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HEAT AND MASS TRANSFER IN TURBULENT FLOWS

CALCULATION OF THE STATISTICAL CHARACTERISTICS OF A TURBULENT FLOW UNDER THE ACTION OF EXTERNAL FORCES

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A study is made of the statistical characteristics of isotropic velocity and scalar fields in supply of the kinetic energy of turbulence from the energy of the average flow. Two models based on the distributions of the kinetic turbulence energy and the intensity of scalar-field pulsations by wave numbers and length scales are used for calculation of the statistical characteristics of turbulent velocity and scalar fields. The calculation results are compared to the data of the direct numerical modeling performed under the same initial conditions.

Introduction. A great deal of chemical reactions realized in industrial devices are "rapid" (i.e., the time of chemical reaction is much shorter than the time of turbulent mixing). In this case, the chemical-reaction rate is determined by the rate of mixing of the reagents to the molecular level. Turbulent mixing seeks to make the scalar field homogeneous, in so doing considerably intensifying this process due to the formation of large scalar gradients in the flow. The joint action of turbulent transfer and diffusion makes the mixing (from a large-scale one to that at the molecular level) efficient.

The formalism of the probability density function of the turbulent pulsations is used to statistically describe turbulent mixing [1]. Models based on the joint probability density function (JPDF) are used to study the turbulent reacting scalar field. Knowledge of a JPDF makes it possible to correctly average strongly nonlinear terms describing chemical interaction in transfer equations for the concentrations of the mixture components and the temperature. Methods of construction of the equations for different JPDFs in turbulent flows have already been developed at present [1–5]. Open equations for a number of JPDFs have been presented in [2]. Data of experiments and direct numerical modeling as well as the assumptions of the Gaussian or another existing form of conditional distribution functions are used to close them.

The conservative-scalar method where a special variable (conservative scalar), the transfer equations for which contain no term describing chemical interaction, is constructed are widely used for description of flows with chemical reactions. The conditional moments from the JPDF of the conservative scalar and its gradient (conditional scalar-dissipation function, flame-surface density, etc.) are then used in the equations for nonconservative scalars. Also, the equation for the JPDF of the scalar and its gradient is used with allowance for the terms characterizing chemical interaction, e.g., when it is necessary to calculate very low concentrations of harmful reaction products [6].

Closed equations for the JPDF of the scalar and its gradient have been presented in [6–8]. The models presented contain the unknown coefficients to determine which one must use experimental results and data of direct numerical modeling or construct additional models.

Since the models mentioned in [6–8] for JPDFs are single-point ones from the viewpoint of the statistics used, their coefficients must allow for the spatial turbulence structure. In the simplest case there are the characteristic space and time scales of turbulence (characteristic frequencies). The presence of the known distribution of the kinetic turbulence energy by length scales or by wave numbers makes it possible to determine these coefficients and those more complex in nature.

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To find the coefficients one can use data of direct numerical modeling which contain the most detailed information on the structure of the flow or flame mixed. However, the methods of direct numerical modeling require considerable computational resources and are restricted to the cases of the simplest geometry and small Reynolds and Péclet numbers; therefore, at the present time, statistical models remain, as previously, the basic means for investigating practical problems of turbulent mixing in both inert flows and flows with chemical reactions.

The present work seeks to extend the capabilities of two models for evaluation of the statistical characteristics of turbulent velocity and scalar fields in the case of generation of kinetic turbulence energy and to compare the results of numerical solution to the corresponding data of direct numerical modeling.

Models for Calculation of the Statistical Characteristics of Turbulent Velocity and Scalar Fields. The closed equation for the JPDF of a scalar and the modulus of its gradient was obtained earlier in [8]. It includes the following statistical characteristics of turbulent velocity and scalar fields as time-dependent coefficients: $\overline{c^2}(t)$, $\varepsilon(t)$, $\chi(t)$, $S_{uc}(t)$, and $D_{cc}^{(\mathrm{IV})}(0,\ t)$.

