in terms of the functions $P_t(r)$ and $P_t^{(C)}(r)$ can be obtained using the analogy between turbulent and molecular diffusion. We define the micro- (Mi) and macrocomponent (Ma) of the turbulent field of the reagent C as

$$\int_0^\infty P_t^{(C)}(r)\,dr = \mathrm{Mi} + \mathrm{Ma}\,, \tag{24}$$

where $\mathrm{Mi} = \int_0^r P_t^{(C)}(\tilde{r})d\tilde{r}$ and $\mathrm{Ma} = \int_0^\infty P_t^{(C)}(\tilde{r})d\tilde{r}$.

Let us write an equation for the macrocomponent Ma. To do this, we will integrate the left- and right-hand sides of Eq. (22) over r from r to ∞:

$$\frac{\partial}{\partial t}\int_r^\infty P_t^{(C)}(\tilde{r})\,d\tilde{r} = -\Pi^{(C)}(r) - 2D\left(\frac{\partial}{\partial r} + \frac{2}{r}\right)P_t^{(C)}(r) - 2\langle \Phi(C)\,c\,(x+r)\rangle\,. \tag{25}$$

Here $\Pi^{(C)}(r)$ is the turbulent flux of the scalar-fluctuation intensity through the point r of the spectrum. By analogy with the molecular transfer, we will assume that the flux $\Pi^{(C)}(r)$ has the form

$$\Pi_t^{(C)}(r) = 2D_{\mathrm{tur}}(r)\left(\frac{\partial}{\partial r} + \frac{2}{r}\right)P_t^{(C)}(r)\,. \tag{26}$$

Formula (26) for the turbulent flux involves the unknown function $D_{\mathrm{tur}}(r)$ representing an analogy of the diffusion coefficient in the expression for the molecular flux. The turbulent diffusion is due to the action of all the vortices with dimensions smaller than r. Therefore, $D_{\mathrm{tur}}(t)$ can be represented as

$$D_{\text{tur}}(r) = \int_0^r d_{\text{tur}}(\tilde{r})\, d\tilde{r}\,. \tag{27}$$

Here $d_{\text{tur}}(\tilde{r})d\tilde{r}$ is the contribution of the vortices with dimensions from $\tilde{r}$ to $\tilde{r} + d\tilde{r}$ to the turbulent-diffusion coefficient $D_{\text{tur}}(r)$. It would appear reasonable that the coefficient $d_{\text{tur}}(\tilde{r})$ depends on the distribution of the energy of the turbulent fluctuations over the length scales $P_t(r)$. Using the reasonings of the dimensionality theory, we write

$$d_{\text{tur}}(\tilde{r}) = \beta \sqrt{P_t(\tilde{r})}\, \tilde{r}\,. \tag{28}$$

Here β is a constant determined experimentally. In view of (28), the expression for the turbulent-diffusion coefficient (27) takes the form

$$D_{\text{tur}}(r) = \beta \int_0^r \sqrt{P_t(\tilde{r})}\, \tilde{r}\, d\tilde{r}\,. \tag{29}$$

In the final analysis, the expression for the turbulent flux of the scalar-fluctuation intensity through the point r can be represented as

$$\Pi_T^{(C)}(r) = 2\beta \int_0^r \sqrt{P_t(\tilde{r})}\, \tilde{r}\, d\tilde{r} \left(\frac{\partial}{\partial r} + \frac{2}{r}\right) P_t^{(C)}(r)\,. \tag{30}$$

Substituting this expression into equality (25) and calculating the derivative of the left- and right-hand sides of the equality obtained with respect to r, we obtain the following equation for $P_t^{(C)}(r)$ in dimensionless form:

$$\frac{\partial P_t^{(C)}(r)}{\partial t} = \frac{\partial}{\partial r}\left\{\left(\frac{2}{\text{Pe}} + 2\beta \int_0^r \sqrt{P_t(\tilde{r})}\, \tilde{r}\, d\tilde{r}\right)\left(\frac{\partial}{\partial r} + \frac{2}{r}\right) P_t^{(C)}(r)\right\} + 2W_t(r)\,. \tag{31}$$

The equation for the distribution of the turbulent scalar fluctuations $P_t^{(C)}(r)$ involves the function $P_t(t)$ describing the distribution of the turbulent fluctuations over various length scales.

