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Many-length scale fractal model for turbulent mixing of reactants

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Abstract

The expression for the probability density function of scalar field pulsation values is derived taking into account the fractal and multiscales structure of turbulence. The evolution of this function was stated by the detailed structure of the probability distribution of length scales of a scalar turbulent field. The expression for the latter has been found using the fractal character of the surfaces separated the regions with the different scalar concentrations in turbulent flows. Analytical expressions for the conditional dissipation rate of scalar fluctuations were proposed using the hypothesis on typical realisations of a scalar turbulent field which were different at various evolution stages. It is possible to consider these expressions as an attempt to explain a sufficiently complicated transformation of the form of conditional dissipation, which were obtained by direct numerical simulation of a turbulent scalar field. The obtained analytical expressions for a conditional dissipation rate can be useful to study the turbulent combustion process in the framework of the laminar diffusion flamelet models.

1. Introduction

When the processes of turbulent mixing of scalar fields, including reacting ones, is described, it is often possible to confine the investigation to the probability density function (PDF) of one scalar quantity $f_t(c)$ [1]. The scalar field c in this case can mean some variables like the Shvab–Zeldovich function used to examine turbulent flows with non-premixed reactants [2] or the progress variable adopted to describe turbulent flows with premixed reactants [3].

For the expression for the function $f_t(c)$ to be derived it is very important to take into account the many-length scale character of the turbulent mixing process [4]. When studying the turbulent mixing of scalar fields, it is easy at a qualitative level to distinguish two aspects of the process, that is the dynamics of length scales and the dynamics of the fluctuation intensity of this field. Consider, for instance, mixing of the scalar field in the isotropic turbulent flow. When in the gas or liquid grid flow some other grid generates the scalar fluctuation field, then the evolution of this scalar field is a rather good example of turbulent mixing. The scalar field near the second grid mainly has only two values: zero and unity, in accordance with the condition of full unmixedness at the molecular level. The typical length scale of unmixed gas volumes is specified by introducing this scalar field into the flow. Different values of this field appear downstream, and at the same time there occurs the whole spectrum of length scales. It is clear that these two aspects of turbulent mixing permanently interact. The evolution of the length scale spectrum creates a steadily varying condition for the effect of molecular diffusion, thereby influencing the dissipation rate of

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Nomenclature

f	the deviation of fractal from topological dimension
$f_t(c)$	probability density function of scalar field
$f_t(c, \lambda)$	one-length scale probability density function of scalar field
$P(\lambda)$	distribution scale of the turbulent length scales
$P(\tau)$	distribution of time scales
Re	Reynolds number
S_T	the area of the surface separating the regions with different scalar concentrations in developed turbulent flow
S_λ	the area of the surface measured with the resolution $\lambda > \eta$

Greek symbols

η	Kolmogorov length scale
$\Theta(\lambda)$	Heaviside function
$\chi(t\|c)$	scalar conditional dissipation rate

scalar field fluctuation intensity. The different parts of the length scale spectrum effect the dissipation rate of the fluctuation intensity in a different way. From physical consideration it is seen that small length scales more strongly influence the structure of the value spectrum. All these effects are different for different fluctuation values and for different parts of the length scale spectrum. These complex dynamics must is some way be taken into consideration in developing the theoretical model of turbulent mixing of reactants.

To describe the turbulent mixing process, use is usually made of the one-point probability function of scalar field fluctuation. However, the presence of the spectrum of length scales is, as a rule, ignored. The state of the scalar field in this relation is taken into account in terms of some average length scale or average dissipation rate of the fluctuation intensity. It is likely, that just the disregard of many scale characters of turbulent mixing is responsible for the absence of quite a satisfactory closed system of equations for the process.

The many-length scale character of turbulent mixing is closely related with the many-time scales character of a turbulent reacting scalar field. As it is shown in [5], the taking into consideration of the distribution of time scales is very important for studying turbulent diffusion flame with kinetic effects.

The many-length scale character of turbulent mixing is closely connected with the fractal property of the turbulent velocity and scalar field [6]. Therefore, any mixing model of scalar fields has to take into consideration the fractal dimensions of surfaces in turbulent flows.

The goal of this work is to demonstrate how it is possible to get the expression for the PDF of the scalar field with the use of the many-length scale and the fractal character of turbulence and to estimate the quantitative difference between the usual and fractal approaches to the mixing problem.