The quantities mentioned can be obtained by solution of an auxiliary system of equations. Two models, i.e., systems of equations of transfer of turbulent energy and intensity of scalar pulsations by length scales [9] and by wave numbers [10], have been proposed as such a system. The system of equations of turbulent-energy transfer and scalar-pulsation intensity by length scales has the form

$$\frac{\partial P(r,t)}{\partial t} = \frac{\partial}{\partial r}\left[\left(\frac{2}{\mathrm{Re}} + 2\gamma \int_0^r \sqrt{rP(\tilde{r},t)}\, d\tilde{r}\right)\left(\frac{\partial}{\partial r} + \frac{4}{r}\right) P(r,t)\right], \tag{1}$$

$$\frac{\partial P^{(c)}(r,t)}{\partial r} = \frac{\partial}{\partial r}\left\{\left(\frac{2}{\mathrm{Pe}} + 2\beta \int_0^r \sqrt{P(\tilde{r},t)\tilde{r}}\, d\tilde{r}\right)\left(\frac{\partial}{\partial r} + \frac{2}{r}\right) P^{(c)}(r,t)\right\}, \tag{2}$$

and that by wave numbers has the form

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

$$\frac{\partial E^{(c)}(k,t)}{\partial t} = -2\frac{\partial}{\partial k}\left[\left[\frac{1}{\mathrm{Pe}} + \sigma \int_k^\infty \sqrt{\frac{E(\tilde{k},t)}{\tilde{k}^3}}\, d\tilde{k}\right] \int_0^k k'^2 E^{(c)}(k',t)\, dk'\right]. \tag{4}$$

The procedures of numerical solution of these systems have been presented respectively in [9] and [10], and the models have been checked by comparing to the data of direct numerical modeling in [11], where consideration has been given to the turbulent velocity field (degenerated with time) without the generation of turbulence energy. The procedure of selection of the constants β, γ, and α, σ of the models was described in this work.

The necessary coefficients can be determined by solution of the systems of equations (1), (2) and (3), (4) according to the relations [11]

$$\overline{c^2}(t) = \int_0^\infty P^{(c)}(r,t)\, dr, \quad \varepsilon(t) = \frac{15}{\mathrm{Re}} P'(0,t), \quad \chi(t) = \frac{3}{\mathrm{Pe}} P^{(c)'}(0,t),$$
$$S_{uc}(t) = \frac{2P^{(c)'''}(0,t)}{3\mathrm{Pe}\, P'(0,t)^{1/2} P^{(c)'}(0,t)}, \quad D_{cc}^{(\mathrm{IV})}(0,t) = 2P^{(c)'''}(0,t); \tag{5}$$

$$\overline{c^2}(t) = \int_0^\infty E^{(c)}(k, t)\, dk\,, \quad \varepsilon(t) = \frac{2}{\mathrm{Re}} \int_0^\infty k^2 E(k, t)\, dk\,, \quad \chi(t) = \frac{1}{\mathrm{Pe}} \int_0^\infty k^2 E^{(c)}(k, t)\, dk\,,$$

$$S_{uc}(t) = -\frac{\sqrt{\frac{3}{40}} \int_0^\infty k^2 T^{(c)}(k, t)\, dk}{\int_0^\infty k^2 E^{(c)}(k, t)\, dk \left(\int_0^\infty k^2 E(k, t)\, dk \right)^{1/2}}\,, \quad D_{cc}^{(\mathrm{IV})}(0, t) = -\frac{2}{5} \int_0^\infty k^4 E^{(c)}(k, t)\, dk\,. \tag{6}$$

Modification of the Models for the Case of Generation of Pulsation Energies. The turbulent velocity field (degenerated with time) with the generation of turbulence energy has been considered in [9–11]. In the case where the external force causing the generation of turbulence energy acts on the hydrodynamic field of turbulent pulsations, the equation of transfer of turbulent energy must be supplemented with a term describing this action. On the basis of the existing ideas of the spectrum of generation of kinetic turbulence energy in the case of homogeneous turbulence [12], the right-hand side of the equation was supplemented with a term allowing for this generation with a prescribed turbulent-energy distribution by length scales:

$$S_{\mathrm{g}}(r) = \frac{4}{3} G_u \frac{r}{L_u^2} \exp\left(-\frac{r^2}{L_u^2} \right), \tag{7}$$

where L_u is the parameter whose value is related to the length scale on which we have the generation of kinetic energy in the flow. The maximum of $S_{\mathrm{g}}(r)$ is accounted for by the scale $r_{\max} = L_u\sqrt{2}$. A factor of 4/3 in the expression results from the fact that Eq. (1) has been written for the intensity of pulsations of one velocity component.