An equation for the function $P_t(r)$ can be obtained in the same approximation and by the same method as in the case of derivation of the equation for $P_t^{(C)}(r)$. However, in this case, the Kármán–Howarth equation is used as the initial equation for the correlation function. This equation in dimensionless form is as follows:

$$\frac{\partial P_t(r)}{\partial t} = \frac{\partial}{\partial r}\left\{\left(\frac{2}{\text{Re}} + 2\gamma \int_0^r \sqrt{P_t(\tilde{r})}\, \tilde{r}\, d\tilde{r}\right)\left(\frac{\partial}{\partial r} + \frac{4}{r}\right) P_t(r)\right\}. \tag{32}$$

Here γ is a constant determined by comparison of the theoretical and experimental data.

To estimate the constants β and γ in (31) and (32), it is necessary to relate them to the constants c and s in the "two-thirds" power law for the corresponding structural functions [7]

$$D(r) = c\varepsilon^{2/3} r^{2/3}\,, \tag{33}$$

$$D^{(C)}(r) = s\chi\varepsilon^{-1/3} r^{2/3}\,. \tag{34}$$

Let us solve (31) and (32) analytically in the inertial and inertial-convective intervals of the scales. The equations for $P_t(r)$ and $P_t^{(C)}(r)$ in these intervals take the form

$$\frac{2}{3}\varepsilon = 2\gamma \int_0^r \sqrt{\tilde{r}P(\tilde{r})\,\tilde{r}}\; d\tilde{r}\left(\frac{d}{dr}+\frac{4}{r}\right)P(r)\,, \tag{35}$$

$$2\chi = 2\beta \int_0^r \sqrt{\tilde{r}P(\tilde{r})\,\tilde{r}}\; d\tilde{r}\left(\frac{d}{dr}+\frac{4}{r}\right)P^{(C)}(r)\,. \tag{36}$$

Here, the functions $P_t(r)$ and $P_t^{(C)}(r)$ are defined, in view of (33) and (34), as

$$P_t(r) = \frac{1}{3} c\varepsilon^{2/3} r^{-1/3}\,, \tag{37}$$

$$P_t^{(C)}(r) = \frac{1}{3} s\chi\varepsilon^{-1/3} r^{-1/3}\,. \tag{38}$$

Substituting expressions (37) and (38) into Eqs. (35) and (36) and performing integration, we obtain formulas relating the constants γ and β to the constants c and s:

$$\gamma = \frac{12}{11\sqrt{13}} c^{-3/2}\,, \quad \beta = \frac{12\sqrt{3}}{5}\frac{1}{\sqrt{c}\, s}\,. \tag{39}$$

Using the experimental values of c and s from [7], we obtain the following assessment: $\gamma = 0.24$ and $\beta = 1.08$.

Simultaneous solution of Eqs. (31) and (32) gives expressions for the functions $P_t^{(C)}(r)$ and $P_t(r)$, necessary for the calculation of the statistical characteristics of the turbulent velocity and scalar fields (18)–(19) which are coefficients in the JPDF equation for $P_t(W, \Gamma)$.

Expressions for Coefficients in the JPDF Equation in Terms of Distributions of the Intensity of Turbulent Fluctuations over the Wave Numbers. An alternative model for determining the coefficients in (1) can be constructed on the basis of the transfer equations for the distributions of the turbulent energy and the intensity of the scalar fluctuations over the spectrum of wave numbers. The transfer equations were closed with the use of the Heisenberg hypothesis. The equation for $E(k, t)$ has the form [7, p. 215]

$$\frac{\partial E(k,t)}{\partial t} = -2\frac{\partial}{\partial k}\left[\left[\frac{1}{\mathrm{Re}} + \alpha\int_k^{\infty}\sqrt{\frac{E(\tilde{k},t)}{\tilde{k}^3}}\,d\tilde{k}\right]\int_0^k k'^2 E(k',t)\,dk'\right]. \tag{40}$$

The constant α in (40) was evaluated by comparison of the Kolmogorov constant calculated based on the solution of this equation to its experimental value (Ko = 1.44). This approach gives $\alpha = 0.54$. This value falls within the range of values of this constant 0.2–0.85 obtained theoretically and experimentally (see [7, p. 220]). The best agreement between the numerical solution of the spectral-transfer equation (40) and the data of the direct numerical simulation performed in [8] has been obtained by us at $\alpha = 0.45$, which conforms with the data of [7], where it has been noted that the best agreement between the experimental data of Stewart and Townsend and the calculations of Tolmin and Meetz for the decaying turbulence downstream of a grid is observed at $\alpha \sim 0.45$.