2. Distribution of turbulent length scales

The expression for the PDF $f_t(c)$ was obtained by the next procedure. First, an expression is written for the one-length scale PDF $f_t(c, \lambda)$ which is the solution of the one-length scale mixing model [4]. The function $f_t(c, \lambda)$ then has to be averaged over the distribution of the turbulent length scale $P(\lambda)$. As a result the expression is obtained for the PDF $f_t(c)$ which has to be correct for the many-length scale turbulent flow.

$$f_t(c) = \int f_t(c, \lambda) P(\lambda)\, d\lambda \tag{1}$$

The physical meaning of the function $P(\lambda)$ consists of the probability of the presence of the pieces of the interface λ in size in the turbulent scalar field. This interface separates the regions with different scalar concentration. In Ref. [4] for this purpose to be implemented the function $P_t^c(\lambda)$ was proposed. This function was defined so that the following quality was warranted

$$\langle c^2(t)\rangle = \int_0^\infty P_t^c(\lambda)\, d\lambda$$

where $\langle c^2(t)\rangle$ is the dispersion of the turbulent scalar field. After the normalisation this function could be interpreted as the probability density function of length scale values. However, the role of the function P_λ may more appropriately be played by the function immediately related with the interface distribution over different length scales.

If in accordance with the results of [6] the surface separating the regions with different scalar concentration in developed turbulent flows is assumed to be fractal, then the area of this surface S_T per unit of fluid volume with the Schmidt number $S_c = 1$, may be found by the formula

