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DERIVATION AND NUMERICAL SOLUTION OF A CLOSED EQUATION FOR THE SPECIFIC ISOSCALAR-SURFACE AREA IN A TURBULENT REACTIVE FLOW

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Based on the equation obtained earlier for the joint probability density function of the fluctuations of an isotropic turbulent scalar field of a reagent and its gradient [Inzh.-Fiz. Zh., **71**, No. 5, 827–849 (1998)] *the authors derived and numerically solved an equation for the specific isoscalar-surface area* $\Sigma_f(\Gamma)$ *in a turbulent reactive flow. The equation for* $\Sigma_f(\Gamma)$ *contains the single-point probability density function for pulsations of a reactive scalar and the time function that depend on the distribution of the energy of turbulent velocity pulsations and the intensity of scalar reagent pulsations by different length scales. The corresponding equations are written for all these functions.*

Introduction. The most significant approach to the modeling of combustion that allows for a deviation from the position of chemical equilibrium is based on the assumption which considers a turbulent flame as an ensemble of thin one-dimensional reaction zones (flamelets). Each zone is found in a locally laminar mixing environment. This description of the turbulent flame was named the laminar diffusion flamelet model. This concept was proposed for the first time in [2] and was extended in a number of papers (see, for example, [3]).

The instantaneous flame consists of localized reactive leafs that are transferred by a flow and are bent and stretched by turbulent vortices but remain identified structures.

The field of application of flamelet models has been the subject of discussion thus far. It is agreed that this concept is applicable in the region of large Damköhler numbers; in this case, the characteristic turbulence scales are much larger than the typical flame thickness. These conditions are satisfied in many practical situations, and the flamelet regime exists in spark-ignition engines, in continuous flows of aircraft engines, in rocket engines, and in industrial burners.

The most important class of flamelet models is associated with a balance equation for the density of the flame surface. This equation describes the transfer of the average reactive surface by a turbulent flow and also the mechanisms of production and destruction of the flame area. The notion of the flame area was already used in the previous combustion models. However, an equation for this quantity was proposed for the first time in [4], where the combustion of unmixed reactants at the early stage is controlled by the competition between the deformation of the elements of the flame and mutual annihilation of the flame area because of the destruction of its adjacent elements. The advantage of the flame model that is based on the equation for the surface area consists of using it to relate the analysis of an individual flamelet to that of the global turbulent field.

Having the calculated area of the flame surface Σ_f, we can easily calculate the average rate of heat release per unit volume or the flow rate of the reagent by the formulas

$$W = Q\Sigma_f\,, \quad W_f = -\frac{Q}{\Delta h_f}\Sigma_f\,. \tag{1}$$

Here Q is the rate of heat release per unit area of the flame; Δh_f is the enthalpy.

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In writing an equation for Σ_f based on intuitive arguments as was done in [4], we have to artificially introduce into the equation all the effects associated with the interaction of the rate of deformation and the combustion surface. At the same time, there is a possibility of deriving the equation for the flame surface on the basis of rigorous relations for the joint probability density function of a scalar and its gradient. Precisely this is the objective of the present investigation. In [5-7], the following formula that relates the specific isoscalar surface to the probability density function of a scalar and its gradient was proposed:

$$\Sigma_{x,t}(\Gamma) = \int_0^\infty W P_{x,t}(W, \Gamma)\, dW . \tag{2}$$

The equation for $P_{x,t}(\Gamma)$ is proposed in the work of Sosinovich et al. [1]. A solution for it remains to be found. However, it can be used as the reference point when an equation for the density function of the flame surface $\Sigma_{x,t}(\Gamma)$ is derived.

A Closed Equation for the Joint Probability Density Function (JPDF) of the Fluctuations of a Reactive Scalar and Its Gradient. The equation for the JPDF $P_t(\vec{W}, \Gamma)$ was obtained in [1] for the case of an isotropic turbulent field (formula (117)). The function $P_t(W, \Gamma)$ that describes the JPDF of the absolute value of the fluctuations of the scalar gradient and the fluctuations of the scalar Γ is related to $P_t(\vec{W}, \Gamma)$ as follows:

$$P_t(W, \Gamma) = 4\pi W^2 P_t(\vec{W}, \Gamma) . \tag{3}$$

We substitute the expression for $P_t(\vec{W}, \Gamma)$ from (3) into Eq. (117) from [1] and, having carried out simple manipulations, obtain the equation for $P_t(W, \Gamma)$:

$$\begin{gathered}
\frac{\partial P_t(W, \Gamma)}{\partial t} = -DW^2 \frac{\partial^2 P_t(W, \Gamma)}{\partial \Gamma^2} + \\
+ \frac{S_{UC}(t)}{2} \sqrt{\left(\frac{\varepsilon(t)}{15\nu}\right)} \left[\left(1 + W\frac{\partial}{\partial W}\right) - \frac{DW^2}{\chi(t)}\left(3 + W\frac{\partial}{\partial W}\right)\right] P_t(W, \Gamma) - \\
- DN_t(\Gamma)\left[\frac{2}{W^2} - \frac{2}{W}\frac{\partial}{\partial W} + \frac{\partial^2}{\partial W^2}\right] P_t(W, \Gamma) - \\
- 2D\frac{\partial}{\partial \Gamma}\left\{X_t(\Gamma)\left[1 + W\frac{\partial}{\partial W}\right] P_t(W, \Gamma)\right\} - \\
- \left[\dot{\omega}(\Gamma)\frac{\partial}{\partial \Gamma} + \frac{\partial \dot{\omega}(\Gamma)}{\partial \Gamma}\left(2 + W\frac{\partial}{\partial W}\right)\right] P_t(W, \Gamma)
\end{gathered} \tag{4}$$

with the initial

$$P_t(W, \Gamma)\big|_{t=0} = P_0(W, \Gamma) \tag{5}$$

and boundary conditions

$$P_t(W, \Gamma)\big|_{W=\infty} = 0 , \quad P_t(W, \Gamma)\big|_{W=0} = 0 , \quad \left.\frac{\partial P_t(W, \Gamma)}{\partial \Gamma}\right|_{\Gamma=0} = 0 ,$$

$$P_t(W, \Gamma)\big|_{|\Gamma| = \Gamma_{\max}} = 0 . \tag{6}$$

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

The first term on the right-hand side of the equation for JPDE (4) describes the effect of the process of diffusion in the space of scalar values, while the second term describes the effect of the structure of turbulent velocity and scalar fields. Here $S_{UC}(t)$ denotes the asymmetry of the joint probability density function of the velocity and scalar fields. This function can be expressed in terms of other moments by the following formula:

$$S_{UC}(t) = \frac{\frac{1}{6} D'''_{LCC}(0, t)}{(\chi(t)/3D)\,(\varepsilon(t)/15\nu)^{1/2}}. \tag{7}$$

Here $D'''_{LCC}(0, t)$ is the third derivative of a double-point structural third-order function of the velocity field and the scalar field with respect to the distance at $r = 0$; $\varepsilon(t)$ is the average dissipation rate of turbulent energy; $\chi(t)$ is the average dissipation rate of the intensity of scalar fluctuations.