The equation for the scalar spectrum $E^{(C)}(k, t)$ can be represented as

$$\frac{\partial E^{(C)}(k,t)}{\partial t} = -2\frac{\partial}{\partial k}\left[\left[\frac{1}{\mathrm{Pe}} + \sigma\int_k^{\infty}\sqrt{\frac{E(\tilde{k},t)}{\tilde{k}^3}}\,d\tilde{k}\right]\int_0^k k'^2 E^{(C)}(k',t)\,dk'\right]. \tag{41}$$

The constant σ in Eq. (41) was initially evaluated by comparison of the Obukhov–Batchelor constant (calculated based on the solution of this equation in the inertial-convective interval) to its experimental value Ba = 0.4, which gives σ

= 1.85. Then this constant was decreased to σ = 1.25 in an attempt to bring the results of the numerical solution into coincidence with the data of the direct numerical simulation [8].

Below we present expressions for the desired coefficients of Eq. (1) in terms of $E(k, t)$ and $E^{(C)}(k, t)$ [9]: the dispersion of the turbulent fields of velocity $\overline{q^2(t)}$ and scalar $\overline{c^2(t)}$:

$$\frac{\overline{q^2(t)}}{2} = \int_0^\infty E(k, t)\, dk\,, \quad \overline{c^2(t)} = \int_0^\infty E^{(C)}(k, t)\, dk\,; \tag{42}$$

the rate of dissipation of the turbulent fields of velocity $\varepsilon(t)$ and scalar $\chi(t)$:

$$\varepsilon(t) = 2\nu \int_0^\infty k^2 E(k, t)\, dk\,, \quad \chi(t) = D \int_0^\infty k^2 E^{(C)}(k, t)\, dk\,; \tag{43}$$

the mixed asymmetry of the derivatives of the fluctuating fields of velocity and scalar $S_{UC}(t)$:

$$S_{UC}(t) = -\sqrt{\frac{3}{40}}\, \frac{\int_0^\infty k^2 T^{(C)}(k, t)\, dk}{\left[\int_0^\infty k^2 E(k, t)\, dk\right]^{1/2} \left[\int_0^\infty k^2 E^{(C)}(k, t)\, dk\right]}\,, \tag{44}$$

where $T^{(C)}(k, t)$ is the function characterizing the transfer of the intensity of the turbulent fluctuations of the scalar through the spectrum of wave numbers in the Corrsin equation for the spectrum $E^{(C)}(k, t)$;

the fourth derivative of the second-order, two-point structural function of the scalar field at a zero value of this variable:

$$D_{CC}^{(\mathrm{IV})}(0, t) = -\frac{2}{5} \int_0^\infty k^4 E^{(C)}(k, t)\, dk\,. \tag{45}$$

Setting of the Initial Conditions in Subsidiary Problems. One of the objectives of the present work is comparison of the data obtained with the data of direct numerical simulation. Therefore, we used initial conditions identical to those of the direct numerical simulation in the corresponding works as well as literature data [8] and data of our direct numerical simulation (hereinafter, the direct numerical simulation of isotropic velocity and scalar fields performed by one of the authors will be referred to as DNS-1).

In [8], the initial conditions were defined by the following relations:

$$E(k, 0) = A_U k^4 \exp(-Bk^2)\,, \quad E^{(C)}(k, 0) = A_C k^4 \exp(-Bk^2)\,, \tag{46}$$

where $A_U = 6\sqrt{\pi} B^{3/2}$, $A_C = 12\sqrt{\pi} B^{3/2}$, and $B = 0.0220971$.

