Journal of Engineering Physics and Thermophysics, Vol. 75, No. 3, 2002

MODEL OF THE SURFACE OF EQUAL CONCENTRATION IN A TURBULENT REACTING FLOW

Yu. V. Zhukova and V. A. Sosinovich UDC 532.517.4

Statistical data on the scalar-field gradient obtained by means of direct numerical simulation of turbulence is used in the present paper to predict the form of the specific area of the isoscalar surface at different stages of evolution of a turbulent flow. From the available literature data on the conditional scalar dissipation rate a suggestion of the form of typical realizations of the turbulent field at different stages of its evolution is made and on this basis the form of the scalar gradient probability density on the isoconcentric surface is proposed. Using this quantity and the idea that the turbulent scalar field is multiscale in nature, it is possible to calculate the dependence of the specific area of equal concentration on the scalar value at the initial, intermediate, and final stages of turbulent mixing. The results of the present work are compared with the results of other theoretical approaches to the calculation of the surface area of equal concentration.

Introduction. The investigation of turbulent combustion is an important topic for many practical applications. The flames of rocket and aircraft engines are turbulent, combustion in internal combustion engines is realized in the turbulent regime, and the main methods of obtaining energy in industry are associated with turbulent combustion. In describing it, many problems that are still far from being completely solved arise. The current approaches to its investigation are associated with flames that are far from the chemical equilibrium state. The most important approach to the modeling of combustion with allowance for the deviation from the state of chemical equilibrium is based on the assumption that the turbulent flame can be considered as an ensemble of one-dimensional thin reaction zones (flamelets), and each zone is in a locally laminar mixed environment (laminar diffusion flamelet model). The development of theoretical models of turbulent combustion that take into account the nonequilibrium effects requires deep knowledge of the statistical properties of the scalar-field gradient. Relatively detailed information on the statistics of the scalar-field gradient is contained in the combined probability density (CPD) of the fluctuation values of the scalar field and its gradient. For this function, by different techniques an equation was derived [1–5]. However, its solution to a degree permitting its practical use has not been found. The main difficulty encountered in attempting to solve the equations for the CPD is associated with their multidimensionality. In this connection, the desire to obtain information on the moments of this function, which are important for developing the theory of turbulent combustion, arises. The second-order CPD moment is the dissipation rate of scalar fluctuations on the isoscalar surface. Suffice it to say that this function is indispensable for solving the equation for the single-point probability density of the scalar in a turbulent reacting flow [6, 7]. The equation for the second-order CPD moment was obtained in [8]. In attempting to solve it numerically, serious difficulties were revealed, since this equation in the space of scalar values in describing the mixing process models the shrinkage of the values of scalar fluctuations to zero. Formally it appears as the presence in the equation of a term with negative diffusion. It is known that the numerical realization of such a calculation leads to the appearance of instability. Although this problem is, in principle, soluble, it requires a special approach and much effort [9].

Analogous difficulties arise in deriving and attempting to solve the equation for the first-order CPD moment by the gradient variable. This moment is nothing but the specific area of the isoscalar surface [10]. The notion of the flame area had been used before in early combustion models. However, the equation for this quantity was proposed for the first time in [11], where it was suggested that the combustion of non-mixed reactants at an early stage was controlled by the competition between the deformation of the flame elements and the mutual annihilation of the flame

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A. V. Luikov Heat and Mass Transfer Institute, National Academy of Sciences of Belarus, Minsk, Belarus; email: svaturb@ns1.hmti.ac.by. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 75, No. 3, pp. 51–62, May–June, 2002. Original article submitted July 11, 2001.

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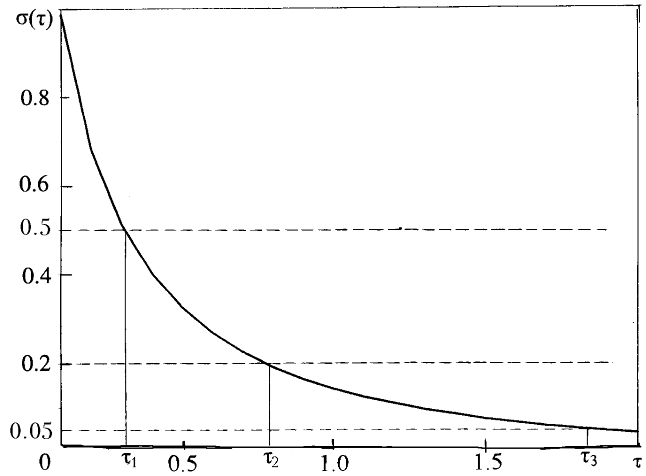

Fig. 1. Evolution of dispersion.

area due to the destruction of its adjacent elements. The advantage of the flame model based on the equation for the surface area is that it is used to relate the analysis of a separate flamelet and the global turbulent field.

Given the calculated flame surface area $\Sigma_\tau(\Gamma)$, we can easily calculate the mean heat release rate per unit volume or the reactant flow rate by the formulas

$$W = Q\,\Sigma_\tau(\Gamma)\,, \quad W_\tau = -\frac{Q}{\Delta h_\tau}\,\Sigma_\tau(\Gamma)\,. \tag{1}$$

The main difficulty in finding $\Sigma_\tau(\Gamma)$ is associated with the closure of the equation of [12] and its numerical solution [10]. To close individual terms of this equation, one normally uses the results of direct numerical simulation of the turbulent scalar-field [13]. Then, using the thus-closed equation, we shall attempt to obtain the form of this function at all times.

In the present paper, an attempt is made to elucidate the form of the isoscalar surface specific area at some instants of the scalar-field evolution, using the known literature results concerning the statistics of the scalar-field gradient without solving the equation for this quantity. In [14], on the basis of the results of direct numerical simulation a form of the conditional scalar dissipation rate of the intensity of scalar fluctuations at different stages of turbulent mixing was proposed. Using this information, we can attempt to reconstruct the conditional probability density of the scalar gradient and calculate the specific area of the isoscalar surface. We can associate each dependence of the conditional scalar dissipation value given in [14] with a typical realization of the scalar field [15], which is the source of such a dependence. Then, using this typical realization, we can calculate the scalar-field gradient and obtain the corresponding gradient probability density at a given value of the scalar. Given such a function and using the notions of the multiscale character of the turbulent mixing process, we can calculate the value of the isoscalar surface for a given stage of evolution of the turbulent scalar field.