The third term on the right-hand side of (4) describes the effect of dissipation in the scalar-gradient space on the joint statistics of the scalar reactive field and its gradient. The function $N_t(\Gamma)$ has the form

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

where

$$T(t) = \frac{\sqrt{2}\,\chi(t)}{3D\sqrt{\left(-\overline{c^2}(t)\, D_{CC}^{(IV)}(0, t)\right)}}. \tag{9}$$

Here $\overline{c^2}(t)$ is the root-mean-square intensity of the scalar fluctuations; $D_{CC}^{(IV)}(0, t)$ is the fourth derivative of a double-point structural function of the scalar turbulent field with respect to the space variable r at the zero value of this variable.

The fourth term on the right-hand side of the equation for the JPDF describes the effect of cross diffusion in the space of values of the scalar and velocity gradient on the joint statistics of the reactive scalar and its gradient. The function $X_t(\Gamma)$ is determined by the expression

$$X_t(\Gamma) = K_t(\hat{\Gamma})\exp\left\{-\alpha(T)\,\hat{\Gamma}^2\right\}. \tag{10}$$

Here we use the following notation:

$$\alpha(T) = \frac{27T^2}{8\,[5 - 9T^2]}, \quad \hat{\Gamma} = \frac{\Gamma}{\sqrt{\left(\overline{c^2}\right)}}, \tag{11}$$

$$K_t(\hat{\Gamma}) = \chi(t)\,\kappa(\hat{\Gamma})\Big/\left(6D\sqrt{\left(\overline{c^2}\right)}\right), \tag{12}$$

$$\kappa(\hat{\Gamma}) = N(n)\,(2n + 1)\,(\hat{\Gamma}/N(n))^{\frac{2n-1}{2n+1}}\left[2n - (2n + 1)\,(\hat{\Gamma}/N(n))^{\frac{2}{2n+1}}\right], \tag{13}$$

$$N(n) = \frac{\sqrt{\pi}\,\Gamma(2n + 2)}{\Gamma(2n + 3/2)}. \tag{14}$$

The quantity n can take on values larger than or equal to zero.

The fifth term on the right-hand side of (4) describes the effect of the chemical-reaction rate on the JPDF.

In principle, we can try to solve Eq. (4) numerically. In this case, we need to complete it with a system of moment equations, from which we could obtain information about the functions $\varepsilon(t)$, $\chi(t)$, $S_{UC}(t)$, and $D_{CC}^{(IV)}(0, t)$.

A Closed Equation for the Specific Isoscalar-Surface Area in a Turbulent Reactive Flow. As is seen from formula (2) the specific area of the isoscalar surface $\Sigma_{\vec{x},t}(W, \Gamma)$ is the first moment of the JPDF $P_{\vec{x},t}$ (W, Γ). For this function, Eq. (4) is written. Using (4), we derive an equation for the function $\Sigma_{\vec{x},t}(W, \Gamma)$.

We multiply the left-hand and right-hand sides of Eq. (4) by W and integrate it from 0 to ∞:

$$\frac{\partial}{\partial t}\int_0^\infty WP_t(W,\Gamma)\,dW = -D\int_0^\infty W^3\frac{\partial^2}{\partial\Gamma^2}P_t(W,\Gamma)\,dW +$$

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

$$-DN_t(\Gamma)\int_0^\infty W\left[\frac{2}{W^2}-\frac{2}{W}\frac{\partial}{\partial W}+\frac{\partial^2}{\partial W^2}\right]P_t(W,\Gamma)\,dW -$$

$$-2D\frac{\partial}{\partial\Gamma}\left[X_t(\Gamma)\int_0^\infty W\left(1+W\frac{\partial}{\partial W}\right)P_t(W,\Gamma)\,dW\right] -$$

$$-\int_0^\infty W\left[\dot{\omega}(\Gamma)\frac{\partial}{\partial\Gamma}+\frac{\partial\dot{\omega}(\Gamma)}{\partial\Gamma}\left(2+W\frac{\partial}{\partial W}\right)\right]P_t(W,\Gamma)\,dW. \tag{15}$$

We write Eq. (15) in symbolic form:

$$\frac{\partial}{\partial t}(0) = (\mathrm{I})+(\mathrm{II})+(\mathrm{III})+(\mathrm{IV})+(\mathrm{V})\,. \tag{16}$$

Let us transform each term of (16). Using determination (2) for the specific isoscalar-surface area, on the left-hand side we obtain

$$(0) = \int_0^\infty WP_t(W,\Gamma)\,dW = \Sigma_t(\Gamma)\,. \tag{17}$$

The subscripts $\vec{x}, t$ in the notation $\Sigma_t(\Gamma)$ are replaced by the subscript t, since we restrict ourselves to the derivation of an equation for $\Sigma_t(\Gamma)$ in the approximation of isotropic turbulence.

We transform term (I):

$$(\mathrm{I}) = -D\int_0^\infty W^3\frac{\partial^2}{\partial\Gamma^2}P_t(W,\Gamma)\,dW = -D\frac{\partial^2}{\partial\Gamma^2}\int_0^\infty W^3P_t(W,\Gamma)\,dW = -D\frac{\partial^2}{\partial\Gamma^2}\Sigma_t^{(3)}(\Gamma)\,. \tag{18}$$

Here the notation

$$\Sigma_t^{(3)}(\Gamma) = \int_0^\infty W^3 P_t(W, \Gamma)\, dW \tag{19}$$

is used for the average conventional value of the cube of the gradient of the reactive scalar field.

For (II) we obtain

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

$$= -\frac{S_{UC}(t)}{2}\sqrt{\left(\frac{\varepsilon(t)}{15\nu}\right)}\left[\Sigma_t(\Gamma) - \frac{D}{\chi(t)}\Sigma_t^{(3)}(\Gamma)\right]. \tag{20}$$

We carry out the transformation of (III):

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

$$= -2DN_t(\Gamma)\,\Sigma_t^{(-1)}(\Gamma). \tag{21}$$

In expression (21), we used the notation

$$\Sigma_t^{(-1)}(\Gamma) = \int_0^\infty W^{-1} P_t(W, \Gamma)\, dW. \tag{22}$$

From (22) it is seen that $\Sigma_t^{(-1)}(\Gamma)$ denotes the conventional average value of the reciprocal of the gradient. For it, as for $\Sigma_t^{(3)}(\Gamma)$, we will obtain an approximate expression in terms of traditional statistics of the scalar and its gradient.