Analogously, Eq. (2) for the distribution $P^{(c)}(r, t)$ in the case of scalar-field-energy generation (caused, for example, by the nonzero gradient of the average scalar field) must contain its own generation term

$$S_{\mathrm{g}}^{(c)}(r) = 4 G_c \frac{r}{L_c^2} \exp\left(-\frac{r^2}{L_c^2} \right), \tag{8}$$

where L_c is the parameter whose value is related to the length scale on which the scalar-field energy is generated and G_c is half the integral rate of generation of scalar-field pulsations.

The rates of generation of pulsations of the velocity G_u and scalar G_c fields are dependent on flow. We can evaluate them, using the following determinations:

$$2G_u = -\langle u_i u_j \rangle \frac{\partial U_i}{\partial x_j}\,, \quad 2G_c = -\langle u_j c \rangle \frac{\partial \langle C \rangle}{\partial x_j}\,. \tag{9}$$

Here we use the ordinary rule of summation by double subscripts.

To close relations (9) we must indicate the method of computation of turbulent momentum and scalar flows $\langle u_i u_j \rangle$ and $\langle u_i c \rangle$. This can be done in a standard manner, just as in the widely used K_{t}–ε model:

$$\langle u_i u_j \rangle = -C_1 \frac{K_{\mathrm{t}}}{\varepsilon} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) + \frac{2}{3} \delta_{ij} K_{\mathrm{t}}\,, \quad \langle u_i c \rangle = -\frac{C_2}{\mathrm{Pr}} \frac{K_{\mathrm{t}}^2}{\varepsilon} \frac{\partial \langle C \rangle}{\partial x_j}$$

or

$$\langle u_i c \rangle = -C_3 \langle u_i u_j \rangle \frac{K_{\mathrm{t}}}{\varepsilon} \frac{\partial \langle C \rangle}{\partial x_j}\,,$$

where $C_1 = 0.09$, $C_2 = 0.255$, $C_3 = 0.3$, and $\mathrm{Pr} = 0.9$.

The parameters of the distributions L_u and L_c have been evaluated by comparing them to the turbulence macroscales. Under the assumption of homogeneous turbulence, the relations

$$L_u = \frac{5\overline{q^2}^{\,3/2}(t)}{\varepsilon(t)}, \quad L_c = \frac{6\overline{c^2}(t)\,\overline{q^2}^{\,1/2}(t)}{\chi(t)}$$

hold true. These evaluations can be refined, if the data of direct numerical modeling or experimental data are available.

Since Eqs. (1) and (2) have been supplemented with the terms of generation of kinetic turbulence energy and intensity of scalar-field pulsations (7) and (8), such terms must also be introduced into Eqs. (3) and (4). For this purpose we applied the transformations [13]

$$E(k, t) = \frac{1}{\pi k}\int_0^\infty \left\{\left[3 - (kr)^2\right]\sin kr - 3kr\cos kr\right\} P(r, t)\, dr, \tag{10}$$

$$E^{(c)}(k, t) = \frac{2}{\pi k}\int_0^\infty \left\{\sin kr - kr\cos kr\right\} P^{(c)}(r, t)\, dr, \tag{11}$$

to (7) and (8), which leads to

$$S_{\mathrm{g}}(k) = \frac{1}{\pi k}\int_0^\infty \left\{\left[3 - (kr)^2\right]\sin kr - 3kr\cos kr\right\} S_{\mathrm{g}}(r)\, dr = \frac{G_u}{12\sqrt{\pi}} k^4 L_u^5 \exp\left(-\frac{1}{4}k^2 L_u^2\right), \tag{12}$$

$$S_{\mathrm{g}}^{(c)}(k) = \frac{2}{\pi k}\int_0^\infty \left\{\sin kr - kr\cos kr\right\} S_{\mathrm{g}}^{(c)}(r)\, dr = \frac{G_c}{2\sqrt{\pi}} k^2 L_c^3 \exp\left(-\frac{1}{4}k^2 L_c^2\right). \tag{13}$$

Calculation Results. The results of numerical solution of systems (1), (2) and (3), (4), where the right-hand sides of Eqs. (1) and (3) are supplemented with the generation terms (7) and (12) respectively, were compared to the data of direct numerical modeling of turbulent velocity and scalar fields [14]. The generation of the intensity of turbulent scalar pulsations was not prescribed ($S_{\mathrm{g}}^{(c)} = 0$). The same spectra as those in testing models (1), (2) and (3), (4) were used as the initial ones [15].

