Short communications

PROBABILITY DENSITY FUNCTION OF SCALAR LENGTH SCALES IN TURBULENT FLOW

ABSTRACT

In this Brief Communication scalar length-scale and time-scale distributions are determined by considering the statistics of the scalar field and its gradient. For this purpose, a relationship between the scalar length-scale probability density function and the joint probability density function for the scalar field and its gradient in the form of the integral relation is established.

Keywords: turbulent flow; scalar; dissipation rate; length scale; probability density function

Statistical approaches, among which is the method based on probability density functions (PDFs), find wide use for solving a variety of problems on complex turbulent flows [1]. It is known that as compared to other methods, the PDF method allows one to describe the influence of turbulent fluctuations on the mixing intensity of scalar fields of temperature or concentration and then to take into account more accurately this influence on chemical processes in reacting flows [2].

The study of turbulent mixing of reacting flows by the PDF method is based on three major approaches. First, mixing is represented in terms of the decay rate of the scalar variance – the scalar dissipation rate. It characterizes mixing of reagents and chemical reaction rate. Second, scalar fields are being investigated with regard to the dynamics and topology of isoscalar surfaces. Third, statistical properties of scalar fields are analyzed by calculating correlation quantities [3].

In the existing mixing models using the above-mentioned approaches, the problem on accounting of the spatial structure of turbulent flows still remains a stumbling block. The existence of different values of scalar length scale provides a basis for different manifestations of turbulent transfer. Evolution of length scales makes the boundary conditions for molecular diffusion vary constantly and affects a decay rate of the scalar variance. In this case, the structure of the scalar fluctuation field depends to a greater extent on small scales that immediately influence the scalar dissipation rate, but not on large scales.

Usually, the equation or the presumed form of one-point scalar PDF is adopted to describe turbulent mixing [1-3]. Unfortunately, the one-point statistics of scalar fields does not supply information on a turbulent scale spectrum. In the one-point models, this information is taken into account empirically or ignored. The models operating with multipoint statistics do not face this task, but as for their realization, they are much more complex and hence are in less use [4].

The key problem of the PDF method is the necessity to model a contribution of fine-grained mixing (micromixing) of a scalar field to the general structure of mixing. Micromixing proceeds by the mechanism of interaction between turbulent fluctuation transfer and molecular diffusion due to small-scale flow motions.

A subsequent approach to solving this problem uses the joint statistics of the scalar field and its gradient that carries information on the microstructure of the scalar field itself [1-2]. Turbulent length and time scales, as a rule, can be obtained from the statistics of fluctuations of the velocity and its gradient. This is not always adequate for a scalar fluctuation field, since relevant Schmidt numbers can differ essentially from unity where the Schmidt number is defined as the ratio of viscosity to scalar diffusivity. In the case of the one-point models, joint statistics of the scalar field and its gradient permits a direct determination of distributions of length and time scales of scalar fluctuations. The scalar gradients are responsible for the diffusion effects and define scalar dissipation rates in turbulent mixing [1-2]. In turn, in theory of combustion, such characteristics of a turbulent flame as flame propagation velocity and combustion completeness depend on the scalar dissipation rate [3, 5].

The problem of determining the typical length and time scales at turbulent mixing still remains necessary, but unsolved up to now [2]. The Direct Numerical Simulation (DNS) shows an essentially non-Gaussian two-mode form of the one-point scalar PDF at intermediate mixing stages [6]. That is why, the structure of the one-point scalar PDF should be specified through all details of the scalar field, but not only through its averaged characteristics: averaged scalar, dispersion, averaged time scale or averaged scalar dissipation rate.

Sosinovich *et al.* [7] obtained the expression for the length scale PDF with regard to the fractal character of surfaces subdivided by different-concentration regions in the turbulent flow. It has also been invoked to derive analytical relations for conditional scalar dissipation rate and surface density function using the hypothesis of typical implementation of a scalar turbulent field at different mixing stages [7-8].

The multi-scale character of turbulent mixing is closely connected with time scale distributions in turbulent flows. Dopazo *et al.* [9] studied the distributions of typical time scales by the DNS for scalar mixing. In studying diffusion flames with kinetic effects it was shown that the regard to time scale distributions is important and the model for an averaged reaction rate uses the presumed time scale PDF [10].