In [14], information on the form of the conditional dissipation rate $\chi_\tau(\Gamma)$ is given for separate time intervals of the scalar-field evolution. These intervals correspond to the initial stage where the scalar-field dispersion amounts to 50% of its initial value ($\sigma(\tau)/\sigma(0) = 0.5$), the intermediate stage where the dispersion amounts to about 20% of its initial value ($\sigma(\tau)/\sigma(0) = 0.2$), and the final stage where the dispersion amounts to 5% of its initial value ($\sigma(\tau)/\sigma(0) = 0.05$). To find the time intervals τ corresponding to the above stages of evolution of the turbulent scalar field, we write the form of the single-point probability density of the scalar-field values in the form [16]

$$f_\tau(\Gamma) = \frac{1}{\sqrt{\pi}}\,\frac{\tau^{1/2}}{\Gamma\,\left|\ln|\Gamma|\right|^{3/2}}\exp\left(-\frac{\tau}{\left|\ln|\Gamma|\right|}\right) \tag{2}$$

and use it to calculate the dispersion evolution

$$\sigma(\tau) = \int_{-1}^{1} \Gamma^2 f_\tau(\Gamma)\, d\Gamma , \tag{3}$$

which is given in Fig. 1. Using this dependence, it can easily be shown that to the initial stage there corresponds the time $\tau_1 = 0.3$, to the intermediate stage there corresponds the time $\tau_2 \approx 0.7$, and to the final stage — $\tau_3 \approx 1.9$. The dimensionless time τ is measured in the characteristic time intervals equal to the time of diffusion mixing on the scale of length l:

$$\tau = \frac{t}{l^2/(3D)} . \tag{4}$$

1. Area of the Nonscalar Surface at the Initial Stage of Evolution of the Turbulent Scalar Field. As shown in [14], by means of direct numerical simulation of turbulence in the initial period of turbulent flow evolution, where the dispersion of scalar-field fluctuations constitutes about 50% of its initial value, the function of the conditional scalar dissipation rate $\chi_\tau(\Gamma)$, i.e., of the dissipation rate realized on the surface $c(x, \tau) = \Gamma$, demonstrates a parabolic form with a maximum at small values of scalar fluctuations. Such a form of the function of the conditional scalar dissipation rate is expected in the case where the scalar field consists essentially of diffusion layers separating the ranges of approximate homogeneity. If we choose a local system of coordinates with the OX axis directed perpendicular to the diffusion layer, then, as a typical realization of a scalar field with a fixed wavelength λ, a sinusoid with a time-decaying amplitude can serve. Such a field can be described by the formula

$$c_1(x, \tau) = \exp\left(-\frac{\tau}{2\lambda^2}\right)\sin\left(\frac{x}{\lambda}\right). \tag{5}$$

The dispersion of the random scalar field $c_1(x, \tau)$ is of the form

$$\sigma_1(\tau) = \frac{1}{2\pi}\int_0^{2\pi} c_1(x, \tau)^2\, dx = \frac{1}{\sqrt{2}}\exp\left(-\frac{\tau}{2\lambda^2}\right). \tag{6}$$

The scalar gradient field can be calculated, taking a derivative of the expression for $c_1(x, \tau)$ with respect to x:

$$z_1(x, \tau) = \frac{1}{\lambda}\exp\left(-\frac{\tau}{2\lambda^2}\right)\cos\left(\frac{x}{\lambda}\right). \tag{7}$$

At a given level of the scalar-field value $c(x, \tau) = \Gamma$ the scalar-field gradient $z_1(x, \Gamma)$ can take on two different values:

$$z_i(\Gamma) = \frac{1}{\lambda}\exp\left(-\frac{\tau^2}{2\lambda^2}\right)\cos\varphi_i(\Gamma) , \quad i = 1, 2 . \tag{8}$$

As seen from Fig. 2, the values of the angles $\varphi_1(\Gamma)$ and $\varphi_2(\Gamma)$ are related by the relation

$$\varphi_2(\Gamma) = \pi - \varphi_1(\Gamma) . \tag{9}$$

The value for $\varphi_1(\Gamma)$ is determined by the ratio of the field value $c(x, \tau) = \Gamma$ at a given point to the maximum value of this field at time τ equal to $\exp(-\tau/2\lambda^2)$. Thus,

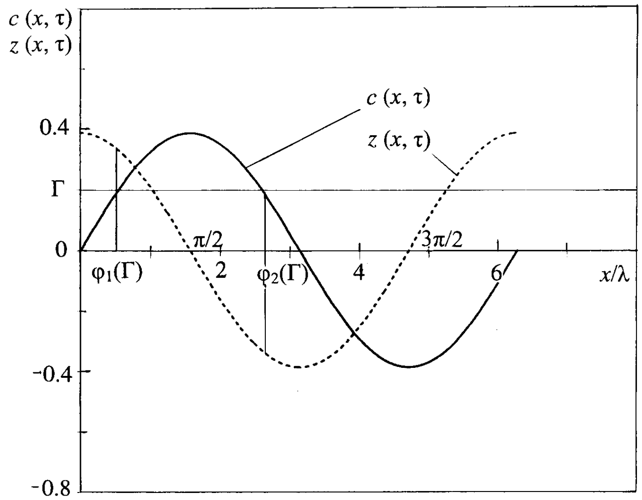

Fig. 2. Realization of the scalar field $c(x, \tau)$ and its gradient $z(x, \tau)$ at the initial stage of evolution $\frac{\sigma(\tau)}{\sigma(0)} \approx 0.5$.

$$\varphi_1(\Gamma) = \arcsin \frac{\Gamma}{\exp\left(-\frac{\tau}{2\lambda^2}\right)} = \arcsin\left(\Gamma \exp\left(\frac{\tau}{2\lambda^2}\right)\right). \tag{10}$$

Using equality (8), we can write the expression for the conditional probability density of the field gradient values:

$$P_\tau(W|\Gamma) = \frac{1}{2}\{\delta[W - z_1(\Gamma)] + \delta[W - z_2(\Gamma)]\}\,\Theta\left[1 - |\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)\right]. \tag{11}$$

The Heaviside function $\Theta\left[1 - |\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)\right]$ in (11) reduces $P_\tau(W|\Gamma)$ to zero beyond the domain of its existence:

$$|\Gamma| < \exp\left(-\frac{\tau}{2\lambda^2}\right). \tag{12}$$

The values of the scalar-field gradient at $\varphi_1(\Gamma)$ and $\varphi_2(\Gamma)$ are equal in magnitude but opposite in sign. Since for our purposes only the probability density of the gradient magnitude is important, for $P_\tau(W|\Gamma)$ we can write

$$P_\tau(W|\Gamma) = \delta[W - z_1(\Gamma)]\,\Theta\left[1 - |\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)\right]. \tag{13}$$