The length scale L_u must be prescribed in expressions for the terms (7) and (12) describing the generation of kinetic turbulence energy in the flow. Since the turbulent energy in the flow is generated for small wave numbers, according to the conditions of direct numerical modeling, the parameter L_u was selected so that, first, the maximum of the distribution (12) was accounted for by small wave numbers and, second, integration of the distribution (12) by all wave numbers yielded the value $G_u = 4.149$. The parameter L_u was selected first for the spectral model (3), but thereafter, using this parameter, we carried out calculations from model (1).

Figure 1 gives the time variation in the variance and dissipation of the field of velocity pulsations for two models (1) and (3) and compares it to the data of direct numerical modeling [14].

In direct numerical modeling, at the initial step of mixing where the variance of the scalar field amounts to 50% of the initial one ($t \sim 0.15$), we observe a sharp growth in the variance of the velocity field; this growth is related to the external energy supply to the flow (Fig. 1a). The dissipation of the velocity field $\varepsilon(t)$ grows nearly linearly to its maximum value at $t \sim 0.45$ (Fig. 1b). From this instant, large vortices begin to disintegrate and their energy is transferred to smaller ones. In the data of direct numerical modeling, the evolution of the variance and dissipation of the velocity field is characterized by the presence of sharp peaks of different time and space scales, which is caused

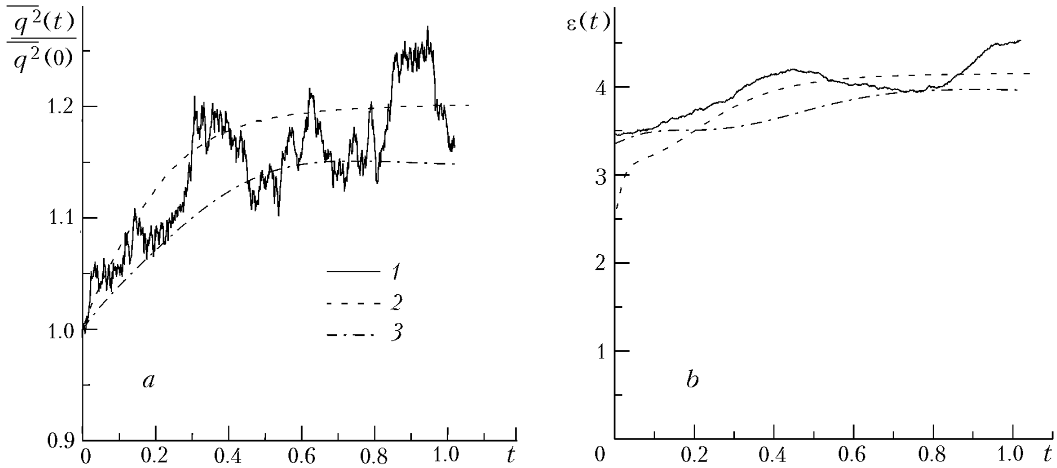

Fig. 1. Time variation in the velocity variance (a) and dissipation (b): 1) direct numerical modeling; 2) calculation from model (1), (2) with the term allowing for the generation of kinetic turbulence energy (8); 3) calculation from model (3), (4) with the term allowing for the generation of kinetic turbulence energy (12).

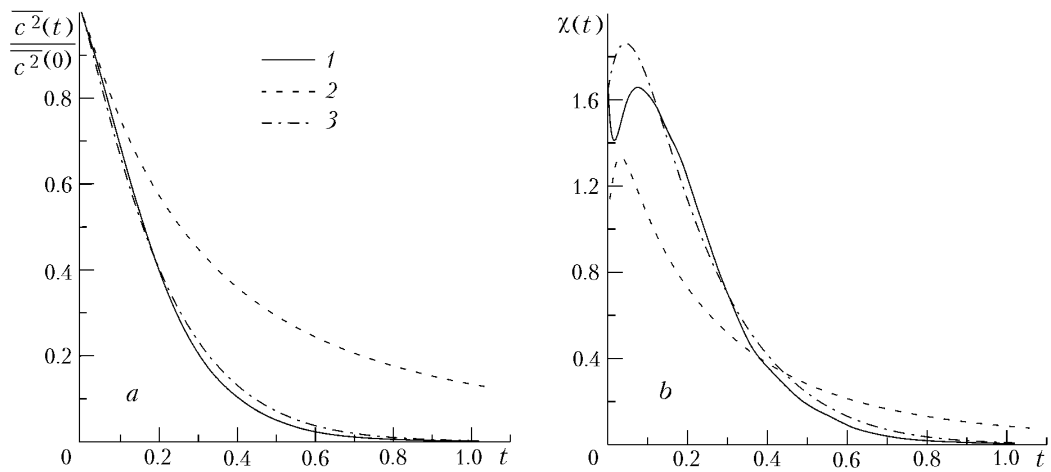

Fig. 2. Time variation in the scalar variance (a) and dissipation (b). The notation is the same as in Fig. 1.

by the influence of the generation and disintegration of individual large vortices. Calculation from statistical models actually represents the time averaging of these data.