$$S_T = S_0(\eta/L)^{-f} \tag{2}$$

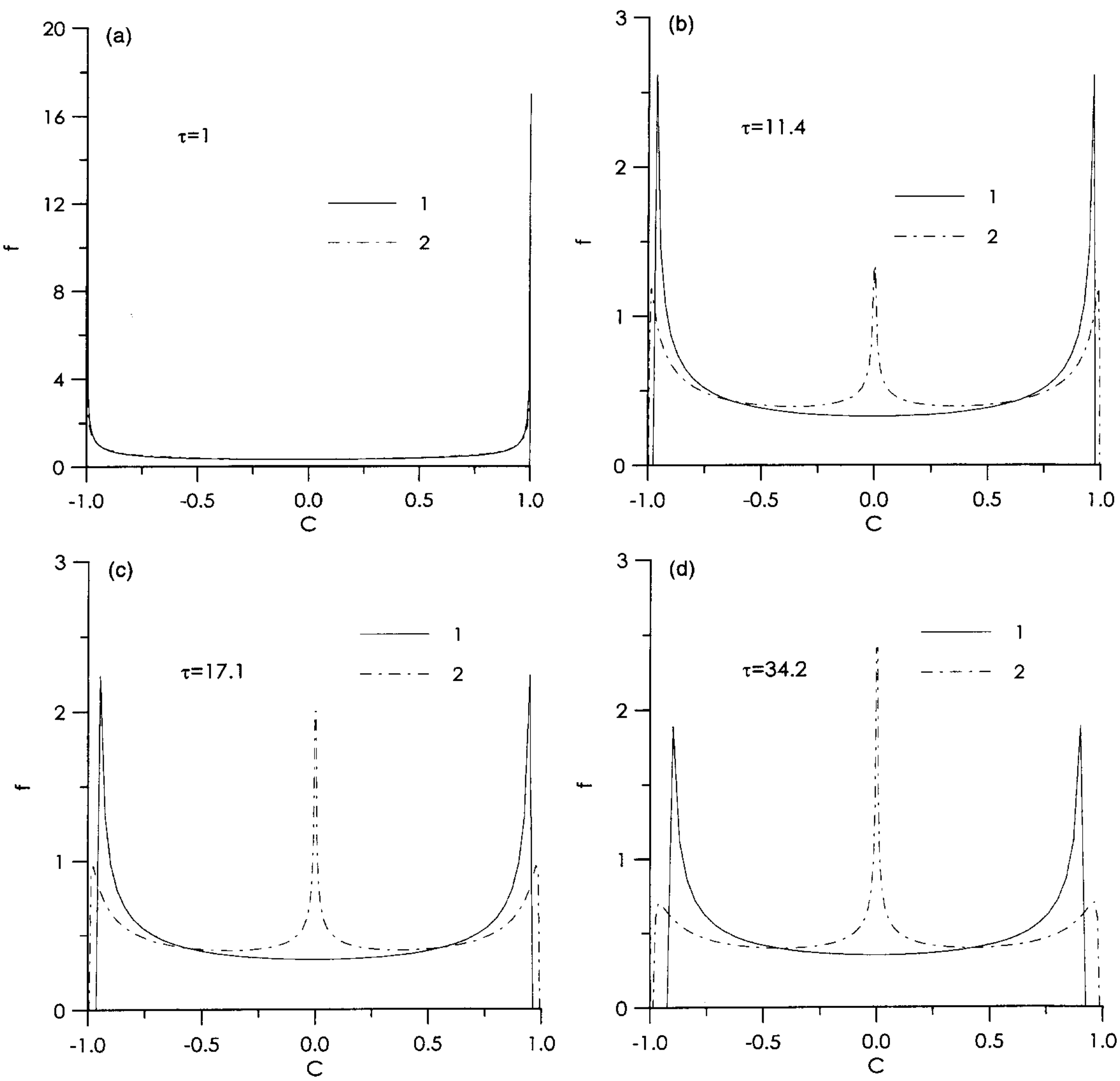

Fig. 1. Form of PDF in accordance with one-scale (1) and many-scale (2) models.

Here S_0 is the surface area measured with resolution L, L being the macroscale of the length, η being the Kolmogorov length scale, $f = D - 2$ is the deviation of fractal from topological dimensions which is equal to two.

The estimates [6] and the straightforward measurements of fractal dimensions of surfaces in different turbulent flows make it possible to assume that the value of D is equal to 2.35. Therefore,

$$f = D - 2 = 0.35 \tag{3}$$

The area of the interface measured with the resolution $\lambda > \eta$ is defined by the formula

$$S_\lambda = S_0(\lambda/L)^{-f} \tag{4}$$

As the hypothesis for the function $P(\lambda)$ to be calculated, the following formula can be used

$$P(\lambda) \sim P(S_\lambda) \sim (\lambda/L)^{-f} \tag{5}$$

Such a hypothesis leads to a plausible dependence of the probability of length scales on the fractal exponent f. The larger the fractal exponent f, the more compactly the surface is embedded in the volume of the fluid, and the smaller the length scale λ, which separated the regions with different concentrations of the scalar field, are more probable. The absence of fractality, $f = 0$, reduces the distribution of length scales to be uniform.

The function $P(\lambda)$ has to be normalised to unity under integration over all length scales λ from the point of $\lambda=0$ to the point of $\lambda=L$. The normalised function $P(\lambda)$ has the form

$$P(\lambda)=\begin{cases}\dfrac{(1-f)\lambda^{-f}}{L^{1-f}[1-(\eta/L)^{1-f}]}, & \text{if } \eta<\lambda<L\\ 0, & \text{if } \lambda<\eta,\ \lambda>L\end{cases} \quad (6)$$

For developed turbulent flow with a large Reynolds number $Re=u'L/\nu$ (u' is the rms value of turbulence fluctuations, ν is the kinematic viscosity coefficient) there exist the relation between Kolmogorov's length scale η and the macroscale L [7].

$$\eta/L=Re^{-3/4} \quad (7)$$

The formula for $P(\lambda)$ in this case has the form

$$P(\bar{\lambda})=(1-f)\bar{\lambda}^{-f}[\Theta(\bar{\lambda}-1)-\Theta(\bar{\lambda}-Re^{-3/4})]$$
$$\times(Re^{-3/4(1-f)}-1)^{-1} \quad (8)$$

with the notation $\bar{\lambda}=\lambda/\eta$ used, Θ being the Heaviside function.

Let us note that formula (6) may also be used to calculate $P(\lambda)$ in non-developed unsteady turbulent flow. In this case, the length scales $L(t)$ and $\eta(t)$ must be calculated from some closed system of the equations like the k–ϵ model or from the closed equation for the length scale energy distribution $P_t(\lambda)$ [8].