Curves of the initial distributions of the velocity and scalar fluctuations in the space of wave numbers obtained by DNS-1 are shown in Fig. 1. The initial field consists of large-scale fluctuations, to which correspond peaks of the distributions at small values of the wave number k. These distributions were converted using the formulas of [7, 10]

$$P_0(r) = 2 \int_0^\infty \left\{ \left[\frac{3}{(kr)^4} - \frac{1}{(kr)^2} \right] \sin(kr) - \frac{3}{(kr)^3} \cos(kr) \right\} kE(k, 0)\, dk\,, \tag{47}$$

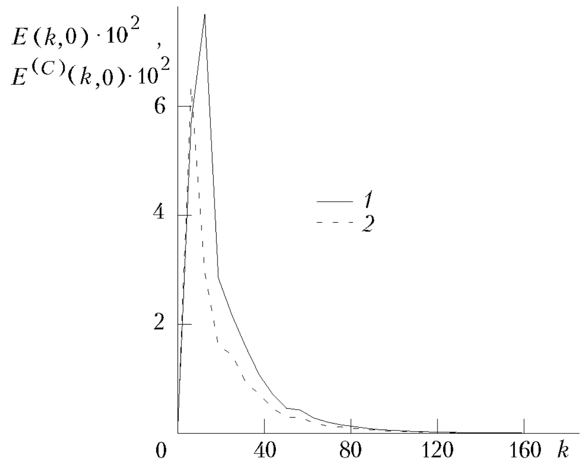


Fig. 1. Initial distributions of the turbulent fields of velocity (1) and scalar (2) obtained by DNS-1.

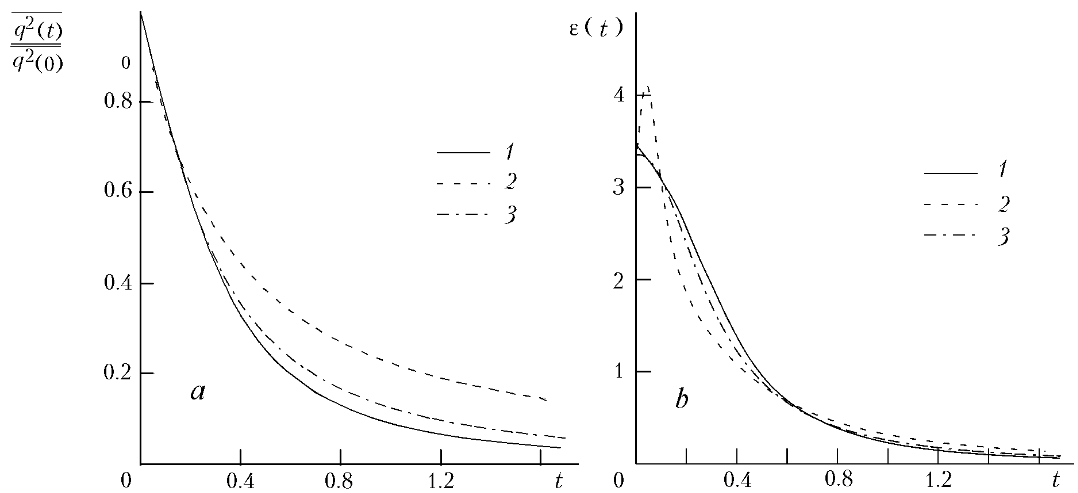


Fig. 2. Evolution of the dispersion (a) and dissipation (b) of the velocity fluctuations: 1) DNS-1; 2) calculation with model (31)–(32); 3) calculation with model (41)–(42).

$$P_0^{(C)}(r) = \int_0^{\infty} \left[\frac{\sin(kr)}{(kr)^2} - \frac{\cos(kr)}{kr} \right] kE^{(C)}(k, 0)\, dk \tag{48}$$

to the space of length scales, and then the calculations were performed on the basis of models (31)–(32) and (40)–(41) in the spaces of r and k.

Initial Conditions of DNS-1. DNS-1 was performed in the computational region of dimension $(2\pi)^3$ with 128^3 nodes, maximum wave number $k = 383.324$, and initial turbulent Reynolds number $\mathrm{Re}_\lambda(0) = u'\lambda/\nu = 56.45$, constructed in the Taylor length scale $\lambda(0) = 0.48157$ at a root-mean-square magnitude of the velocity fluctuation $u'(0) = 1.407$. The scalar field transferred by the velocity field is homogeneous, isotropic, and chemically inertial; in this case, the Prandtl number Pr = 0.7 and the kinematic viscosity $\nu = 0.012$. Mixing occurs at a practically segregated scalar field with an average value close to 0.7. The Reynolds and Peclet numbers are $\mathrm{Re} = UL/\nu = 736.7$ and $\mathrm{Pe} = 515.7$. Below, the data of DNS-1 are presented in dimensionless form. To bring the data to the dimensionless form, we used the scales of length $L_0 = 2\pi$, velocity $U_0 = u'(0) = \sqrt{\overline{q^2}(0)/3} = 1.407$, time $t_0 = L_0/U_0$, and scalar $\sqrt{\overline{c^2}(0)}$.