For (IV), we have

$$(\mathrm{IV}) = -2D\frac{\partial}{\partial\Gamma}\left\{X_t(\Gamma)\int_0^\infty W\left(1 + W\frac{\partial}{\partial W}\right)P_t(W, \Gamma)\, dW\right\} =$$

$$= -2D\frac{\partial}{\partial\Gamma}X_t(\Gamma)\left\{\Sigma_t(\Gamma) - 2\Sigma_t(\Gamma)\right\} = 2D\frac{\partial}{\partial\Gamma}\left[X_t(\Gamma)\,\Sigma_t(\Gamma)\right]. \tag{23}$$

For (V), we obtain

$$(\mathrm{V}) = \left[-\dot{\omega}(\Gamma)\frac{\partial}{\partial\Gamma} - 2\frac{\partial\dot{\omega}(\Gamma)}{\partial\Gamma} + 2\frac{\partial\dot{\omega}(\Gamma)}{\partial\Gamma}\right]\Sigma_t(\Gamma) = -\dot{\omega}(\Gamma)\frac{\partial}{\partial\Gamma}\Sigma_t(\Gamma). \tag{24}$$

We substitute the results of the calculation of expressions (0)-(V) into equality (16):

$$\frac{\partial\Sigma_t(\Gamma)}{\partial t} = -D\frac{\partial^2}{\partial\Gamma^2}\Sigma_t^{(3)}(\Gamma) - \frac{S_{UC}(t)}{2}\sqrt{\left(\frac{\varepsilon(t)}{15\nu}\right)}\left[\Sigma_t(\Gamma) - \frac{D}{\chi(t)}\Sigma_t^{(3)}(\Gamma)\right] -$$

$$-2DN_t(\Gamma)\,\Sigma_t^{(-1)}(\Gamma) + 2D\frac{\partial}{\partial\Gamma}\left[X_t(\Gamma)\,\Sigma_t(\Gamma)\right] - \dot{\omega}(\Gamma)\frac{\partial}{\partial\Gamma}\Sigma_t(\Gamma). \tag{25}$$

To close Eq. (25) for the specific isoscalar surface it is necessary to propose a method for expressing the functions $\Sigma_t^{(3)}(\Gamma)$ and $\Sigma_t^{(-1)}(\Gamma)$ in terms of the known statistical quantities. It is also necessary to prescribe a particular form of the function $\omega(\Gamma)$ that describes the reaction rate as a function of the concentration field.

Expressions for the functions $\Sigma_t^{(3)}(\Gamma)$ and $\Sigma_t^{(-1)}(\Gamma)$ can be represented in the form

$$\Sigma_t^{(-1)}(\Gamma) = \int_0^{\infty} W^{-1} P_t(W|\Gamma)\, dW f_t(\Gamma)\,, \tag{26}$$

$$\Sigma_t^{(3)}(\Gamma) = \int_0^{\infty} W^{3} P_t(W|\Gamma)\, dW f_t(\Gamma)\,. \tag{27}$$

Here $P_t(W|\Gamma)$ is the conventional probability density function of the scalar gradient calculated with a prescribed scalar field $c(\vec{x},t) = \Gamma$; $f_t(\Gamma)$ is the single-point probability density function for the scalar field. We rewrite formulas (26) and (27) in the form

$$\Sigma_t^{(-1)}(\Gamma) = \overline{W_t^{(-1)}}(\Gamma) f_t(\Gamma)\,, \tag{28}$$

$$\Sigma_t^{(3)}(\Gamma) = \overline{W_t^{(3)}}(\Gamma) f_t(\Gamma)\,, \tag{29}$$

where

$$\overline{W_t^{(-1)}}(\Gamma) = \int_0^{\infty} W^{-1} P_t(W|\Gamma)\, dW\,, \tag{30}$$

$$\overline{W_t^{(3)}}(\Gamma) = \int_0^{\infty} W^{3} P_t(W|\Gamma)\, dW\,. \tag{31}$$

The conventional function $P_t(W|\Gamma)$ in equalities (30) and (31) is determined as

$$P_t(W|\Gamma) = \frac{P_t(W,\Gamma)}{f_t(\Gamma)}\,. \tag{32}$$

To evaluate the integrals on the right-hand side of equalities (30) and (31) we can resort to the distribution law of the modulus of a three-dimensional vector (see [8], p. 435):

$$P_t(W|\Gamma) = \begin{cases} 0\,, & -\infty < W < 0\,, \\ \sqrt{\left(\dfrac{2}{\pi}\right)} \dfrac{1}{\sigma^3} W^2 \exp\left\{-\dfrac{W^2}{2\sigma^2}\right\}, & 0 < W < +\infty\,. \end{cases} \tag{33}$$

Calculating by formulas (30) and (31) with account for (28) and (29) yields

$$\Sigma_t^{(-1)}(\Gamma) = \frac{2}{\sqrt{2\pi}} \left(\frac{3D}{\chi(t)}\right)^{1/2} f_t(\Gamma)\,, \tag{34}$$

$$\Sigma_t^{(3)}(\Gamma) = \frac{16}{\sqrt{2\pi}} \left(\frac{\chi(t)}{3D} \right)^{3/2} f_t(\Gamma) . \tag{35}$$

With this approximation of the function $\Sigma_t^{(3)}(\Gamma)$ the first term on the right-hand side of the equation for $\Sigma_t(\Gamma)$ will involve the second derivative of the function $f_t(\Gamma)$, which presents significant difficulties in numerical solution of this equation. Since the form of the first term resulted from an approximation of the function $\Sigma_t^{(3)}(\Gamma)$, we can propose, for the first term in (25), another expression for $\Sigma_t^{(3)}(\Gamma)$ that will present no numerical difficulties in solving the equation for $\Sigma_t(\Gamma)$.

We write formula (19) for $\Sigma_t^{(3)}(\Gamma)$ in the form

$$\Sigma_t^{(3)}(\Gamma) = \frac{\Sigma_t^{(3)}(\Gamma)}{\Sigma_t(\Gamma)} \Sigma_t(\Gamma) = \frac{W_t^{(3)}(\Gamma)}{W_t^{(1)}(\Gamma)} \Sigma_t(\Gamma) . \tag{36}$$

Here $W_t^{(3)}(\Gamma)$ is determined by formula (31), while $W_t^{(1)}(\Gamma)$ is determined by the following expression:

$$W_t^{(1)}(\Gamma) = \int_0^\infty W P_t(W \mid \Gamma)\, dW . \tag{37}$$

Using (33) for $P_t(W \mid \Gamma)$ we find (38)

$$W_t^{(1)}(\Gamma) = \frac{2}{\sqrt{2\pi}} \int_0^\infty \frac{W}{[\chi(t)/3D]^{3/2}} \exp\left\{ -\frac{W^2}{2\chi(t)/3D} \right\} dW = \frac{4}{\sqrt{2\pi}} \left[\frac{\chi(t)}{3D} \right]^{1/2} .$$

By employing (31) and (33) we obtain

$$W_t^{(3)}(\Gamma) = \frac{16}{\sqrt{2\pi}} \left[\frac{\chi(t)}{3D} \right]^{1/2} . \tag{39}$$

With account for (38) and (39)

$$\Sigma_t^{(3)}(\Gamma) = 4 \left(\frac{\chi(t)}{3D} \right) \Sigma_t(\Gamma) . \tag{40}$$