Using formula (7) for $\varphi_1(\Gamma)$, we obtain

$$P_\tau(W|\Gamma) = \delta\left[W - \frac{1}{\lambda}\exp\left(-\frac{\tau}{2\lambda^2}\right)\cos\varphi_1(\Gamma)\right]\Theta\left[1 - |\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)\right] =$$

$$= \delta\left[W - \frac{1}{\lambda}\exp\left(-\frac{\tau}{2\lambda^2}\right)\cos\left(\arcsin \exp\left(\frac{\tau}{2\lambda^2}\right)\Gamma\right)\right]\Theta\left[1 - |\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)\right] =$$

$$= \delta\left[W - \frac{1}{\lambda}\exp\left(-\frac{\tau}{2\lambda^2}\right)\left(1 - \exp\left(\frac{\tau}{\lambda^2}\right)\Gamma^2\right)^{1/2}\right]\Theta\left[1 - |\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)\right]. \tag{14}$$

The formula for calculating the specific area of the surface in a turbulent flow with a given scale of λ is of the form

$$\Sigma_\tau(\Gamma, \lambda) = \int_0^\infty W P_\tau(W \mid \Gamma) f_\tau(\Gamma, \lambda)\, dW . \tag{15}$$

Using (14), we obtain

$$\Sigma_\tau(\Gamma, \lambda) = \frac{1}{\lambda} \exp\left(-\frac{\tau}{2\lambda^2}\right)\left(1 - \exp\left(\frac{\tau}{\lambda^2}\right)\Gamma^2\right)^{1/2} f_\tau(\Gamma, \lambda)\, \Theta\left[1 - |\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)\right]. \tag{16}$$

The symbol λ in the argument of the functions $\Sigma_\tau(\Gamma, \lambda)$ and $f_\tau(\Gamma, \lambda)$ denotes that they have been calculated in a single-scale approximation, i.e., under the assumption that the scalar turbulent field is sinusoidal with a wavelength λ. In this approximation, the function $f_\tau(\Gamma, \lambda)$ can be given in the form [16]

$$f_\tau(\Gamma, \lambda) = \exp\left(\frac{\tau}{\lambda^2}\right) f_0\left(\Gamma \exp\left(\frac{\tau}{\lambda^2}\right)\right). \tag{17}$$

Here $f_0(\Gamma)$ is the form of the probability density function at the initial instant of time. The choice of this form is largely arbitrary. In the case where the initial scalar field is totally segregated, the function

$$f_0(\Gamma) = \frac{1}{2}\left[\delta(\Gamma - 1) + \delta(\Gamma + 1)\right].$$

Then for $f_\tau(\Gamma, \lambda)$ we obtain

$$f_\tau(\Gamma, \lambda) = \frac{1}{2}\left[\delta\left(\Gamma \exp\left(\frac{\tau}{\lambda^2}\right) + 1\right) + \delta\left(\Gamma \exp\left(\frac{\tau}{\lambda^2}\right) - 1\right)\right] \exp\left(\frac{\tau}{\lambda^2}\right). \tag{18}$$

With the use of this formula, taking into account the symmetry in Γ and $-\Gamma$, the single-scale specific area of the surface will be given by the expression

$$\Sigma_\tau(\Gamma, \lambda) = \frac{\exp\left(\frac{\tau}{2\lambda^2}\right)}{\lambda}\left(1 - \exp\left(\frac{\tau}{\lambda^2}\right)\Gamma^2\right)^{1/2} \delta\left(\Gamma \exp\left(\frac{\tau}{\lambda^2}\right) - 1\right)\Theta\left[1 - |\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)\right]. \tag{19}$$

To write the specific surface function, which will hold for the multiscale field, it is necessary to average the expression for $\Sigma_\tau(\Gamma, \lambda)$ over the distribution of the length scales $P(\lambda)$, which was chosen in the following form [16]:

$$P(\lambda) = 2\lambda \exp(-\lambda^2) . \tag{20}$$

Then

$$\Sigma_\tau(\Gamma) = \int_0^\infty \Sigma_\tau(\Gamma, \lambda) P(\lambda)\, d\lambda = 2 \int_0^\infty \exp\left(\frac{\tau}{2\lambda^2} - \lambda^2\right)\left(1 - \exp\left(\frac{\tau}{\lambda^2}\right)\Gamma^2\right)^{1/2} \times$$

$$\times\, \Theta\left[1 - |\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)\right] \delta\left(\Gamma \exp\left(\frac{\tau}{\lambda^2}\right) - 1\right). \tag{21}$$

We take into account the presence in the integrand in (21) of a Dirac δ-function and realize integration with respect to the variable λ. We make use of the following formulas of [17] (p. 31, formula (6.5)):

$$\delta\,[\varphi\,(x)] = \sum_s \frac{\delta\,(x - x_s)}{|\,\varphi'\,(x_s)\,|}\,. \tag{22}$$

Here x_s denotes the simple roots of the equation

$$\varphi\,(x) = 0 \tag{23}$$

lying in the interval under consideration. In our case,

$$\varphi\,(\lambda) = \Gamma \exp\left(\frac{\tau}{\lambda^2}\right) - 1\,. \tag{24}$$

Solving Eq. (23) for this case, we obtain

$$|\,\Gamma\,| \exp\left(\frac{\tau}{\lambda^2}\right) - 1 = 0\,, \tag{25}$$

which is equivalent to the equation

$$\exp\left(\frac{\tau}{\lambda^2}\right) = \frac{1}{|\,\Gamma\,|}\,. \tag{26}$$

The calculation of the logarithm of the left- and right-hand sides yields

$$\frac{\tau}{\lambda^2} = \ln \frac{1}{|\,\Gamma\,|}\,. \tag{27}$$

We take into account that $|\,\Gamma\,| < 1$:

$$\lambda^2 = \frac{\tau}{|\ln\,|\,\Gamma\,|\,|}\,. \tag{28}$$

Consequently,

$$\lambda_{1,2} = \pm \sqrt{\frac{\tau}{|\ln\,|\,\Gamma\,|\,|}}\,. \tag{29}$$

We find the value of the derivative $\varphi'(\lambda)$:

$$\varphi'\,(\lambda) = -\frac{2\tau}{\lambda^3}\,|\,\Gamma\,| \exp\left(\frac{\tau}{\lambda^2}\right). \tag{30}$$