Results. In Figs. 2–9, the data of the numerical solution of the model equations (31)–(32) and (40)–(41) are shown in comparison to the data of [8] and the data of DNS-1.

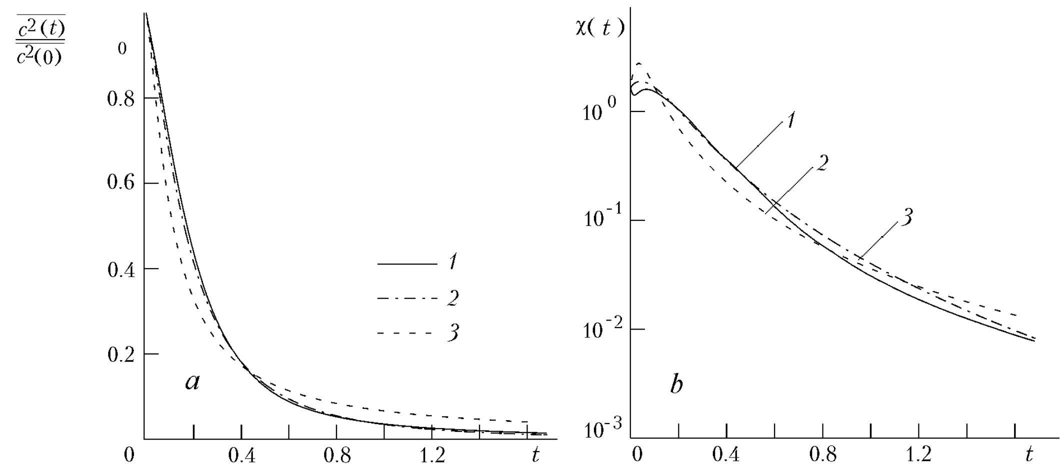


Fig. 3. Evolution of the dispersion (a) and dissipation (b) of the scalar fluctuations. The designations are the same as in Fig. 2.

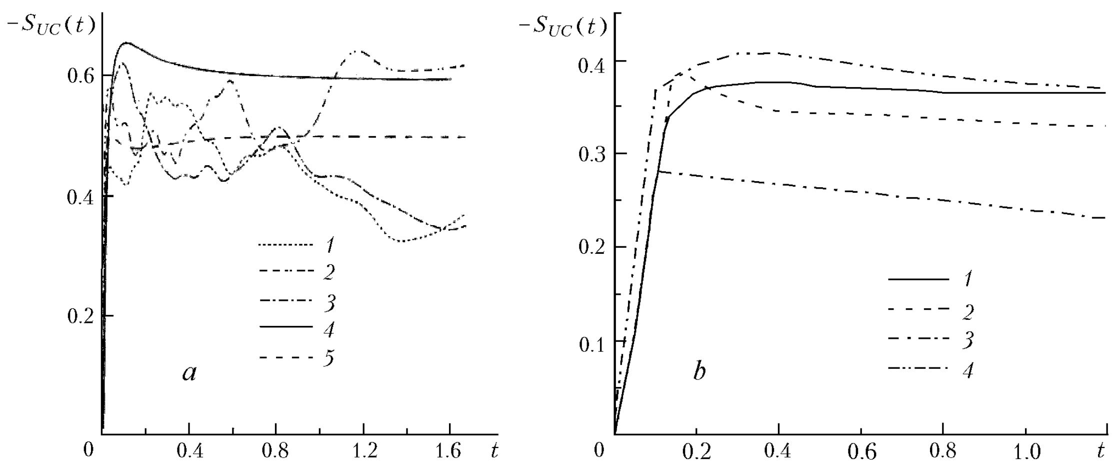


Fig. 4. Evolution of the mixed skewness of the derivatives of the fluctuating fields of velocity and scalar $S_{UC}(t)$: a): 1–3) DNS-1 ($S_{UC}(t)$ is calculated by three different components of the velocity and scalar gradient); 4) calculation with model (31)–(32); 5) calculation with model (41)–(42); b): 1) DNS-1 [8]; 2) direct-interaction approximation [8]; 3) test-field model [8]; 4) calculation in the space of wave numbers with model (41)–(42).