In accordance with the growth in the variance, we have a growth in the rate of dissipation of scalar-field pulsations $\varepsilon(t)$; it lasts to the instant of time $t \sim 0.8$, reaching the stationary value. As is seen in Fig. 1, model (3) for the distributions by wave numbers better describes, on the whole, the data of direct numerical modeling for both the variance of velocity pulsations and the rate of dissipation of kinetic energy than model (1). It is noteworthy that the dissipation-rate maxima in the calculations based on Eq. (3) are smaller in value and are shifted toward shorter times, unlike the data of direct numerical modeling.

Analogous comparisons for the variance and dissipation of the scalar field have shown that the best agreement with direct numerical modeling is demonstrated by model (3), (4) (Fig. 2).

Also, the calculation has shown that the mixed asymmetry is conservative to external actions (Fig. 3a). The asymptotic value of $S_{uc}(t)$ throughout the time interval in question is close to a constant $S_{uc} \approx -0.5$, which differs only slightly from the case considered earlier without turbulent-energy supply [15].

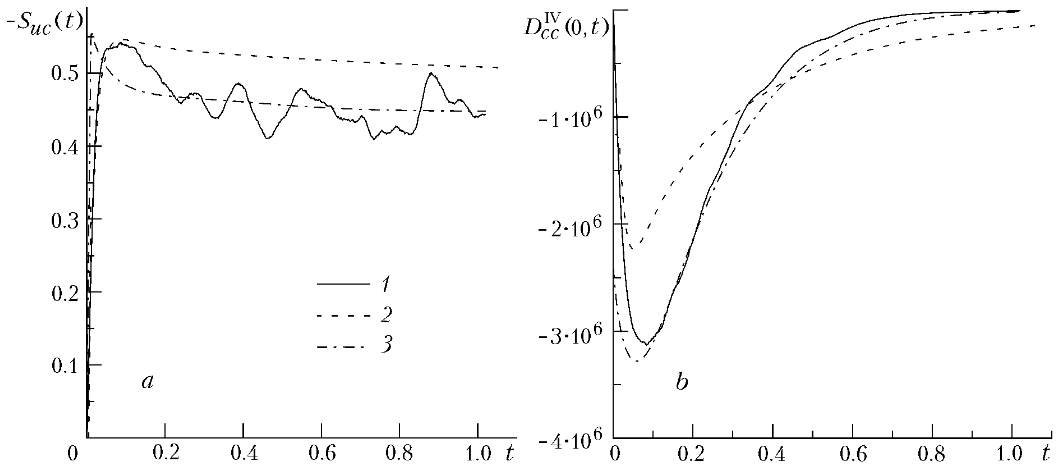

Fig. 3. Time variation in the mixed asymmetry of the derivatives of pulsatory velocity and scalar fields (a) and the derivative of fourth order of the structural function of second order of the scalar field with respect to the space variable for the zero value of the space variable (b). The notation is the same as in Fig. 1.