Using (29) and taking into consideration (26), we obtain

$$|\,\varphi'\,(\lambda_{1,2})\,| = \frac{2\,|\ln\,|\,\Gamma\,|\,|^{3/2}}{\tau^{1/2}}\,. \tag{31}$$

The account of (22) for $\Sigma_\tau(\Gamma)$ yields

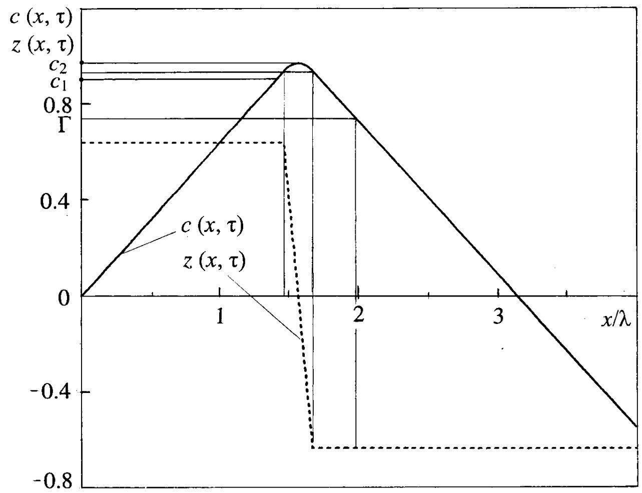

Fig. 3. Realization of the scalar field $c(x, \tau)$ and its gradient $z(x, \tau)$ at the intermediate stage of evolution $\frac{\sigma(\tau)}{\sigma(0)} \approx 0.2$.

$$\Sigma_\tau(\Gamma) = 2\frac{1}{|\Gamma|^{1/2}}\exp\left(-\frac{\tau}{|\ln|\Gamma||}\right)\left(1-\frac{1}{|\Gamma|}\Gamma^2\right)^{1/2}\frac{\tau^{1/2}}{2|\ln|\Gamma||^{3/2}}\Theta\left(1-|\Gamma|\frac{1}{|\Gamma|^{1/2}}\right). \tag{32}$$

Thus, the expression for the specific area of the isoscalar surface at the initial stage of turbulent scalar-field evolution is of the form

$$\Sigma_\tau^{(I)}(\Gamma) = \frac{\tau^{1/2}(1-|\Gamma|)^{1/2}}{|\Gamma|^{1/2}|\ln|\Gamma||^{3/2}}\exp\left(-\frac{\tau}{|\ln|\Gamma||}\right)\Theta(1-|\Gamma|^{1/2}). \tag{33}$$

2. Area of the Isoscalar Surface at the Intermediate Stage of Evolution. At intermediate times, as shown by means of direct numerical simulation in [14], the conditional scalar dissipation function $\chi_\tau(\Gamma)$ turns out to be almost flat. This corresponds to the time where the scalar-field dispersion constitutes 20% of its initial value. Such a form of the function of the conditional scalar dissipation rate can be expected in the case where the scalar field consists essentially of curves resembling a saw whose edges represent rectangular portions. The assumed form of the scalar-field realization typical of the intermediate stage of evolution is shown in Fig. 3.

Exactly such a form of the scalar field leads to the dependence of the conditional dissipation rate on the value of the scalar field on the major portion of the $c(x, \tau)$ curve. In this case, the analytical expression for the scalar field is of the form

$$c_2(x,\tau) = \sqrt{\frac{3}{2}}\exp\left(-\frac{\tau}{2\lambda^2}\right)\begin{cases} \frac{2}{\pi}\frac{x}{\lambda}, & -\frac{\pi}{2}+\delta < \frac{x}{\lambda} < \frac{\pi}{2}-\delta, \\ a\sin\left(\omega\frac{x}{\lambda}\right), & \frac{\pi}{2}-\delta < \frac{x}{\lambda} < \frac{\pi}{2}+\delta, \\ -\frac{2}{\pi}\frac{x}{\lambda}, & \frac{\pi}{2}+\delta < \frac{x}{\lambda} < \frac{3\pi}{2}-\delta, \\ a\sin\left[\omega\left(\frac{x}{\lambda}-\frac{3\pi}{2}\right)\right], & \frac{3\pi}{2}-\delta < \frac{x}{\lambda} < \frac{3\pi}{2}+\delta. \end{cases} \tag{34}$$

The value of δ should be chosen small ($\sigma \to 0$). The parameters a and ω are calculated by the formulas

$$a = 1-\frac{\delta}{\pi}; \quad \omega = \sqrt{\frac{2}{\pi\delta}} \tag{35}$$

and are chosen so that the expressions for $c_2(x, \tau)$ and its first derivative are continuous at points $\frac{x}{\lambda} = \frac{\pi}{2} \pm \delta$ and $\frac{x}{\lambda} = \frac{3\pi}{2} \pm \delta$. The smooth connection of the rectangular portions of the $c_2(x, \tau)$ curve with opposite gradients is explained by the fact that the sharp gradients in the turbulent flow are smoothed due to the action of the molecular mechanism of diffusion. In this case, the field of the scalar gradient is described by the expression

$$z_2(x, \tau) = \frac{1}{\lambda}\sqrt{\frac{3}{2}}\exp\left(-\frac{\tau}{2\lambda^2}\right)\begin{cases} \frac{2}{\pi}, & -\frac{\pi}{2} + \delta < \frac{x}{\lambda} < \frac{\pi}{2} - \delta, \\ a\omega\cos\left(\omega\frac{x}{\lambda}\right), & \frac{\pi}{2} - \delta < \frac{x}{\lambda} < \frac{\pi}{2} + \delta, \\ -\frac{2}{\pi}, & \frac{\pi}{2} + \delta < \frac{x}{\lambda} < \frac{3\pi}{2} - \delta, \\ a\omega\cos\left[\omega\left(\frac{x}{\lambda} - \frac{3\pi}{2}\right)\right], & \frac{3\pi}{2} - \delta < \frac{x}{\lambda} < \frac{3\pi}{2} + \delta. \end{cases} \tag{36}$$

If the level of the scalar field $c(x, \tau) = \Gamma$, where

$$|\Gamma| < c_1 = \sqrt{\frac{3}{2}}\exp\left(-\frac{\tau}{2\lambda^2}\right)\left(1 - \frac{2\delta}{\pi}\right), \tag{37}$$

then, as seen from Fig. 3, the scalar-field gradient $z_2(x, \tau)$ assumes only two values:

$$z_2(x, \tau) = \pm\left(\frac{3}{2}\right)^{1/2}\frac{2}{\pi\lambda}\exp\left(-\frac{\tau}{2\lambda^2}\right). \tag{38}$$