Figure 2 shows the evolution of the dispersion and the dissipation rate of the velocity-fluctuation field. Since turbulent-energy sources are absent in an isotropic field, the kinetic energy of turbulence $K_{tur} = \overline{q^2}(t)/2$ and the rate of its dissipation $\varepsilon(t)$ degenerate. The model constructed in the space of length scales (31)–(32), unlike the DNS-1 and the spectral model (40)–(41), gives a nonmonotonic dependence of the dissipation rate on time at the initial stage of the evolution. The nonmonotonic behavior of the dissipation rate (Fig. 2b) is characteristic of a low-dissipation initial field of the velocity fluctuations. At the initial stage, competing processes of increasing the dissipation rate occur because of the breakdown of large vortices, the increase in the velocity gradients, and the decrease in the dissipation rate as a result of the decay of turbulence and the decrease in the kinetic energy of turbulence as a whole. As a consequence, $\varepsilon(t)$ increases and reaches a maximum value for a dimensionless time equal approximately to unity, which corresponds, in order of magnitude, to one turnover of an energy vortex.

Analogous graphs of change in the relative dispersion and the dissipation rate of the scalar field are presented in Fig. 3. The initial field of the scalar fluctuations is more large-scale as compared to the corresponding field of velocity fluctuations (see Fig. 1); therefore, for all the calculations (DNS-1 and models (31)–(32) and (40)–(41)) the rate

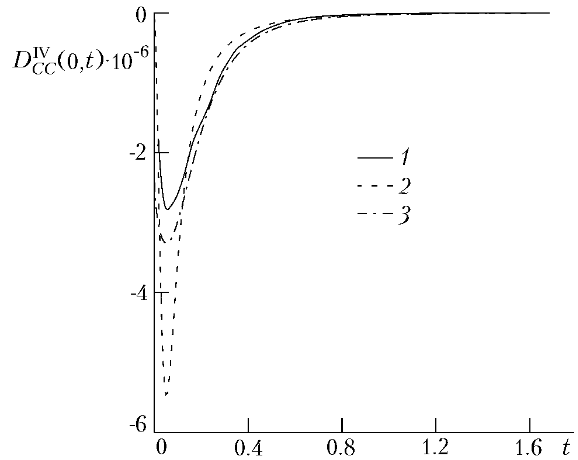


Fig. 5. Evolution of the fourth derivative of the second-order, two-point structural function of the scalar field with respect to the spatial variable *r* at a zero value of *r*. The designations are the same as in Fig. 2.

of dissipation of the scalar field increases in the initial period because of the increase in its gradients. By and large, the data on the evolution of the dispersion of the fluctuations of the scalar field and the rate of its dissipation obtained by the two coefficient models and DNS-1 are in satisfactory agreement.

Figure 4 shows the results of the calculation of the third moment — the mixed skewness of the derivatives of the fluctuating velocity and scalar fields. The mixed skewness $S_{UC}(t)$ describes the influence of the turbulent velocity-gradient field on the scalar-gradient field.

It was originally believed [11] that $S_{UC}(t) \to 0$ at Schmidt numbers $\mathrm{Sc} \ll 1$. However, it was subsequently shown [12] that S_{UC} remains practically unchanged and equal to –0.5 for $0.1 < \mathrm{Sc} < 1$. According to [13], the skewness of the gradient $S_{UC}(t)$ = –0.4 at Sc = 3 and, according to [14], $S_{UC}(t)$ = –0.4 at Sc = 0.04 and $S_{UC}(t)$ = –0.5 at Sc = 144.

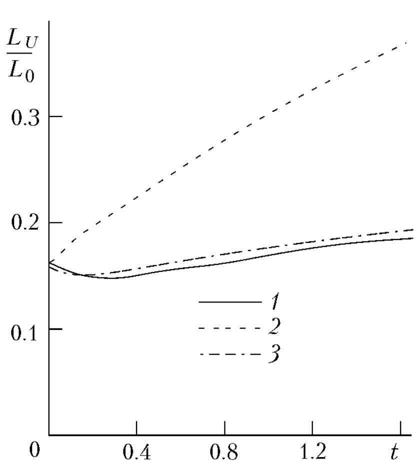
It is known that the asymptotic value of $S_{UC}(t)$ is related to the corresponding value of the gradient skewness of the fluctuating velocity field $S(t)$ by the relation [7]

$$\frac{5}{3} S^2_{UC}(t) + \frac{7}{18} S_{UC}(t)\, S(t) = \frac{2}{3}\,. \tag{49}$$

The value of $S(t)$ = –0.4 has been measured experimentally [15]. The mixed skewness of the gradients $S_{UC}(t)$ calculated by formula (49) is $S_{UC}(t) \approx -0.6$. In Fig. 4a, the calculation data obtained with models (31)–(32) and (40)–(41) are compared to the data of DNS-1 and, in Fig. 4b, the calculation data obtained with the spectral model (40)–(41) are compared to the data of the direct numerical simulation performed in [8] and to the data of other models in [8].