3. Many-length scale probability function

In Ref. [4] the expression for the PDF $f_t(c,\lambda)$ was derived for the one-length scale of the scalar field. This function, in dimensionless variables ($\hat{c}=c/a$, $\tau=3tD/\eta^2$ where a is the maximal value of scalar concentration and D is the coefficient of molecular diffusion) has the form

$$f_\tau(c,\lambda)=e^{\tau/\lambda^2}f_0(\hat{c}\,e^{\tau/\lambda^2}) \quad (9)$$

where $f_0(\hat{c})$ is the initial form of PDF. Expression (9) coincides with the one for PDF which may be obtained by the mean square estimation theory of the conditional expected value $E(c'|c)$ [9]. The defect of this closure had been discussed [1] and alternative approximations were suggested [10]. The derivation of this form for the PDF, which was done in [4], points clearly to the one-length scale character of this model. If expression (9) is substituted into (1), then the following formula can be obtained

$$f_\tau(\hat{c})=\int e^{\tau/\lambda^2}f_0(c\,e^{\tau/\lambda^2})P(\lambda)\,d\lambda \quad (10)$$

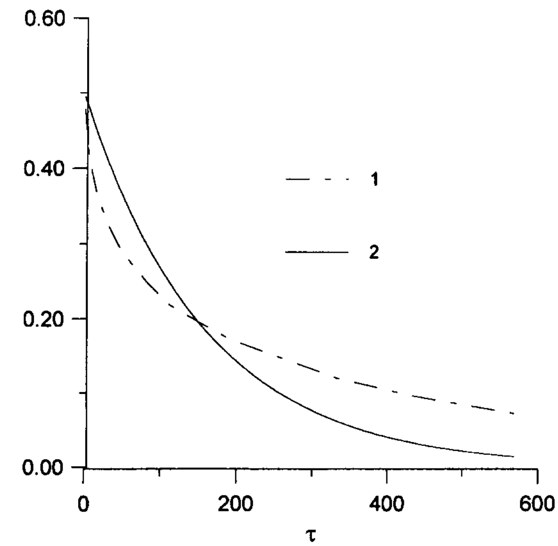

Fig. 2. Evolution of dispersion of scalar fluctuation in the case of taking the fractality into consideration (1) and without it (2).

Let us choose the initial PDF $f_0(\hat{c})$ as corresponding to the sine form of the concentration field. The solution of the one-length model (9) conserves this unchanged forever. After taking many-length scales into account, in accidence with (10), this solution essentially changes. If $P(\lambda)$ form (8) is chosen, which corresponds to developed turbulence, then we will get the following expression for $f_\tau(\hat{c})$

$$f_\tau(\hat{c})=(1-f)\pi^{-1}[Re^{-3/4(1-f)}-1]^{-1}\int_1^{Re^{-3/4}}\lambda^{-f}$$
$$e^{\tau/2\lambda^2}\Theta[1-|c|\,e^{\tau/2\lambda^2}][1-c^2\,e^{\tau/2\lambda^2}]^{-1}\,d\lambda \quad (11)$$

The bracketed expression in formula (11) defines the region of non-zero values of the function $f_\tau(\hat{c})$. This expression for the PDF $f_\tau(\hat{c})$ describes the turbulent mixing process of the scalar field, starting with segregated conditions of the scalar field up to the terminal conditions in the form of $f_\tau(\hat{c})=\delta(\hat{c})$.

In the latter case the entire mixture becomes mixed up to the molecular level. As is seen from Fig. 1a–d, the many length scale model reflects the turbulent mixing process more realistically than a one-length scale model, demonstrating all values of concentrations at intermediate times of evolution.

The bimodal form of the PDF reflects the possibility of the simultaneous presence of the fresh unmixed regions and mixtures mixed up to molecular level in the flow. Such a form qualitatively corresponds to the experimental data [2] and results of the calculation of