The objective of this Brief Communication is to determine length-scale and time-scale distributions considering the statistics of the scalar field and its gradient and to establish a relationship between the scalar length-scale PDF and the joint PDF for the scalar field and its gradient in the form of the integral relation.

For this objective to be achieved, let's consider turbulent mixing of a dynamically passive scalar field [11]. For modeling purposes, common practice is based on the statistics of two quantities: a conserved scalar C representing a mixture fraction, or inert impurity concentration, and a norm of its gradient $|\nabla C|$ related to the dissipation rate of scalar fluctuations $c = C - \bar{C}$ in the turbulent flow where the overbar indicates the Reynolds averaging operator [1, 2, 3, 5]. In this case, the scalar field behavior is governed by the well-known convection-diffusion equation [2-3]. Let's consider statistically homogeneous velocity and scalar fields. The disappearance of heterogeneities in the turbulent flow then follows from the dynamics of velocity and scalar fluctuations u_i and c (henceforth c is referred to as the scalar). For this case the scalar transport equation in non-dimensional form is valid:

$$\frac{\partial c}{\partial t} + \frac{\partial (u_i c)}{\partial x_i} = \frac{1}{\mathrm{Pe}} \frac{\partial^2 c}{\partial x_i^2}. \qquad (1)$$

Here the dimensional variables are non-dimensionalised as $c = \hat{c} / c_0$, $u_i = \hat{u}_i / u_0$, $x_i = \hat{x}_i / l_0$, $t = \hat{t} u_0 / l_0$ where l_0, u_0, c_0 are the dimensional reference quantities of length, velocity and scalar. The hat denotes the dimensional term for the variables. The Péclet number Pe is defined as the ratio of the advective transport rate to the diffusive transport rate ($\mathrm{Pe} = \frac{u_0 l_0}{D}$ where D is the diffusivity).

Having multiplied equation (1) by c and having taken into account the continuity equation $\frac{\partial u_i}{\partial x_i} = 0$, the following equation can be obtained

$$\frac{\partial c^2}{\partial t} + \frac{\partial (u_i c^2)}{\partial x_i} = \frac{1}{\mathrm{Pe}} \frac{\partial^2 c^2}{\partial x_i^2} - 2\chi. \qquad (2)$$

Here $\chi = \frac{1}{\mathrm{Pe}} \frac{\partial c}{\partial x_i} \frac{\partial c}{\partial x_i} = \frac{1}{\mathrm{Pe}} |\nabla c|^2$ is the instantaneous scalar dissipation rate. The use of the Reynolds averaging for equation (2) yields an equation for the scalar dispersion $\overline{c^2}\,(t)$. In the case of homogeneous turbulence, the relation for $\overline{c^2}$ and the averaged scalar dissipation rate $\overline{\chi}$ is represented as $\partial \overline{c^2} / \partial t = -2\overline{\chi}(t)$.

The averaged time $t_C\,(t)$ and length $l_C\,(t)$ scales of the scalar are the integral characteristics of spectral state of mixing and are related as $t_C = \frac{\overline{c^2}}{2\overline{\chi}} = \frac{l_C^2\,\mathrm{Pe}}{6}$ [2, 3, 5]. The physical meaning of the scalar length scale $l_C = \sqrt{\frac{3}{\mathrm{Pe}} \frac{\overline{c^2}}{\overline{\chi}}}$ is identical to that of Taylor's velocity microscale $l_\mathrm{T} = \sqrt{\frac{15}{\mathrm{Re}} \frac{u_\mathrm{rms}^2}{\varepsilon}}$ where Re is the Reynolds number, u_rms is the root-mean-square velocity fluctuation, ε is the turbulence dissipation rate.