The results of the calculation of the higher moment $D^{(IV)}_{CC}(0,\ t)$ — the fourth derivative of the structural function — are presented in Fig. 5. All three curves agree qualitatively; however; the best quantitative agreement between the calculation data for $D^{(IV)}_{CC}(0,\ t)$ and the analogous data of DNS-1 have been obtained with the spectral model (40)–(41). It should be noted that the coefficient $D^{(IV)}_{CC}(0,\ t)$ has a small value and therefore is of little importance in Eq. (1). The most important higher moment is the coefficient $S_{UC}(t)$ of the term responsible for the action of the hydrodynamic field on the field of the scalar fluctuations.

The characteristic scales of the turbulent field are shown in Figs. 6–9. Here the Reynolds number of turbulence $\mathrm{Re}_\lambda = \lambda u'/\nu$ is constructed in the Taylor microscale of the velocity field with regard for the root-mean-square magnitude of the velocity fluctuations. The dimensionless Taylor microscale $\lambda(t)$ was determined from the relation $\lambda^2(t) = 10K_{\mathrm{tur}}/(\mathrm{Re}_0\varepsilon(t))$. The microscale L_U was calculated based on the solution of problem (31)–(32) by the formula $L_U = \int_0^\infty rP_t r(dr)/\int_0^\infty P_t r(dr) = \frac{3}{2K_{\mathrm{tur}}}\int_0^\infty rP_t(r)dr$ and the time scale was calculated by the formula $T_U = L_U/\sqrt{\frac{2}{3}K_{\mathrm{tur}}}$.



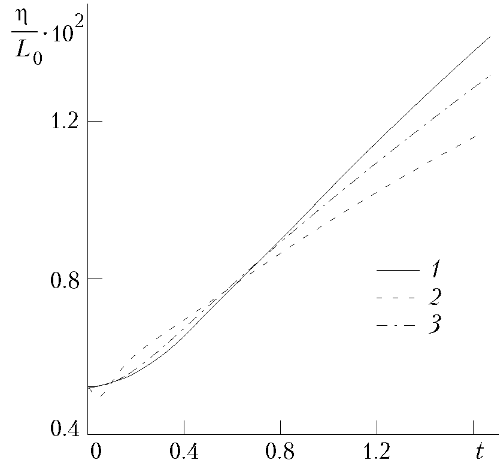
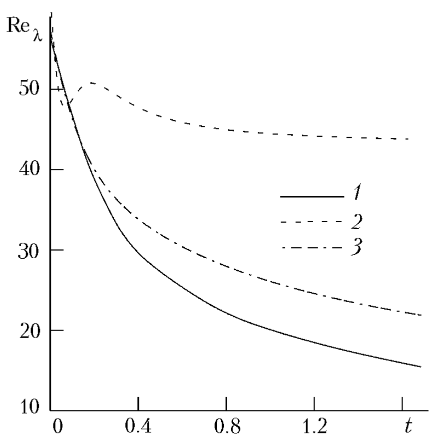


Fig. 6. Evolution of the integral length scale. The designations are the same as in Fig. 2.

Fig. 7. Evolution of the turbulent Reynolds number. The designations are the same as in Fig. 2.



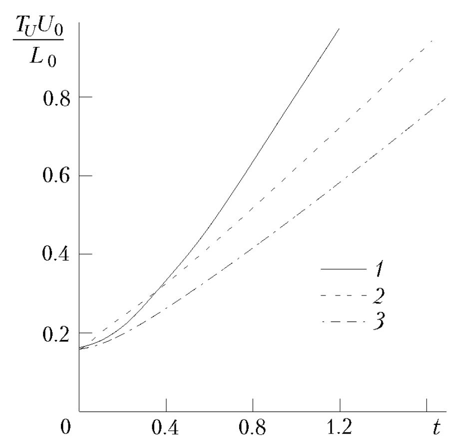


Fig. 8. Evolution of the Kolmogorov length. The designations are the same as in Fig. 2.