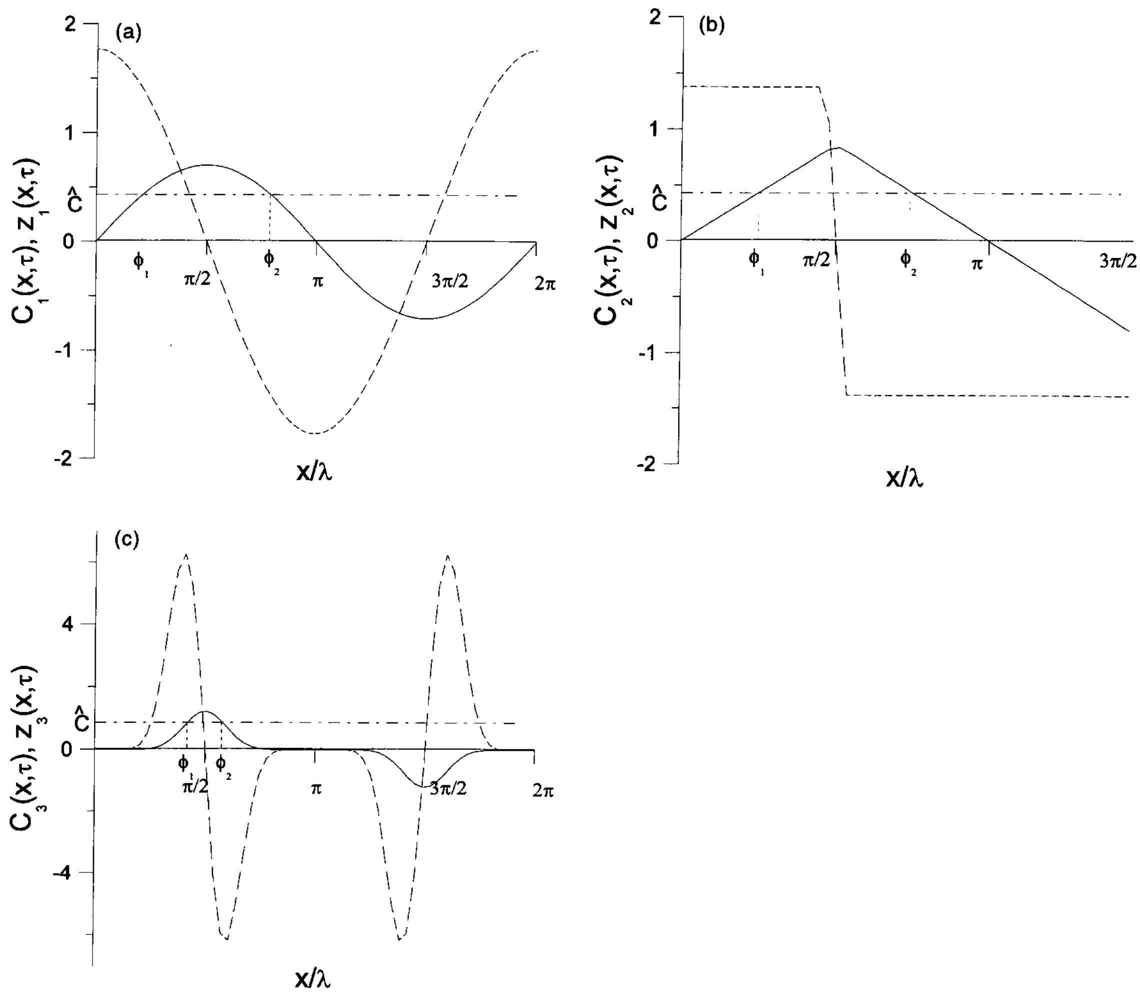

Fig. 3. Typical realisation of scalar field and its gradient. Initial stage of evolution. (b) Typical realisation of scalar field and its gradient. Intermediate stage of evolution. (c) Typical realisation of scalar field and its gradient. Developed stage of evolution.

PDF by the linear eddy mixing model [11], when wide-band length scale distribution is used.

The significance of taking into account the fractality of the turbulent field for calculation of the turbulent mixing rate can be evaluated by comparing the evolution of the intensity of the turbulent scalar field of fluctuations predicted by the formula

$$\sigma = \langle c^2(\tau)\rangle = \int \hat{c}^2 f_\tau(\hat{c})\, d\hat{c} \tag{12}$$

with $f_\tau(\hat{c})$ in the form (11) at the values of the fractal exponent $f = 0$ and $f = 0.35$.

As is seen from Fig. 2 the account of the fractality brings a noticeable difference in the rate of scalar intensity dissipation, especially during the initial period of mixing. It is clear that for the chemical reaction rate to be calculated taking into account the fractality may appear to be more essential as yet.

As mentioned above, the many-length scale distribution is associated with the many-time scale character of the turbulent reacting scalar field [5]. If length scale λ is the thickness of the interface in the turbulent scalar field, then the characteristic time scale of molecular diffusion on this scale has to be [7]

$$\tau = \lambda^2 \tag{13}$$

Hence, the distribution of time scales related with length scales distribution (8) has the form

$$P(\tau) = (1-f)\tau^{-1/2(1+f)}[\Theta(\tau-1) - \Theta(\tau - Re^{3/2})] \times (2\,Re^{3/4(1-f)} - 1)^{-1} \tag{14}$$

This distribution of the time scale is connected with the fractal structure of turbulent surfaces.