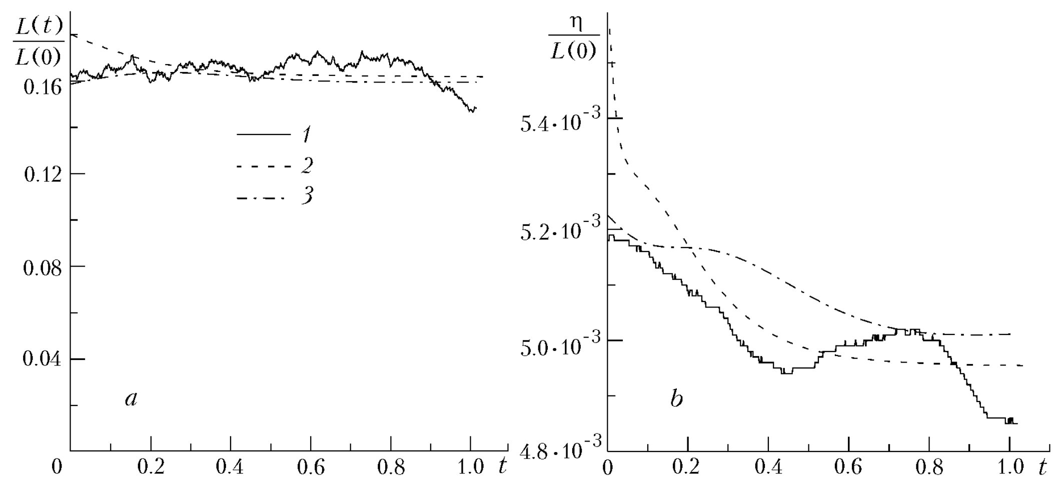

Fig. 4. Time variation in the integral (a) and Kolmogorov (b) length scales. The notation is the same as in Fig. 1.

Allowance for the external action on the hydrodynamic field has not affected, in practice, the character of time variation in the function $D_{cc}^{(IV)}(0,\ t)$. The changes are true only for the maximum of $D_{cc}^{(IV)}(0,\ t)$ as compared to the case without the generation of kinetic energy in the flow [11] (Fig. 3b).

For model (3), (4), there is a good agreement with direct numerical modeling relative to the time variation in the integral length scale $L(t) = \dfrac{\int_0^\infty rP(r,t)dr}{\int_0^\infty P(r,t)dr} = \dfrac{3\pi}{4}\dfrac{\int_{k_{\min}}^\infty \frac{E(k,t)}{k}dk}{\int_{k_{\min}}^\infty E(k,t)\,dk}$ (Fig. 4a) and the Kolmogorov length scale $\eta(t)$ (Fig. 4b). The integral scale is held at a constant level, which is due to the fact that the stationary level of the variance of velocity pulsations has been reached. The Kolmogorov length scale on the initial portion decreases once the stationary regime has been reached because of the growth (caused by the total growth in the kinetic energy in the flow) in the dissipation of the velocity field.

Conclusions. The results of the calculations of the statistical characteristics of a homogeneous turbulent flow carried out from the models for the turbulent-energy distributions by length scales and wave numbers with allowance for the supply of kinetic turbulence energy show a good agreement with the data of direct numerical modeling. A better agreement is given by model (3), (4). Both statistical models can be used for calculation of turbulent mixing using more complex models based on the formalism of the probability density function. In particular, they can be used as additional models for determination of the coefficients involved in the equation for the JPDF of a scalar and its gradient and for the conditional moments of this function [15].

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NOTATION

$\overline{c^2}(t)$, variance of scalar-field pulsations squared; $\langle C\rangle$, average value of the scalar field; $D_{cc}^{(IV)}(0, t)$, derivative of fourth order of the structural function of second order of the scalar field with respect to the space variable for the zero value of the space variable; $E(k, t)$ and $E^{(c)}(k, t)$, distributions of the energy of turbulent velocity pulsations and the energy of turbulent scalar pulsations by wave numbers respectively; G_u, integral rate of generation of kinetic energy; k, wave number; K_t, kinetic turbulence energy; $L(t)$, macroscale; Pe, Péclet number; Pr, Prandtl number; $P(r, t)$ and $P^{(c)}(r, t)$, distributions of turbulent velocity pulsations and turbulent scalar pulsations by different length scales respectively; $\overline{q^2}(t) = 2K_t$, doubled kinetic turbulence energy; r, length scale; Re, Reynolds number; $S_{uc}(t)$, mixed asymmetry of the gradient fields of velocity and scalar pulsations; t, time; u_j, velocity-field pulsations; U_i and U_j; average flow velocity; α, β, γ, and δ, constants; δ_{ij}, Kronecker symbol; $\varepsilon(t)$, rate of dissipation of velocity-field pulsations; $\eta(t)$, Kolmogorov length scale; λ, Taylor microscale; $\chi(t)$, rate of dissipation of scalar-field pulsations. Subscripts and superscripts: c, quantity describing the scalar field; g, generation of turbulence energy; t, turbulence; u, quantity describing the velocity field; uc, quantity describing the mutual influence of turbulent velocity and scalar fields; max, maximum; min, minimum; ′, derivative; ~, integration variable.

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