Only in a narrow range of values of the scalar-field where

$$c_1(x, \tau) < |\Gamma| < c_2(x, \tau), \tag{39}$$

where $c_1(x, \tau)$ is given by formula (37) and

$$c_2(x, \tau) = \left(\frac{3}{2}\right)^{1/2}\exp\left(-\frac{\tau}{2\lambda^2}\right)\left(1 - \frac{\delta}{\pi}\right), \tag{40}$$

can the field gradient assume values determined by the second and fourth lines in (36):

$$z_2(x, \tau) = \pm\left(\frac{3}{2}\right)^{1/2}\exp\left(-\frac{\tau}{2\lambda^2}\right)\frac{1}{\lambda}a\omega\cos\left(\omega\frac{x}{\lambda}\right). \tag{41}$$

We now express the value of $\cos\left(\omega\frac{x}{\lambda}\right)$ in terms of $c_2(x, \tau)$. This can be done by making use of the second line in (34):

$$c_2(x, \tau) = \left(\frac{3}{2}\right)^{1/2}\exp\left(-\frac{\tau}{2\lambda^2}\right)a\sin\left(\omega\frac{x}{\lambda}\right). \tag{42}$$

Hence

$$\sin\left(\omega\frac{x}{\lambda}\right) = \frac{c_2(x, \tau)}{\left(\frac{3}{2}\right)^{1/2}\exp\left(-\frac{\tau}{2\lambda^2}\right)a}. \tag{43}$$

We express $\cos\left(\omega \frac{x}{\lambda}\right)$ in terms of $\sin\left(\omega \frac{x}{\lambda}\right)$:

$$\cos\left(\omega \frac{x}{\lambda}\right) = \left(1 - \sin^2\left(\omega \frac{x}{\lambda}\right)\right)^{1/2} = \left(1 - \frac{c_2^2(x, \tau)}{\frac{3}{2}\exp\left(-\frac{\tau}{\lambda^2}\right)a^2}\right)^{1/2}. \tag{44}$$

Using this expression in the formula for $z_2(x, \tau)$ and invoking formulas (35) for α and ω, we obtain

$$z_2(x, \tau) = \left(\frac{3}{2}\right)^{1/2} \exp\left(-\frac{\tau}{2\lambda^2}\right)\frac{1}{\lambda}\left(1 - \frac{\delta}{\pi}\right)\left(\frac{2}{\pi\delta}\right)^{1/2}\left(1 - \frac{c_2^2(x, \tau)}{\frac{3}{2}\exp\left(-\frac{\tau}{\lambda^2}\right)\left(1 - \frac{\delta}{\pi}\right)^2}\right)^{1/2}. \tag{45}$$

By transformation and replacement of $c(x, \tau)$ for Γ we find

$$z_2(x, \tau) = \left(\frac{3}{\pi\delta}\right)^{1/2} \exp\left(-\frac{\tau}{2\lambda^2}\right)\frac{1}{\lambda}\left(1 - \frac{\delta}{\pi}\right)\left(1 - \frac{2\Gamma^2 \exp\left(\frac{\tau}{\lambda^2}\right)}{3\left(1 - \frac{\delta}{\pi}\right)^2}\right)^{1/2}. \tag{46}$$

Having used formulas (37)–(40) and (46), we write the expression for the conditional probability density of the scalar gradient value

$$P_\tau(W|\Gamma) = \frac{1}{2}\Theta(c_1 - |\Gamma|)\,[\delta(W - z_2) + \delta(W + z_2)] +$$

$$+ \frac{1}{2}[\Theta(|\Gamma| - c_1)\,\Theta(c_2 - |\Gamma|]\,[\delta(W - z_2) + \delta(W + z_2)] \tag{47}$$

or, writing in detail and taking into account that we are only interested in the scalar gradient value, we obtain

$$P_\tau(W|\Gamma) = \Theta\left(\left(\frac{3}{2}\right)^{1/2}\exp\left(-\frac{\tau}{2\lambda^2}\right)\left(1 - \frac{2\delta}{\pi}\right) - |\Gamma|\right)\delta\left(W - \left(\frac{3}{2}\right)^{1/2}\frac{2}{\pi\lambda}\exp\left(-\frac{\tau}{2\lambda^2}\right)\right) +$$

$$+ \left[\Theta\left(|\Gamma| - \left(\frac{3}{2}\right)^{1/2}\exp\left(-\frac{\tau}{2\lambda^2}\right)\left(1 - \frac{2\delta}{\pi}\right)\right) - \Theta\left(\left(\frac{3}{2}\right)^{1/2}\exp\left(-\frac{\tau}{2\lambda^2}\right)\left(1 - \frac{\delta}{\pi}\right) - |\Gamma|\right)\right] \times$$

$$\times \left[\delta\left(W - \left(\frac{3}{\pi\delta}\right)^{1/2}\exp\left(-\frac{\tau}{2\lambda^2}\right)\frac{1}{\lambda}\left(1 - \frac{\delta}{\pi}\right)\left(1 - \frac{2\Gamma^2\exp\left(\frac{\tau}{\lambda^2}\right)}{3\left(1 - \frac{\delta}{\pi}\right)^2}\right)^{1/2}\right)\right]. \tag{48}$$

We now make use of formula (48) and calculate $\Sigma_\tau(\Gamma)$, whose value is given by formula (15). The expression for the surface area in the single-scale approximation, taking into account the formula for $P_\tau(W|\Gamma)$, upon integration with respect to W will take on the form

$$\Sigma_\tau(\Gamma,\lambda) = \frac{1}{\lambda}\left(\frac{3}{2}\right)^{1/2}\frac{2}{\pi}\exp\left(-\frac{\tau}{2\lambda^2}\right)\exp\left(\frac{\tau}{\lambda^2}\right)\delta\left(\Gamma\exp\left(\frac{\tau}{\lambda^2}\right)-1\right)\times$$

$$\times\Theta\left(\left(\frac{3}{2}\right)^{1/2}\exp\left(-\frac{\tau}{2\lambda^2}\right)\left(1-\frac{2\delta}{\pi}\right)-|\Gamma|\right)+\frac{1}{\lambda}\left(\frac{3}{\pi\delta}\right)^{1/2}\exp\left(-\frac{\tau}{2\lambda^2}\right)\times$$