Let us emphasise that the present method makes it possible to calculate the one-point PDF depending on the fluctuation length scale whose influence should be allowed for.

4. Scalar conditional dissipation rate

One of the most important characteristics of the turbulent flow necessary for different theoretical descriptions of turbulent combustion is the scalar condition dissipation rate $\chi(\tau|\hat{c})$ [12]. This function was obtained in [13] as a result of direct numerical simulations of evolution of a turbulent scalar field. It was shown that during evolution the form of this function underwent essential changes, from the parabolic form with a maximum under small fluctuations to the form independent on the value of the latter, then again to the parabolic form but with a minimum under small fluctuations. Such a behaviour of conditional dissipation is verified by experimental study of this function in different turbulent flows [14]. The proposed analytical models for this function do not reflect its ability to transform its form essentially in the process of evolution [15].

It seems plausible to assume that such a complicated transformation of conditional dissipation is related with a change of typical modes of a scalar field in turbulent flow. If it is assumed that the typical modes of a scalar field evolve from a sine-shaped form responsible for the beginning of turbulent mixing through a saw-tooth form to a sharp form of scalar fluctuations, then these modes of scalar field will be consistent with different forms of scalar gradients, hence, with different forms of conditional dissipation (Fig. 3a–c).

Rather simple calculations performed for every case separately result in the following analytical expression for conditional dissipation

$$\chi_1(\tau,\lambda \mid \hat{c}) = \Theta(1-\mid c\mid)\frac{1}{\lambda^2}e^{-\tau/\lambda^2}(1-c^2) \tag{15}$$

Here and later on

$$c = \hat{c}\, e^{\tau/\lambda^2} \tag{16}$$

$$\chi_2(\tau,\lambda \mid \hat{c}) = \Theta(c_1-\mid c\mid)\frac{6}{\pi^2\lambda^2}e^{-\tau/\lambda^2} + [\Theta(\mid c\mid - c_1) - \Theta(\mid c\mid - c_2)]\left(1-\frac{\delta}{\pi}\right)^2\frac{3}{\pi\lambda^2\delta}e^{-\tau/\lambda^2} \times \left[1-\frac{2\hat{c}}{3(1-\delta/\pi)^2}\right] \tag{17}$$

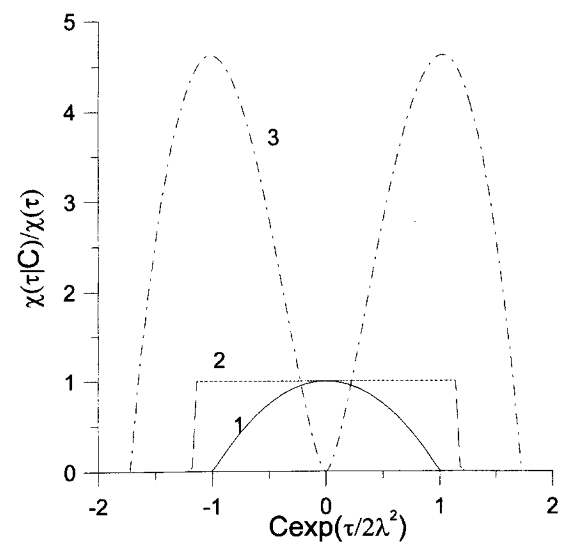

Fig. 4. Conditional dissipation rate for one-length scale model. 1. According to (15), 2. according to (17), 3. according to (19).

where

$$c_1 = \sqrt{\frac{3}{2}}\left(1-2\frac{\delta}{\pi}\right),\quad c_2 = \sqrt{\frac{3}{2}}\left(1-\frac{\delta}{\pi}\right),\quad \delta\to 0 \tag{18}$$

$$\chi_3(\tau,\lambda \mid \hat{c}) = \Theta\left[1-\frac{\mid c\mid}{N}\right]\frac{(2n+1)^2}{\lambda^2}N^2 e^{-\tau/(2\lambda^2)} \times \left(\frac{c}{N}\right)^{2n/(2n+1)}\left[1-\frac{(\mid c\mid)^{2/(2n+1)}}{N}\right] \tag{19}$$

Here

$$N = \sqrt{\frac{(4n+2)!!}{2(4n+1)!!}} \tag{20}$$

The parameter n must be chosen rather large ($n \approx 10$).