Substituting (34) for $\Sigma_t^{(-1)}(\Gamma)$ and (40) for $\Sigma_t^{(3)}(\Gamma)$, we obtain the final form of the equation for $\Sigma_t(\Gamma)$

$$\frac{\partial \Sigma_t(\Gamma)}{\partial t} =$$

$$= -\frac{4}{3} \chi(t) \frac{\partial^2}{\partial \Gamma^2} \Sigma_t(\Gamma) - S_{UC}(t) \sqrt{\left(\frac{\varepsilon(t)}{15\nu} \right)} \left[\frac{\Sigma_t(\Gamma)}{2} - \frac{8}{3\sqrt{2\pi}} \left(\frac{\chi(t)}{3D} \right)^{1/2} f_t(\Gamma) \right] -$$

$$- DN_t(\Gamma) \frac{4}{\sqrt{2\pi}} \left(\frac{3D}{\chi(t)} \right)^{1/2} f_t(\Gamma) + 2D \frac{\partial}{\partial \Gamma} \left[X_t(\Gamma) \Sigma_t(\Gamma) \right] - \dot{\omega}(\Gamma) \frac{\partial}{\partial \Gamma} \Sigma_t(\Gamma) . \tag{41}$$

Derivation of the Equation for $f_t(\Gamma)$. An equation for the single-point probability density function of a reactive scalar can be obtained from the equation for the JPDF $P_t(W, \Gamma)$ using the formula

$$f_t(\Gamma) = \int_0^{\infty} P_t(W, \Gamma)\, dW\,, \tag{42}$$

whence it is seen that $f_t(\Gamma)$ is the zero-order moment of the JPDF $P_t(W, \Gamma)$. Integrating the left-hand sides of (4) with respect to W from 0 to ∞ and taking (42) into account, we obtain the equation for $f_t(\Gamma)$ in the following form:

$$\frac{\partial}{\partial t} f_t(\Gamma) = -\frac{\partial^2}{\partial \Gamma^2}[\chi_t(\Gamma) f_t(\Gamma)] - \frac{\partial}{\partial \Gamma}[\dot{\omega}(\Gamma) f_t(\Gamma)]\,. \tag{43}$$

It contains the unknown function $\chi_t(\Gamma)$, i.e., the conventional rate of scalar dissipation (CRSD). For this function, we can derive an equation from (4) if we resort to the formula

$$\chi_t(\Gamma) = \frac{D \int_0^{\infty} W^2 P_t(W, \Gamma)\, dW}{f_t(\Gamma)}\,. \tag{44}$$

It is seen from (44) that the conventional dissipation rate is the second-order moment of the JPDF $P_t(W, \Gamma)$. A closed equation for $\chi_t(\Gamma)$ in the case of a nonreactive scalar field was derived in [9].

Supplementing the equation derived in [9] for $\chi_t(\Gamma)$ with a source chemical term, we obtain (see Eq. (19) in [9])

$$\frac{\partial [\chi_t(\Gamma) f_t(\Gamma)]}{\partial t} = -\frac{\partial^2 [\overline{\chi_t^2(\Gamma)} f_t(\Gamma)]}{\partial \Gamma^2} - \left\{ S_{UC}(t) \sqrt{\left(\frac{\varepsilon}{15\nu}\right)} \left[\chi_t(\Gamma) - \frac{\overline{\chi_t^2(\Gamma)}}{\chi(t)}\right]\right\} f_t(\Gamma) -$$
$$- 6D^2 N_t(\Gamma) f_t(\Gamma) + 4D \frac{\partial}{\partial \Gamma}[X_t(\Gamma)\chi_t(\Gamma) f_t(\Gamma)] - \dot{\omega}(\Gamma)\frac{\partial}{\partial \Gamma}[\chi_t(\Gamma) f_t(\Gamma)] +$$
$$+ \frac{\partial \dot{\omega}(\Gamma)}{\partial \Gamma}[\chi_t(\Gamma) f_t(\Gamma)]\,. \tag{45}$$

The equation for $\chi_t(\Gamma)$ involves the unknown function $\overline{\chi_t^2(\Gamma)}$, i.e., the mean square of the conventional rate of scalar dissipation. We take the following function as a hypothesis for modeling the unknown function $\overline{\chi_t^2(\Gamma)}$:

$$\overline{\chi_t^2(\Gamma)} = k_2 \chi_t(\Gamma)\, \chi_t(\Gamma)\,. \tag{46}$$

In writing formula (46) for $\overline{\chi_t^2(\Gamma)}$, we assume that the effect of the pulsations of the conventional rate of scalar dissipation on the evolution of this function is insignificant. The coefficient k_2 will be determined below.

The equations for $\Sigma_t(\Gamma)$ and $\chi_t(\Gamma)$ contain a number of functions that must be calculated from supplementary equations. These are the functions $S_{UC}(t)$, i.e., the asymmetry of the joint probability density function of the fields of the velocity gradient and the scalar, $D_{CC}^{(\mathrm{IV})}(0, t)$, i.e., the fourth derivative of the structural double-point function of the difference of concentrations at two points of an isotropic turbulent flow with respect to the distance when this distance is zero; $\varepsilon(t)$, i.e., the average dissipation rate of the energy of the turbulent velocity field; $\chi(t)$, i.e., the average dissipation rate of scalar-fluctuation intensity, and $\overline{c^2}(t)$, i.e., the square of the variance of the scalar field.

The evolution of the above functions can be found from solution of a coupled system of equations for the functions that describe the distribution of the energy and intensity of scalar reagent pulsations by different length scales. The system of equations for these functions is given in [1] (see formulas (122)-(126)) and [10].

Numerical Solution of the System of Equations for the Specific Isoscalar-Surface Area. We determine dimensionless variables by the formula

$$A = \bar{A} A_C , \tag{47}$$

where A_C is the characteristic variable A. We select the characteristic quantities: $C_C = |C_{\max}|$ is the concentration; it is taken to be equal to the maximum value of the concentration; $L_C = L_C(0)$ is the length scale equal to the initial scale of the scalar field length; $\Sigma_C = 1/L_C$ is the specific isoscalar-surface area; $f_C = 1/C_C$ is the single-point probability density function; $q_C = \sqrt{q^2(0)}$ is the square of the velocity pulsation; it is selected to be equal to the initial square of the velocity pulsation; $t_C = L_C/q_C$ is time; it is selected to be equal to the time of one rotation of an energy-containing vortex; $\chi_C = C_C^2/t_C$ is the scalar dissipation; $\varepsilon_C = q_C^2/t_C$ is the dissipation rate of the turbulent velocity field; $P_C^{(\xi)} = C_C^2/L_C$ is the magnitude of the function $P_t^2(r)$; $(D_{LCC}''')_C = q_C C_C^2/L_C^3$ is the magnitude of the function $D_{LCC}'''(0, t)$; $\mathrm{Pe} = q_C L_C/D$ is the Péclet number; $\mathrm{Re} = q_C L_C/\nu$ is the Reynolds number; $\mathrm{Sc} = \nu/D$ is the Schmidt number; $\mathrm{Da} = t_C/t_r$ is the Damköhler number; t_r is the chemical-reaction time.