$$\times\left(1-\frac{\delta}{\pi}\right)\left(1-\frac{2\Gamma^2\exp\left(\frac{\tau}{\lambda^2}\right)}{3\left(1-\frac{\delta}{\pi}\right)^2}\right)^{1/2}\exp\left(\frac{\tau}{\lambda^2}\right)\delta\left(\Gamma\exp\left(\frac{\tau}{\lambda^2}\right)-1\right)\times$$

$$\times\left[\Theta\left(|\Gamma|-\sqrt{\frac{3}{2}}\exp\left(-\frac{\tau}{2\lambda^2}\right)\left(1-\frac{2\delta}{\pi}\right)\right)-\Theta\left(\sqrt{\frac{3}{2}}\exp\left(-\frac{\tau}{2\lambda^2}\right)\left(1-\frac{\delta}{\pi}\right)-|\Gamma|\right)\right]. \tag{49}$$

As in deriving the multiscale model for the initial stage of evolution, we turn to the multiscale model by averaging $\Sigma_\tau(\Gamma,\lambda)$ over the scales of length λ with weight $P(\lambda)$ given by formula (20):

$$\Sigma_\tau(\Gamma) = \int_0^\infty \Sigma_\tau(\Gamma,\lambda)\,P(\lambda)\,d\lambda = 2\int_0^\infty \exp\left(\frac{\tau}{2\lambda^2}-\lambda^2\right)\frac{\sqrt{6}}{\pi}\,\Theta\left(\left(\frac{3}{2}\right)^{1/2}\exp\left(-\frac{\tau}{2\lambda^2}\right)\left(1-\frac{2\delta}{\pi}\right)-|\Gamma|\right)\times$$

$$\times\delta\left(\Gamma\exp\left(-\frac{\tau}{\lambda^2}\right)-1\right)d\lambda+2\int_0^\infty\exp\left(\frac{\tau}{2\lambda^2}-\lambda^2\right)\left(\frac{3}{\pi\delta}\right)^{1/2}\left(1-\frac{\delta}{\pi}\right)\left(1-\frac{2\Gamma^2\exp\left(\frac{\tau}{\lambda^2}\right)}{3\left(1-\frac{\delta}{\pi}\right)^2}\right)^{1/2}\times$$

$$\times\delta\left(\Gamma\exp\left(\frac{\tau}{\lambda^2}\right)-1\right)\left[\Theta\left(|\Gamma|-\left(\frac{3}{2}\right)^{1/2}\exp\left(-\frac{\tau}{2\lambda^2}\right)\left(1-\frac{2\delta}{\pi}\right)\right)-\Theta\left(\left(\frac{3}{2}\right)^{1/2}\exp\left(-\frac{\tau}{2\lambda^2}\right)\left(1-\frac{\delta}{\pi}\right)-|\Gamma|\right)\right]. \tag{50}$$

We make use of the fact that the integrands in (50) contain Dirac δ-functions and realize integration with respect to the variable λ, taking into account thereby (22)–(31). For $\Sigma_\tau(\Gamma)$ we obtain

$$\Sigma_\tau(\Gamma) = 2\frac{1}{\Gamma^{1/2}}\exp\left(-\frac{\tau}{|\ln\Gamma|}\right)\frac{\sqrt{6}}{\pi}\,\Theta\left(\left(\frac{3}{2}\right)^{1/2}\left(1-\frac{2\delta}{\pi}\right)\Gamma^{1/2}-|\Gamma|\right)\frac{\tau^{1/2}}{2|\ln\Gamma|^{3/2}}+$$

$$+2\frac{1}{\Gamma^{1/2}}\exp\left(-\frac{\tau}{|\ln\Gamma|}\right)\left(\frac{3}{\pi\delta}\right)^{1/2}\left(1-\frac{\delta}{\pi}\right)\left(1-\frac{2|\Gamma|}{3\left(1-\frac{\delta}{\pi}\right)^2}\right)^{1/2}\frac{\tau^{1/2}}{2|\ln\Gamma|^{3/2}}\times$$

$$\times\left[\Theta\left(|\Gamma|-\left(\frac{3}{2}\right)^{1/2}\Gamma^{1/2}\left(1-\frac{2\delta}{\pi}\right)\right)-\Theta\left(\left(\frac{3}{2}\right)^{1/2}\Gamma^{1/2}\left(1-\frac{\delta}{\pi}\right)-|\Gamma|\right)\right]. \quad (51)$$

Thus, the expression for the specific area of the isoscalar surface at the intermediate stage of evolution, where the scalar-field dispersion constitutes 20% of its initial value, is of the form

$$\Sigma_\tau^{(II)}(\Gamma)=\frac{\tau^{1/2}\exp\left(-\frac{\tau}{|\ln\Gamma|}\right)}{\Gamma^{1/2}\,|\ln\Gamma|^{3/2}}\times$$

$$\times\left[\frac{\sqrt{6}}{\pi}\Theta\left(\sqrt{\frac{3}{2}}\left(1-\frac{2\delta}{\pi}\right)-|\Gamma|^{1/2}\right)+\sqrt{\frac{3}{\pi\delta}}\left(1-\frac{2|\Gamma|}{3\left(1-\frac{\delta}{\pi}\right)^2}\right)^{1/2}\times\right.$$

$$\left.\times\left[\Theta\left(|\Gamma|^{1/2}-\sqrt{\frac{3}{2}}\left(1-\frac{2\delta}{\pi}\right)\right)-\Theta\left(\sqrt{\frac{3}{2}}\left(1-\frac{\delta}{\pi}\right)-|\Gamma|^{1/2}\right)\right]\right]. \quad (52)$$

3. Area of the Isoscalar Surface at the Final Stage of Evolution. In [14], which is devoted to the results of direct numerical simulation, it is shown that at the final stage of evolution, where the scalar-field dispersion is of the order of 5% of its initial value, the function describing the conditional scalar dissipation rate becomes parabolic again with a minimum at small values of fluctuations. A typical realization of the scalar field corresponding to such a situation is a curve slightly resembling a sinusoid but pointed so that the gradient maximum of this curve is realized at values close to the maximum value of the scalar field. As the analytical expression for such a realization, we can propose the following expression:

$$c_3(x,\tau)=N(n)\exp\left(-\frac{\tau}{2\lambda^2}\right)\left[\sin\left(\frac{x}{\lambda}\right)\right]^{2n+1}, \quad (53)$$

where n is an integer. If we choose $N(n)$ in the form

$$N(n)=\sqrt{\frac{(4n+2)\,!!}{2\,(4n+1)\,!!}}, \quad (54)$$

the dispersion of the scalar field (53) will be

$$\sigma_3(\tau)=\frac{1}{\sqrt{2}}\exp\left(-\frac{\tau}{2\lambda^2}\right). \quad (55)$$