Let's introduce a similar definition for a local time scale of scalar dissipation due to molecular diffusion on a local scalar length scale λ_C:

$$\tau_C = \frac{c^2}{2\chi} = \frac{\lambda_C^2\,\mathrm{Pe}}{6},$$

where the scalar length scale, on which the scalar fluctuation is realized, is defined as:

$$\lambda_C = \sqrt{\frac{3}{\mathrm{Pe}} \frac{c^2}{\chi}} = \sqrt{3} \frac{|c|}{|\nabla c|}. \qquad (3)$$

Physically, this scalar length scale is characteristic of heterogeneity in a turbulent scalar field (thickness of diffusion layers which separate different concentration regions), and the corresponding PDF shows the existence probability of such scales in the flow [3].

Relation (3) is indicative of the fact that λ_C is determined as a quotient of absolute values of the scalar and its gradient, i.e., it is found from the statistics of c and $|\nabla c|$ which can be expressed in terms of the joint PDF $P(\Gamma,W)$ where Γ and W are the probabilistic variables for c and $|\nabla c|$ with the domain for these variables $\Gamma_{\min} \le \Gamma \le \Gamma_{\max}$ and $0 \le W \le +\infty$ and also $\Gamma_{\min} < 0$, where $\Gamma_{\max}$, $\Gamma_{\min}$ are the maximum and minimum scalar values.

In order to derive a relation for the scalar length scale PDF $P^{\lambda}(\varphi)$, the fundamental approaches of probability theory are used [12]. Consider some joint PDF $P(\psi_1, \psi_2)$ of two random variables ϕ_1 and ϕ_2 with probabilistic variables ψ_1 and ψ_2, respectively. Assume that the domain for these variables is $\phi_{\min} \le \phi_1 \le \phi_{\max}$ and $0 \le \phi_2 \le +\infty$ and also $\phi_{\min} < 0$. The quotient is marked as $\lambda = |\phi_1|/\phi_2$. The cumulative distribution function of a random variable λ is $F(\varphi)=\mathrm{Prob}\{|\psi_1|/\psi_2 \le \varphi\}$ by definition where φ is the probabilistic variable for λ. The desired probability then equals that of a composition space point (ϕ_1, ϕ_2) to obey the inequality $-\varphi\phi_2 \le \phi_1 \le \varphi\phi_2$, i. e.:

$$F(\varphi)=\int_{0}^{+\infty} d\psi_2\left[\int_{\phi_{\min}}^{\phi_{\max}} P(\psi_1,\psi_2)d\psi_1\right]- \\ -\int_{0}^{\phi_{\max}/\varphi} d\psi_2\left[\int_{\varphi\psi_2}^{\phi_{\max}} P(\psi_1,\psi_2)d\psi_1\right]-\int_{0}^{-\phi_{\min}/\varphi} d\psi_2\left[\int_{\phi_{\min}}^{-\varphi\psi_2} P(\psi_1,\psi_2)d\psi_1\right]. \tag{4}$$

As the first integral with the PDF normalization is equal to unity, relation (4) yields:

$$F(\varphi)=1-\int_{0}^{\phi_{\max}/\varphi} \Phi_1(\psi_2,\varphi)d\psi_2-\int_{0}^{-\phi_{\min}/\varphi} \Phi_2(\psi_2,\varphi)d\psi_2=1-F_{+}-F_{-},$$

where $\Phi_1(\psi_2,\varphi)=\int_{\varphi\psi_2}^{\phi_{\max}} P(\psi_1,\psi_2)d\psi_1$ and $\Phi_2(\psi_2,\varphi)=\int_{\phi_{\min}}^{-\varphi\psi_2} P(\psi_1,\psi_2)d\psi_1$.

The last equality is differentiated over the variable φ to obtain the PDF of the quotient $\lambda=|\phi_1|/\phi_2$. Use the below formula for differentiating the integral dependent on some parameter:

$$\frac{d}{dy}\int_{\alpha(y)}^{\beta(y)} f(x,y)dx=\int_{\alpha(y)}^{\beta(y)}\frac{\partial f(x,y)}{\partial y}dx+f(\beta(y),y)\frac{d\beta(y)}{dy}-f(\alpha(y),y)\frac{d\alpha(y)}{dy}. \tag{5}$$