We write the system of equations for $\Sigma_t(\Gamma)$, $f_t(\Gamma)$, and $\chi_t(\Gamma)$ in dimensionless form. In what follows, we omit the overbar in the corresponding dimensionless functions and variables.

The equation for $\Sigma_t(\Gamma)$ in dimensionless form appears as

$$\begin{aligned} \frac{\partial \Sigma_t(\Gamma)}{\partial t} &= -\frac{4}{3}\chi(t)\frac{\partial^2}{\partial \Gamma^2}\Sigma_t(\Gamma) - \\ &- \sqrt{\left(\frac{\mathrm{Re}\,\varepsilon(t)}{15}\right)} S_{UC}(t)\left[\frac{\Sigma_t(\Gamma)}{2} - \frac{8\sqrt{\mathrm{Pe}}}{3\sqrt{6\pi}}\chi(t)^{1/2}\frac{\partial F_t(\Gamma)}{\partial \Gamma}\right] + \\ &+ \frac{2D_{CC}^{(\mathrm{IV})}(0,t)}{\sqrt{6\pi}\,\mathrm{Pe}^{3/2}}\tilde{N}_t(\hat{\Gamma})\frac{\dfrac{\partial F_t(\Gamma)}{\partial \Gamma}}{\chi(t)^{1/2}} + \frac{\chi(t)}{3\sqrt{\left(\overline{c^2(t)}\right)}}\frac{\partial}{\partial \Gamma}\left[\kappa(\hat{\Gamma})\exp\left\{-\alpha(T)\hat{\Gamma}^2\right\}\Sigma_t(\Gamma)\right] - \\ &- \mathrm{Da}\,\dot{\omega}(\Gamma)\frac{\partial}{\partial \Gamma}\Sigma_t(\Gamma) . \end{aligned} \tag{48}$$

Here we used the notation

$$\tilde{N}_t(\hat{\Gamma}) = \left[5 - 3T^2(t)\left(1 - \frac{\hat{\Gamma}^2}{4}\right)\right]\exp\left\{-\alpha(T)\hat{\Gamma}^2\right\} . \tag{49}$$

In the equation for $\Sigma_t(\Gamma)$, instead of $f_t(\Gamma)$, we introduced the function $F_t(\Gamma)$, which is related to the former by

$$F_t(\Gamma) = \int_0^{r} f_t(\tilde{\Gamma})\,d\tilde{\Gamma} . \tag{50}$$

Its behavior is smoother than the behavior of the differential function $f_t(\Gamma)$. The equation for the function $F_t(\Gamma)$ has the form

$$\frac{\partial F_t(\Gamma)}{\partial t} = -\frac{\partial}{\partial \Gamma}\left[\chi_t(\Gamma)\frac{\partial}{\partial \Gamma}F_t(\Gamma)\right] - \mathrm{Da}\,\dot{\omega}(\Gamma)\frac{\partial F_t(\Gamma)}{\partial \Gamma} . \tag{51}$$

We need only to write the equation for $\chi_t(\Gamma)$ in dimensionless form:

$$\frac{\partial \chi_t(\Gamma)}{\partial t} = -\chi_t(\Gamma)\frac{\partial^2 \chi_t(\Gamma)}{\partial \Gamma^2} - 2\left(\frac{\partial \chi_t(\Gamma)}{\partial \Gamma}\right)^2 - \frac{\partial\,[\chi_t(\Gamma)]^2}{\partial \Gamma}\frac{\partial \ln \dfrac{\partial F_t(\Gamma)}{\partial \Gamma}}{\partial \Gamma} -$$

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

$$+\frac{D_{CC}^{(\mathrm{IV})}}{\mathrm{Pe}^2}\tilde{N}_t(\hat{\Gamma}) + \frac{2}{3}\frac{\chi(t)}{\sqrt{\left(\overline{c^2(t)}\right)}}\left[\frac{\partial \ln \dfrac{\partial F_t(\Gamma)}{\partial \Gamma}}{\partial \Gamma} + \frac{\partial}{\partial \Gamma}\right] X_t(\Gamma)\,\chi_t(\Gamma) +$$

$$+\mathrm{Da}\left[2\frac{\partial \dot{\omega}(\Gamma)}{\partial \Gamma} - \dot{\omega}(\Gamma)\frac{\partial}{\partial \Gamma}\right]\chi_t(\Gamma)\,. \tag{52}$$

The solved system of dimensionless partial differential equations consists of Eq. (48) for the density of the flame surface, Eq. (51) for the single-point probability density function, and Eq. (52) for the conventional rate of scalar dissipation. To allow for a particular type of chemical reaction in (48), (51), and (52), we must determine the function $\dot{\omega}(\Gamma)$ and the parameter, i.e., the Damköhler number Da. For simplicity we assume that an expression for $\dot{\omega}(\Gamma)$ is prescribed as the first-order reaction rate $\dot{\omega}(\Gamma) = \Gamma$. This formula can describe a binary chemical reaction in the situation where one reactant is in very short supply [6]. In this case, the system solved can be written as

$$\frac{\partial \Sigma_t(\Gamma)}{\partial t} = -2D(t)\sqrt{\left(\overline{c^2(t)}\right)}\frac{\partial^2 \Sigma_t(\Gamma)}{\partial \Gamma} - A(t)\left[\frac{\Sigma_t(\Gamma)}{2} - \frac{8\sqrt{\mathrm{Pe}}}{3\sqrt{6\pi}}\chi(t)^{1/2} f_t\right] +$$

$$+\frac{2C(t)\sqrt{\mathrm{Pe}}}{\sqrt{6\pi}}\tilde{N}_t(\Gamma)\frac{\dfrac{\partial F_t(\Gamma)}{\partial \Gamma}}{\chi(t)^{1/2}} +$$

$$+\frac{D(t)}{2}\frac{\partial}{\partial \Gamma}\left[\kappa(\hat{\Gamma})\exp\left\{-\alpha(T)\hat{\Gamma}^2\right\}\Sigma_t(\Gamma)\right] - \mathrm{Da}\,\Gamma\frac{\partial \Sigma_t}{\partial \Gamma}\,, \tag{53}$$

$$\frac{\partial F_t(\Gamma)}{\partial t} = \frac{\partial}{\partial \Gamma}\left[\chi_t(\Gamma)\frac{\partial F_t(\Gamma)}{\partial \Gamma}\right] - \mathrm{Da}\,\Gamma\frac{\partial F_t(\Gamma)}{\partial \Gamma}\,, \tag{54}$$

$$\frac{\partial \chi_t(\Gamma)}{\partial t} = k_1 A(t)\left(1 - k_2\frac{\chi_t}{\chi(t)}\right)\chi_t(\Gamma) - C(t)\tilde{N}_t(\Gamma) - \chi_t(\Gamma)\frac{\partial^2 \chi_t(\Gamma)}{\partial \Gamma^2} -$$

$$-2f_t^{-1}(\Gamma)\frac{\partial \chi_t(\Gamma)}{\partial \Gamma}\frac{\partial}{\partial \Gamma}\left[\chi_t(\Gamma)\frac{\partial F_t(\Gamma)}{\partial \Gamma}\right] +$$

$$+D(t)\frac{1}{f_t(\Gamma)}\frac{\partial}{\partial \Gamma}\left\{\Gamma\exp\left[-\alpha(T)\Gamma^2\right]\chi_t(\Gamma) f_t(\Gamma)\right\} - \mathrm{Da}\left(2\chi_t(\Gamma) - \Gamma\frac{\partial \chi_t(\Gamma)}{\partial \Gamma}\right), \tag{55}$$

where

$$A(t)=\sqrt{\left(\frac{\mathrm{Re}}{15}\varepsilon(t)\right)}S_{UC}(t)\,;\quad C(t)=-\frac{D_{CC}^{(\mathrm{IV})}(0,t)}{\mathrm{Pe}^2}\,;\quad D(t)=\frac{2}{3}\frac{\chi(t)}{\sqrt{\left(\overline{c^2}\right)}}\,. \tag{56}$$