The scalar-gradient field is described by the derivative of (53):

$$z_3(x,\tau)=\frac{(2n+1)\,N(n)}{\lambda}\exp\left(-\frac{\tau}{2\lambda^2}\right)\cos\left(\frac{x}{\lambda}\right)\left[\sin\left(\frac{x}{\lambda}\right)\right]^{2n}. \quad (56)$$

The maximum value of the scalar gradient is located close to the points with maximum values of the scalar field (see Fig. 4). Therefore, it is hoped that the conditional dissipation rate calculated from this typical realization will

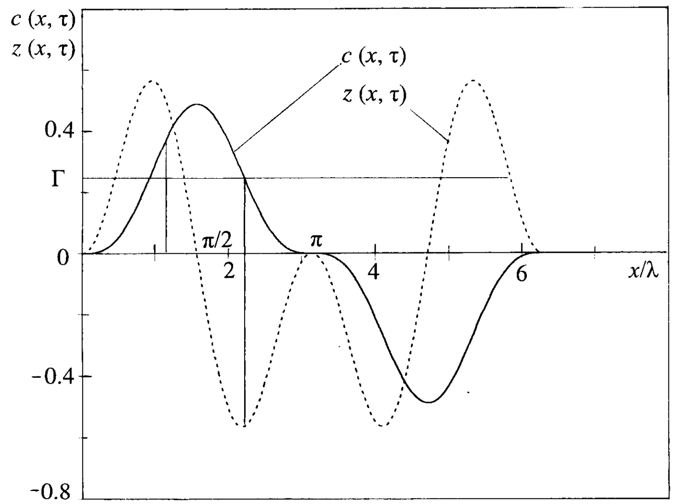

Fig. 4. Realization of the scalar field $c(x, \tau)$ and its gradient $z(x, \tau)$ at the final stage of evolution $\frac{\sigma(\tau)}{\sigma(0)} \approx 0.05$.

have the form of a parabola with a maximum value at large values of scalar fluctuations. Direct calculation corroborates this proposal [15].

From the dependence of the field $c_3(x, \tau)$ and its gradient $z_3(x, \tau)$ it is seen that at a given level of the scalar field $c_3(x, \tau) = \Gamma$ the field gradient can assume, in a half-period, two values equal in magnitude but opposite in sign:

$$W_i(\Gamma) = \pm \frac{(2n+1)}{\lambda} N(n) \exp\left(-\frac{\tau}{2\lambda^2}\right) \cos\varphi_i(\Gamma)\,[\sin\varphi_i(\Gamma)]^{2n}, \quad i = 1, 2\,. \tag{57}$$

The value of the angle $\varphi_1(\Gamma)$ can be calculated with the aid of formula (53). If we assume that $c(x/\lambda) = \Gamma$ and $\sin(x/\lambda) = \sin\varphi_1(\Gamma)$, then

$$\varphi_1(\Gamma) = \arcsin\left\{\left[\frac{\Gamma \exp\left(\frac{\tau}{2\lambda^2}\right)}{N(n)}\right]^{\frac{1}{2n+1}}\right\}. \tag{58}$$

For the conditional probability density of the scalar gradient, we can write

$$P_\tau(W|\Gamma) = \frac{1}{2}\,\Theta\left[1 - \left(\frac{\Gamma \exp\left(\frac{\tau}{2\lambda^2}\right)}{N(n)}\right)^{\frac{1}{2n+1}}\right][\delta(W - W_1(\Gamma))] + [\delta(W + W_1(\Gamma))]\,. \tag{59}$$

Taking into account formulas (58), the expression for $W_1(\Gamma)$ takes on the form

$$W_1(\Gamma) = \frac{2n+1}{\lambda} N(n) \exp\left(-\frac{\tau}{2\lambda^2}\right)\left[1 - \left(\frac{|\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)}{N(n)}\right)^{\frac{2}{2n+1}}\right]^{1/2}\left(\frac{|\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)}{N(n)}\right)^{\frac{2n}{2n+1}} \tag{60}$$

or, upon transformations,

$$W_1(\Gamma) = \frac{2n+1}{\lambda} N(n)^{\frac{1}{2n+1}} \exp\left(-\frac{\tau}{2\lambda^2(2n+1)}\right) |\Gamma|^{\frac{2n}{2n+1}} \left[1 - \frac{|\Gamma|^{\frac{2}{2n+1}} \exp\left(\frac{\tau}{\lambda^2(2n+1)}\right)}{N(n)^{\frac{2}{2n+1}}}\right]^{1/2} . \tag{61}$$

Since for calculating $\Sigma_\tau(\Gamma)$ only the value of the scalar gradient is important, instead of (59) we can propose the following expression:

$$P_\tau(W|\Gamma) = \Theta\left[1 - \left(\frac{|\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)}{N(n)}\right)^{\frac{1}{2n+1}}\right] [\delta(W - W_1(\Gamma))] , \tag{62}$$

where the expression for $W_1(\Gamma)$ is given by (61). Using the formula for the isoscalar surface area in the single-scale approximation, we obtain

$$\Sigma_\tau(\Gamma, \lambda) = \frac{1}{2} \Theta\left[1 - \left(\frac{|\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)}{N(n)}\right)^{\frac{1}{2n+1}}\right] \frac{2n+1}{\lambda} N(n)^{\frac{1}{2n+1}} \exp\left(-\frac{\tau}{2\lambda^2(2n+1)}\right) |\Gamma|^{\frac{2n}{2n+1}} \times$$

$$\times \left[1 - \frac{|\Gamma|^{\frac{2}{2n+1}} \exp\left(\frac{\tau}{\lambda^2(2n+1)}\right)}{N(n)^{\frac{2}{2n+1}}}\right]^{1/2} \exp\left(\frac{\tau}{2\lambda^2}\right) \delta\left[|\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right) - 1\right]. \tag{63}$$