The Heaviside function $\Theta(x)$ defines the domain of the existence of the functions $\chi_i(\tau,\lambda|\hat{c})$. The parameter λ determines the length scale of a scalar field.

With typical realisation as in Fig. 3a, when the values of scalar fluctuations are small, the gradient (hence, the dissipation rate) has a maximum, and vice versa, the gradient is small when the values of scalar fluctuations are large. This results in a parabolic form of conditional dissipation (15) (curve 1 in Fig. 4).

As demonstrated in Fig. 3b, the gradient value remains invariable for any values of scalar fluctuations. The dissipation rate does not change either. At the points where the scalar field has a maximum the gradient is equal to zero. Therefore, the dissipation rate in these points tends to zero (17) (curve 2 in Fig. 4).

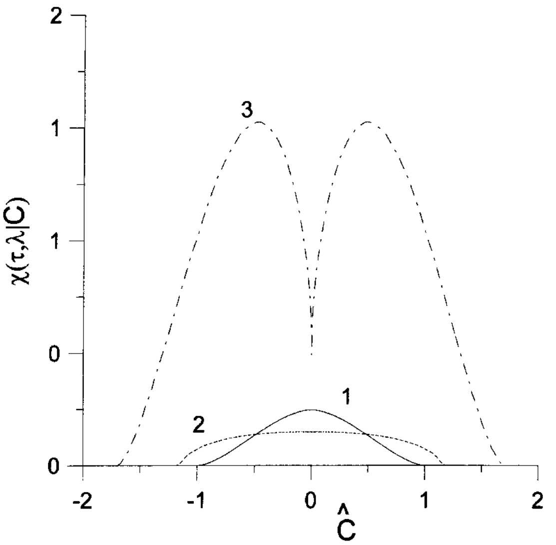

Fig. 5. Conditional dissipation rate for many-length scale model.

With typical realisation as in Fig. 3c, the gradient maximum is seen at values of the scalar field large enough. When the values of scalar fluctuations are small the gradient values are small as well. The behaviour of the inner part of the conditional dissipation curve is just associated with this. At the maximum values of the scalar field the gradient passes through zero, thus decreasing the dissipation rate under maximum scalar fluctuations. With this in view, the branches of curve 3 in Fig. 4 descend.

The obtained expressions for the scalar conditional dissipation rate are said to be a one-length scale model for this function because typical realisations only with a one-length scale were used for deriving these expressions. It is possible to obtain more realistic expressions for conditional dissipation by averaging expressions (15), (17) and (19) over the probability distribution of length scales $P(\lambda)$ defined by formula (8)

$$\chi_i(\tau, \hat{c}) = \int_\lambda \chi_i(\tau, \lambda \mid \hat{c}) P(\lambda)\, \mathrm{d}\lambda, \quad i = 1, 2, 3 \tag{21}$$

The forms of conditional dissipation calculated by this formula for three examined stages of evolution of a scalar field are demonstrated in Fig. 5. As seen from comparison of Figs. 4 and 5, account of many scales does not radically change conditional dissipation. It is possible that the influence of many scales manifests itself in the transformation rate of the forms of the function.

5. Conclusions

An expression for the one-point probability density function of scalar turbulent field $f_\tau(c)$ was derived using the concept about the many-length scale characters of the turbulent mixing process. The evolution of this function was stated by the detailed structure of the probability distribution of length scales of the scalar turbulent field $P(\lambda)$. The expression for the function $P(\lambda)$ has been found using the fractal character of the surfaces separated by the regions with the different scalar concentrations in turbulent flows. The many-length scale model of PDF can be of practical importance for describing the essentially non-Gaussian situation demonstrating the two-modal form of this function.

Analytical expressions for the conditional dissipation rate of scalar fluctuations were proposed using the hypothesis on typical realisations of a scalar turbulent field which were different at various evolution stages. It is possible to consider these expressions as an attempt to explain a sufficiently complicated transformation of the form of conditional dissipation, which were obtained by direct numerical simulation of a turbulent scalar field [13]. The obtained analytical expressions for a conditional dissipation rate can be useful to study the turbulent combustion process in the framework of the laminar diffusion flamelet models.

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