The coefficient k_1 results from the fact that a simplifying assumption of the equality of several similar moments to one is made in deriving Eq. (4) in [1]. In physical meaning, k_1 must be of the order of unity. Having appropriately selected the coefficients k_1 and k_2, we can approximately satisfy the normalization conditions $\int\chi_t(\Gamma)f_t(\Gamma)d\Gamma=\chi(t)$ and $\int\Gamma^2 f_t(\Gamma)d\Gamma=\overline{c^2(t)}$.

Taking into account the symmetry of the functions $\Sigma_t(\Gamma)$ and $\chi_t(\Gamma)$ and the antisymmetry of the function $F_t(\Gamma)$ relative to the origin of coordinates, we will consider half of their domain of definition, $0\leq\Gamma\leq 1$. The boundary conditions have the form

$$\left.\frac{\partial\Sigma_t(\Gamma)}{\partial\Gamma}\right|_{\Gamma=0}=\Sigma_t(1)=\left.\frac{\partial\chi_t(\Gamma)}{\partial\Gamma}\right|_{\Gamma=0}=(\chi_t)\,|_{\Gamma=1}=F_t\,|_{\Gamma=0}=0\,,\quad F_t\,|_{\Gamma=1}=\frac{1}{2}\,. \tag{57}$$

The numerical solution of the boundary-value problem (53)-(57) is strongly complicated by the presence of terms with "negative" viscosity $-D(t\sqrt{\overline{c^2}}\,\frac{\partial^2\Sigma_t(\Gamma)}{\partial\Gamma^2}$, $-\partial/\partial\Gamma[\chi_t\partial F_t/\partial\Gamma]$, and $-\chi_t[\partial^2\chi_t/\partial\Gamma^2]$ that characterize antidiffusion in the phase space of the values of the scalar Γ.

The presence of the "antidiffusion" terms makes problem (53)-(57) similar to classical inverse problems. An extensive literature is available on the theory of solution of inverse problems [11-43] using different variants of the regularization method. However, there are few appropriate examples of numerical solution of the so-called retrospective problems on rather large time intervals without a critical dependence on the regularization parameter that fails to be selected so small as to prevent a substantial dependence of the solution itself on it.

To avoid numerical instability, we solved problem (53)-(57) in the opposite direction with respect to time, beginning with the "starting" time t_s and advancing to smaller values of t. We employed the method of solving the system of partial equations (the method of straight lines in the form of the MOLCH standard numerical procedure from the IMSL package [15]).

There is good reason to indicate the "starting" functions $\Sigma_t(\Gamma)$, $\chi_t(\Gamma)$, and $F_t(\Gamma)$ at the end of a mixing process. The selection of the analytical form for "starting" values of the functions $\chi_t(\Gamma)$ and $F_t(\Gamma)$ was based on the fact that at the end of the mixing process the single-point distribution function $f_t(\Gamma)$ has a Gaussian form. As is known, the single-point probability density function (PDF) tending to a Gaussian form is due to the fact that the CRSD becomes independent of the scalar [16]. Using this fact, we can select, as the "starting" functions for calculating, the Gaussian form for the single-point PDF and the form of the CRSD independent of the scalar field.

The "starting" distributions of the functions $F_t(\Gamma)$ and $f_t(\Gamma)$ in this state were prescribed according to model analytical expressions (see formulas (42) in [9]). The "starting" value for the function $\Sigma_t(\Gamma)$ is prescribed by the formula $\Sigma_{t_s}(\Gamma)=f_{t_s}(\Gamma)\chi_{t_s}(\Gamma)$ that expresses the statistical independence of the scalar-field gradient and the scalar at the final step of mixing [6]:

$$\Sigma_{t_s}(\Gamma)=f_{t_s}\chi_{t_s}=\frac{\beta}{\alpha^2+\Gamma^2}\frac{2\chi_{t_s}}{\pi}\arctan\left((1-\Gamma)/\gamma\right). \tag{58}$$

Usually, the process of integration of equations in the opposite direction began from the instant t_s = 25–30, which corresponds almost totally to the mixed state. This corresponds to a sharp maximum of the function f_t at $\Gamma=0$ and to nearly zero values of f_t when $\Gamma>0$.