We now turn to the writing of the multiscale model of $\Sigma_\tau(\Gamma)$ by using formula (20) for $P(\lambda)$:

$$\Sigma_\tau(\Gamma) = (2n+1) N(n)^{\frac{1}{2n+1}} \int_0^\infty \exp\left(-\lambda^2 - \frac{\tau}{2\lambda^2(2n+1)}\right) |\Gamma|^{\frac{2n}{2n+1}} \left[1 - \frac{|\Gamma|^{\frac{2n}{2n+1}} \exp\left(\frac{\tau}{\lambda^2(2n+1)}\right)}{N(n)^{\frac{2}{2n+1}}}\right]^{1/2} \times$$

$$\times \exp\left(\frac{\tau}{2\lambda^2}\right) \delta\left[|\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right) - 1\right] \Theta\left[1 - \left(\frac{|\Gamma| \exp\left(\frac{\tau}{2\lambda^2}\right)}{N(n)}\right)^{\frac{1}{2n+1}}\right] d\lambda . \tag{64}$$

Taking into account the presence in the integrand of the Dirac δ-function and formulas (22)–(31), upon integration with respect to λ, we obtain the expression for $\Sigma_\tau(\Gamma)$:

$$\Sigma_\tau^{(\mathrm{III})}(\Gamma) = (2n+1) N(n)^{\frac{1}{2n+1}} \exp\left(-\frac{\tau}{|\ln|\Gamma||}\right) |\Gamma|^{-\frac{n}{2n+1} + \frac{2n}{2n+1}} \left[1 - \frac{|\Gamma|^{\frac{2}{2n+1}} |\Gamma|^{-\frac{1}{2n+1}}}{N(n)^{\frac{2}{2n+1}}}\right]^{1/2} \times$$

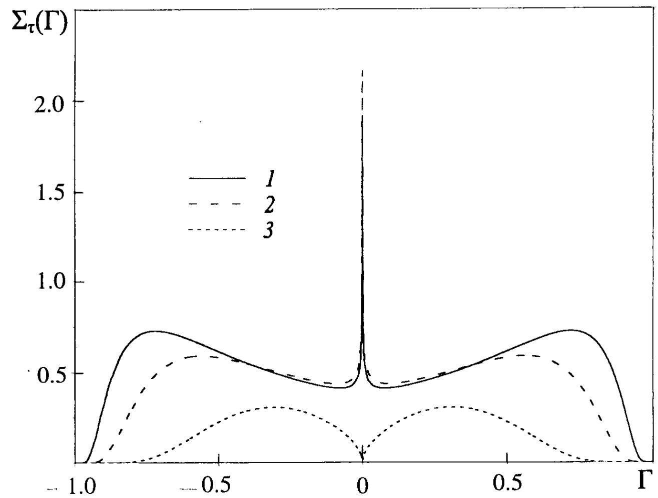

Fig. 5. Evolution of the specific area of the isoscalar surface $\Sigma_\tau(\Gamma)$ at different stages of the scalar-field development: 1) first model, $\tau_1 = 0.3$; 2) second model, $\tau_2 = 0.7$; 3) third model, $\tau_3 = 1.9$.

$$\times \frac{\tau^{1/2}}{2\,|\ln|\Gamma||^{3/2}}\,\Theta\left[1-\left(\frac{|\Gamma|}{N(n)}\frac{1}{|\Gamma|^{1/2}}\right)^{\frac{1}{2n+1}}\right]. \tag{65}$$

Thus, the expression for the specific area of the isoscalar surface at the final stage of evolution is of the form

$$\Sigma_\tau^{(\mathrm{III})}(\Gamma) = (2n+1)\,N(n)^{\frac{1}{2n+1}}\frac{\tau^{1/2}\exp\left(-\frac{\tau}{|\ln|\Gamma||}\right)|\Gamma|^{\frac{n}{2n+1}}}{|\ln|\Gamma||^{3/2}}\times$$

$$\times\left[1-\frac{|\Gamma|^{\frac{1}{2n+1}}}{N(n)^{\frac{2}{2n+1}}}\right]^{1/2}\Theta\left[1-\left(\frac{|\Gamma|^{1/2}}{N(n)}\right)^{\frac{1}{2n+1}}\right]. \tag{66}$$

Figure 5 shows the evolution of the specific area of the isoscalar surface at different stages of the scalar-field development. As mentioned above, to the initial stage there corresponds the model described in Section 1 for $\sigma(\tau)/\sigma(0) = 0.5$ and time $\tau_1 \approx 0.3$, to the intermediate stage – the model described in Section 2 for $\sigma(\tau)/\sigma(0) = 0.2$ and time $\tau_2 \approx 0.7$, and to the final stage – the model described in Section 3 for $\sigma(\tau)/\sigma(0) = 0.05$ and time $\tau_3 \approx 1.9$.

Conclusions. Comparing the form of the specific area of the isoscalar surface at the final stage of evolution obtained in the present paper with the results of the solution of the closed system of equations for this function obtained in [10], one can easily see the differences in the behavior of $\Sigma_\tau(\Gamma)$ at small values of Γ. As seen from formula (15), the function $\Sigma_\tau(\Gamma)$ is a result of the convolution of two functions: $P_\tau(W|\Gamma)$ and $f_\tau(\Gamma)$, i.e., $\Sigma_\tau(\Gamma \sim P_\tau(W|\Gamma)\,f_\tau(\Gamma)$. The sharpening of the $\Sigma_\tau(\Gamma)$ form in the course of the scalar-field evolution is due to the sharpening of the single-point FPD $f_\tau(\Gamma)$. This tendency is seen from Fig. 5. However, as shown in [14, 15], at the final stage of the scalar-field evolution the behavior of the first factor in (15) becomes determining, since $P_\tau(W|\Gamma) \to 0$ at $\Gamma = 0$. As a result, $\Sigma_\tau(\Gamma)$ tends to zero at $\Gamma = 0$. This feature was not revealed in [10]. This work was supported by the INTAS (project 001-353).

NOTATION

$\Sigma_\tau(\Gamma)$, area of the flame surface; Q, heat release rate per unit area of the flame; Δh_τ, enthalpy; D, diffusion coefficient; l, characteristic scale of length; τ, time; λ, scale of spatial inhomogeneity of L, $\lambda = L/l$; x, dimensionless distance on the OX axis, $x = X/l$; $P_\tau(W|\Gamma)$, conditional probability density of the scalar gradient value; $f_\tau(\Gamma)$, single-point probability density of the scalar-field values; $f_\tau(\Gamma, \lambda)$, single-point probability distribution function of the values of scalar fluctuations; $P(\lambda)$, distribution of length scales; $\sigma(\tau)$, scalar-field dispersion.

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