Fig. 9. Evolution of the integral time scale. The designations are the same as in Fig. 2.

These length and time scales were analogously determined based on the solution of the problem on spectral distributions (41)–(42). For this purpose, the above formula for determining the macroscale was converted to the space k with the use of transform (47), which gives $L_U = \frac{3}{4}\pi \int_0^\infty \frac{E(k)}{k}dk / \int_0^\infty E(k)dk = \frac{3}{2K_{\text{tur}}}\frac{\pi}{2}\int_0^\infty \frac{E(k)}{k}dk$.

The length and time scales calculated by these two coefficient models have marked quantitative differences. This is especially true for the characteristic length scales — the macroscale (Fig. 6) and the Taylor microscale. The linear scales (Figs. 6, 7, and 8) determined based on the solution of the problem in the space r (31)–(32) agree worse with those obtained by DNS-1 as compare to the analogous scales determined based on the solution of problem (40)–(41). The reverse situation is observed for the time scale (see Fig. 9). In this case, the data obtained with model (31)–(32) agree most closely with the data of DNS-1. The initial portion is followed by the portion of near-linear increase in the macroscale L_U and in the Kolmogorov scale η, which corresponds to the theoretical representations.

CONCLUSIONS

Two complementary models for determining the coefficients of the equation for the joint probability density of a scalar and its gradient (1) have been constructed. They allow one to predict the evolution of all the coefficients in Eq. (1) for an isotropic, degenerate field of velocity and scalar fluctuations.

The coefficient models (31)–(32) and (40)–(41) have been tested by comparison of the data obtained with them to the data of direct numerical simulation performed for the same conditions. The data obtained with the spectral-transfer model based on the Heisenberg hypothesis agree most closely with the data of the direct numerical simulation. The data obtained with both models for the coefficients that are of considerable importance in Eq. (1) ($\overline{c^2}(t)$, $\chi(t)$, and $S_{UC}(t)$) agree satisfactorily. Using the two alternative models for the coefficients of Eq. (1), one can close the equation for the joint probability density of a scalar and its gradient without recourse to experimental data.

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NOTATION

$\overline{c^2}(t)$, dispersion of the scalar-field fluctuations; D, diffusion coefficient; $D_{CC}^{(\mathrm{IV})}(0, t)$, fourth-order derivative of the second-order structural function of the scalar field with respect to the spatial derivative at a zero value of the latter; $E(k, t)$, distributions of the energy of the turbulent velocity fluctuations over the wave numbers; $E^{(C)}(k, t)$, distributions of the energy of the turbulent scalar fluctuations over the wave numbers; L_U, macroscale; Pe = LU_0/D, Peclet number; $P_t(r)$, distribution of the turbulent velocity fluctuations over the length scales; $P_t^{(C)}(t)$. distribution of the turbulent scalar fluctuations over the length scales; $P_t(W, \Gamma)$, joint probability density of the scalar and its gradient; $\overline{q^2(t)}$, dispersion of the velocity-field fluctuations; Re = LU_0/ν, Reynolds number; $\mathrm{Re}_\lambda = \lambda U_0/\nu$, turbulent Reynolds number constructed in the Taylor length scale; s_0, scale of the scalar field; $S_{UC}(t)$, mixed skewness of the fields of the gradients of the velocity and scalar fluctuations; $T^2(t)$, square of the correlator between the fields of the scalar and its second spatial derivative; T_U, time scale; t, time; U_0, scale of the velocity field; $W = \sqrt{W_1^2 + W_2^2 + W_3^2}$, modulus of the scalar gradient; Γ, magnitude of the scalar fluctuations; $\varepsilon(t)$, rate of dissipation of the velocity-field fluctuations; η, Kolmogorov length scale; λ, Taylor microscale; ρ, density; ν, coefficient of viscosity; $\chi(t)$, rate of dissipation of the scalar-field fluctuations; $\omega(\Gamma)$, rate of a chemical reaction. Subscripts: t, fixed instant of time; U, means that a characteristic is related to the turbulent velocity field; C, means that a characteristic is related to the turbulent scalar field; UC, means that a characteristic is related to the mutual influence of the turbulent fields of velocity and scalar; tur, turbulence.

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