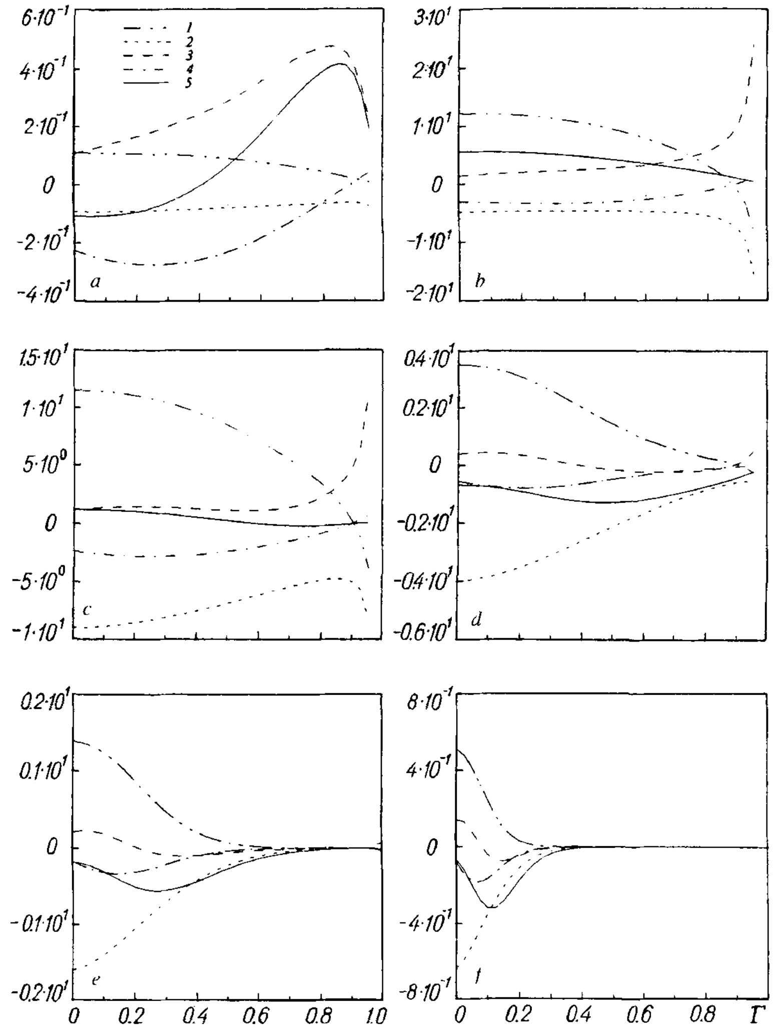

Fig. 1. Individual terms of the right-hand side of Eq. (53) for the conditions of the specific isoscalar-surface area at Da = 0 [a) at the instant t = 0; b) 0.5; c) 1; d) 2.5; e) 5; f) 10]: 1) "source"; 2) "dissipation"; 3) "antidiffusion"; 4) "transfer" in the space Γ; 5) sum of all the terms on the right-hand side.

In test calculations, we checked the sensitivity of the numerical solution to the setting of starting conditions. Thus, the same conditions were set at different starting instants in the interval $t_s \in (15, 30)$ or two more sets of model analytical dependences for the "starting" distributions were used. These calculations showed that the features of setting the starting conditions are smoothed on the time interval $\Delta t \sim 1.5$, and further in calculating we obtain a behavior of the functions of system (53)-(57) that is close to a universal behavior independent of the starting conditions.

Results of the Numerical Solution of the System of Equations for $\Sigma_t(\Gamma)$, $F_t(\Gamma)$, and $\chi_t(\Gamma)$. Since the equation obtained above for $\Sigma_t(\Gamma)$ is new and has not been described earlier in the literature, it is appropriate to study its individual terms that are responsible for different effects. Figures 1 and 2 give a change in the magnitude of individual effects on the right-hand side of Eq. (53) and $\Sigma_t(\Gamma)$ at different evolution times and Damköhler numbers. Here the "source" is used to refer to the term that is proportional to $S_{UC}(t)$ and describes the influence of the turbulent velocity field on the distribution of the isoscalar surface. This is the only term in Eq. (53) for $\Sigma_t(\Gamma)$ in which the characteristics of the turbulent velocity field appear directly. The influence of

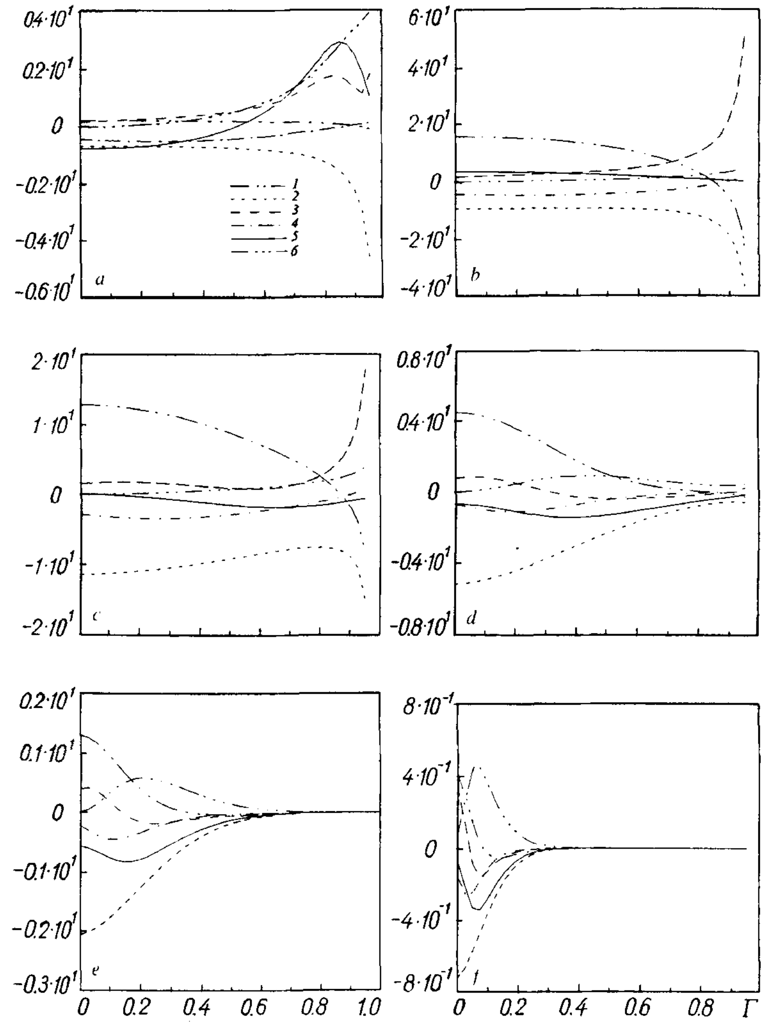

Fig. 2. Individual terms of the right-hand side of Eq. (53) for the conventional specific area of the isoscalar surface at Da = 0.25: a-f) 1-5) notation is the same as in Fig. 1; 6) "chemical reacting."

the velocity field on the density of the isoscalar surface is realized in terms of the "source." As the figures show, the source term is positive at almost all Γ, its small magnitude being attained with small fluctuations. This behavior of the "source" is due to the fact that the correlation of the pulsations of the scalar and the specific surface area is larger with small pulsations and accordingly smaller with large ones. This term can change its sign at the initial steps of mixing in the vicinity of the point $\Gamma = 1$, which is associated with the δ-like character of the distribution of the function $f_t(\Gamma)$ at this point. Therefore, the source term characterizes not only the increase in the flame surface density function (FSDF) due to the mixing by the turbulent velocity field but also such a redistribution of the FSDF for which this function increases in the region of moderate concentrations ($\Gamma = 0$) and decreases at limiting concentrations.

Comparing the "source" at the same evolution times but different Damköhler numbers, we can note that the maximum of this term at small Γ increases with chemical action. At large evolution times and in the presence of the chemical action, the "source" has a minimum at small Γ. It is not improbable that this phenomenon is associated with the peaking of characteristic realizations of the scalar-gradient field at small Γ.

Figures 1 and 2 show the behavior of dissipation in Eq. (53) at different evolution times and Damköhler numbers. The dissipation term in Eq. (53) is proportional to the derivative of the structural function

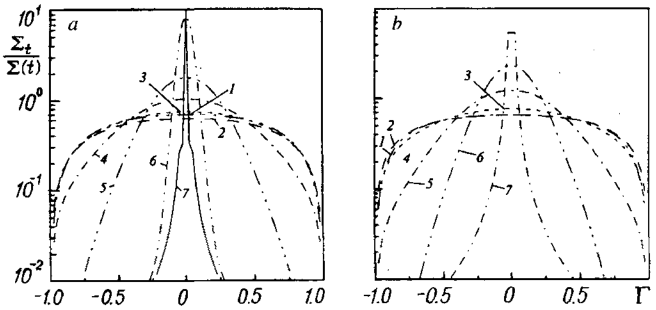

Fig. 3. Variation in the form of the profile of the conventional density of the reacting surface with time [a) Da = 0; b) 0.25]: 1) t = 0; 2) 0.5; 3) 1.4; 4) 2.5; 5) 5; 6) 15; 7) 20.