Then

$$\frac{\partial F_{+}}{\partial\varphi}=\frac{\partial}{\partial\varphi}\left\{\int_{0}^{\phi_{\max}/\varphi}\Phi_1(\psi_2,\varphi)d\psi_2\right\}=\int_{0}^{\phi_{\max}/\varphi}\frac{\partial\Phi_1(\psi_2,\varphi)}{\partial\varphi}d\psi_2,$$

$$\frac{\partial F_{-}}{\partial\varphi}=\frac{\partial}{\partial\varphi}\left\{\int_{0}^{-\phi_{\min}/\varphi}\Phi_2(\psi_2,\varphi)d\psi_2\right\}=\int_{0}^{-\phi_{\min}/\varphi}\frac{\partial\Phi_2(\psi_2,\varphi)}{\partial\varphi}d\psi_2.$$

Formula (5) is applied to get integrals in these relations:

$$\frac{\partial \Phi_1(\psi_2,\varphi)}{\partial \varphi}=\frac{\partial}{\partial \varphi}\int_{\varphi\psi_2}^{\phi_{\max}} P(\psi_1,\psi_2)d\psi_1=\int_{\varphi\psi_2}^{\phi_{\max}} \frac{\partial P(\psi_1,\psi_2)}{\partial \varphi}d\psi_1+\frac{\partial \phi_{\max}}{\partial \varphi}P(\phi_{\max},\psi_2)-$$

$$-\frac{\partial(\varphi\psi_2)}{\partial \varphi}P(\varphi\psi_2,\psi_2)=-\psi_2 P(\varphi\psi_2,\psi_2),$$

$$\frac{\partial \Phi_2(\psi_2,\varphi)}{\partial \varphi}=\frac{\partial}{\partial \varphi}\int_{\phi_{\min}}^{-\varphi\psi_2} P(\psi_1,\psi_2)d\psi_1=\int_{\phi_{\min}}^{-\varphi\psi_2} \frac{\partial P(\psi_1,\psi_2)}{\partial \varphi}d\psi_1+\frac{\partial(-\varphi\psi_2)}{\partial \varphi}P(-\varphi\psi_2,\psi_2)-$$

$$-\frac{\partial \phi_{\min}}{\partial \varphi}P(\phi_{\min},\psi_2)=-\psi_2 P(-\varphi\psi_2,\psi_2).$$

Hence it follows that the desired PDF of the quotient λ is equal to:

$$P^{\lambda}(\varphi)=\int_0^{\phi_{\max}/\varphi}\psi_2 P(\varphi\psi_2,\psi_2)d\psi_2+\int_0^{-\phi_{\min}/\varphi}\psi_2 P(-\varphi\psi_2,\psi_2)d\psi_2\,. \qquad (6)$$

The correspondence of the variable ϕ_1 to the scalar c and of ϕ_2 to its gradient norm $|\nabla c|$ consistent with the joint PDF $P(\Gamma,W)$ is now introduced in formula (6) to have the following expression for the scalar length scale PDF:

$$P^{\lambda}(\varphi)=\int_0^{\sqrt{3}\Gamma_{\max}/\varphi} WP(\varphi W/\sqrt{3},W)dW+\int_0^{-\sqrt{3}\Gamma_{\min}/\varphi} WP(-\varphi W/\sqrt{3},W)dW\,, \qquad (7)$$

where φ is the probabilistic variable for the scale λ_C.

Thus, if the joint PDF of the scalar and its gradient norm or the closed equation for this PDF [13-14] is known, then the scalar length scale PDF is found by relation (7) or by deriving and solving the relevant transfer equation for the desired function.

Knowledge of this function also allows the typical averaged scalar length and time scales to be determined by these relations:

$$\bar{\lambda}_C = \int_0^{+\infty} \varphi P^{\lambda}(\varphi) d\varphi, \qquad \bar{\tau}_C = \frac{\mathrm{Pe}}{6} \int_0^{+\infty} \varphi^2 P^{\lambda}(\varphi) d\varphi .$$

It is worth noting that formula (7) is valid for an arbitrary scalar that not necessarily possesses the property of considered conserved scalar. For further studies, in the premixed reacting flows, a progress variable can be chosen as a scalar, and its equation contains chemical terms [3].

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