$D_{CC}^{(IV)}(0, t)$. It describes the action of molecular dissipation on the isoscalar surface. As is seen from Fig. 1, the dissipation at all the evolution times is negative, which agrees with its physical meaning. At small times, excluding the region in the vicinity of $\Gamma = 1$, the value of the dissipation is independent of Γ. When $t \geq 1$ the dissipation term has a negative maximum at small Γ that increases with further evolution. This behavior of the dissipation is associated with the structure of the function $N_t(\Gamma)$, to be more precise – with the presence of the exponential factor in the expression for $N_t(\Gamma)$. The form of the function $N_t(\Gamma)$ is determined by the conventional statistics of the second derivatives of the scalar field. Comparison of Figs. 1 and 2 shows that the noted features of the behavior of dissipation remain basically the same even when the chemical reaction is taken into account. We can only note a somewhat larger peaking of the maximum of the curve with small fluctuations. Starting with the instant $t = 1$, the source and dissipation terms are the largest effects in Eq. (53); however, since their signs are opposite, the remaining effects also exert a pronounced influence on the evolution of the function $\Sigma_t(\Gamma)$.

The "antidiffusion" term $-2D\sqrt{\overline{c^2}(t)}\ \dfrac{\partial^2\Sigma_t(\Gamma)}{\partial\Gamma^2}$ is called such because it describes a shift of the distribution of $\Sigma_t(\Gamma)$ to the center of the phase space Γ in the process of evolution. Its function is governed by the physics of the process of mixing. As the scalar field is mixed, the probability of small fluctuations must increase. In the phase space Γ, this means a shift of the distribution function to the center of the space, i.e., antidiffusion.

As Fig. 1 shows, in the equation for $\Sigma_t(\Gamma)$ this term first is positive with a maximum at larger fluctuations. When $t > 2.5$, the maximum shifts toward smaller Γ. This behavior of "antidiffusion" is associated with the evolution of the distribution function in the process of turbulent mixing. First the influence of "antidiffusion" shows up with large fluctuations, and as they decrease the zone of this influence shifts to the center of the phase space. Comparison of Figs. 1 and 2 indicates that taking into account the chemical action introduces no substantial change into the character of the behavior of the "antidiffusion" term.

The term that is called transfer – the fourth on the right-hand side of Eq. (53) for $\Sigma_t(\Gamma)$ – is associated with taking into account the correlation between the scalar and its second derivative. Unlike the dissipation that is proportional to the square of the second derivative of the scalar field, the "transfer" in the space Γ is associated with the first degree of the second derivative. As is seen from Fig. 1, this term is always negative in the process of evolution. Its form remains practically constant in evolution. Taking into account the chemical action on the scalar field does not substantially change the transfer and the character of its influence on $\Sigma_t(\Gamma)$ (see Figs. 1 and 2) either.

As is seen from Figs. 1 and 2, the sum of the actions of these effects on the right-hand side of Eq. (53) on the evolution of $\Sigma_t(\Gamma)$ undergoes a rather complex evolution. First, this sum changes the sign in the phase space Γ. The right-hand side of Eq. (53) is negative at small Γ and positive at large Γ, which governs the change in the form of the profile of the function $\Sigma_t(\Gamma)$ to a flatter one when $t \sim 1$. After this instant, the right-hand side again becomes alternating for a time (see Figs. 1c and 2c at $t = 1$) but now, conversely, with

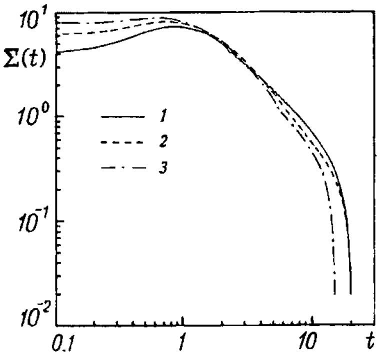

Fig. 4. Evolution of the specific density of the reacting surface $\Sigma(t)$ at different Damköhler numbers Da: 1) Da = 0; 2) 0.1; 3) 0.25.

a minimum at large Γ, which indicates a new rearrangement of the form of the $\Sigma_t(\Gamma)$ profile. With evolution, the right-hand side of the equation for $\Sigma_t(\Gamma)$ levels off, and at larger times the basic processes of change in the function $\Sigma_t(\Gamma)$ are concentrated in the region of small Γ with a maximum at small Γ and a minimum at intermediate ones.

This change in the right-hand side of Eq. (53) causes a rather complex evolution of the form of the specific isoscalar-surface area (see Fig. 3). As the presented graphs show, the evolution of the function $\Sigma_t(\Gamma)$ lies in the peaking of its form from a nearly flat form first to a parabolic one, and subsequently when $t > 6$ its form resembles a δ function narrowing with mixing time.

Taking into account the chemical interaction does not substantially change the character of evolution of the specific isoscalar-surface area. Figure 4 shows a change in the function $\Sigma(t) = \int_0^\infty \Sigma_t(\Gamma)d\Gamma$ that is integral over all values at different Damköhler numbers. It is seen that the general tendency is for a gradual decrease in the value of this function. The increase in $\Sigma(t)$ at the initial step of evolution is associated with the turbulent splitting of the scalar field. The influence of the chemical reacting is rather complex in character. At the beginning of the evolution, the total reacting surface with allowance for the chemical reaction is larger than in the inert scalar field. However, subsequently the chemical action leads to a more rapid decrease in the reacting surface.

As is seen from formulas (53) and (55), the structure of the equations for $\Sigma_t(\Gamma)$ is similar. This is associated with the fact that the functions $\Sigma_t(\Gamma)$ and $\chi_t(\Gamma)$ are, respectively, the first and second statistical moments of the joint probability density function of the scalar and its gradient. The similarity of the equations for $\chi_t(\Gamma)$ and $\Sigma_t(\Gamma)$ is expressed in the fact that the equation for $\chi_t(\Gamma)$ contains the terms of the same meaning as the equation for $\Sigma_t(\Gamma)$ does, i.e., the source term 1, the dissipation term 2, the antidiffusion term 3, and the term of transfer in the space Γ 4. The evolution of the function $\chi_t(\Gamma)$ without allowance for the chemical reaction is presented in [9].

Conclusions. The evolution of $\Sigma_t(\Gamma)$ resulting from the solution of the system of equations is in agreement with the results of direct numerical modeling of the turbulent velocity and scalar fields.

The closed system of equations developed can be employed in calculating chemical reactions in turbulent flows and the processes of turbulent combustion within the framework of the flamelet approach. The results obtained can be used in the development of practical devices for dispersion and homogenization of fuel emulsions with the aim of improving the efficiency of their combustion.

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