STATISTICAL MODEL FOR THE CONDITIONAL DISSIPATION RATE AND SURFACE DENSITY FUNCTION OF SCALAR TURBULENT FLUCTUATION INTENSITY

Valery A. Sosinovich, Valery A. Babenko, Julia V. Zhukova
Luikov Heat & Mass Transfer Institute
National Academy of Sciences of Belarus
15 P. Brovka Str., Minsk, Belarus

ABSTRACT

A closed system of the equations for one-point probability density function (PDF) $f_t(\Gamma)$, surface density function (SDF) $\Sigma_t(\Gamma)$, and a conditional scalar dissipation rate (CSDR) $\chi_t(\Gamma)$ have been derived and solved numerically. These equations were derived through the closed equation for the joint probability density function (JPDF) of a scalar and the value of its gradient, $P_t(W,\Gamma)$.

CLOSED EQUATION FOR THE JPDF

Modern approaches to turbulent combustion are related with studying the flames being far from chemical equilibrium. The development of theoretical turbulent combustion models demands a deep knowledge of statistical characteristics of the turbulent scalar field gradient. Specifically, it turns out that for turbulent combustion flows with non-premixed reactants to be described with regards to states close to extinction, one must know the probability density distribution for dissipation rate of mixture fraction fluctuations on the stoichiometric surface (Peters, 1983). To calculate such a function it is necessary to develop and solve the equation for the joint probability distribution function (JPDF) of a mixture fraction and its gradient $P_t(W,\Gamma)$. Up to date such a task was not done in the extent sufficient to practical application, though some attempts had been undertaken, (Meyers, O'Brien, 1981), (Gao, O'Brien, 1991).

In work Sosinovich et al. (1998) the closed equation for the JPDF was deduced, which is of the following form

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

The first term in the r.h.s. of (1) describes the diffusion influence in a scalar space (this term may be rather called anti-diffusion, because of its sign), the second one describes the influence of turbulent velocity and scalar fields structure on the JPDF. Here, $S_{UC}(t)$ stands for asymmetry of the joint probability distribution of velocity and scalar fields, $\varepsilon(t)$ is the mean dissipation rate of turbulence kinetic energy, $\chi(t)$ is the mean dissipation rate of scalar fluctuation intensity.

The third term in the r.h.s. of (1) presents an influence of dissipation in scalar gradient space on the joint statistics of reacting scalar field and the value of scalar gradient. The function $N_t(\Gamma)$ takes the form

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

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

where

$$\alpha(T) = \frac{27T^2}{8\left[5 - 9T^2\right]}, \quad \hat{\Gamma} = \Gamma / \sqrt{\overline{c^2(t)}} \quad (3)$$

$$T(t) = \sqrt{2}\chi(t) \Big/ \left(3D\sqrt{-\overline{c^2(t)}D_{CC}^{(IV)}(0,t)}\right) \quad (4)$$

Here $\overline{c^2(t)}$ is the squared scalar fluctuation intensity, $D_{CC}^{(IV)}(0,t)$ is the forth derivative of the two-point structural function of scalar turbulent field over distance r at zero r.

The forth term in the r.h.s of the equation for the JPDF describes an influence of mixed cross diffusion in space of a scalar and scalar gradient on the joint statistics of reacting scalar and its gradient. The function $X_t(\Gamma)$ is presented by the expression

$$X_t(\Gamma) = K_t(\hat{\Gamma})\exp\left\{-\alpha(T)\hat{\Gamma}^2\right\} \quad (5)$$

In (5) the following designations are used:

$$K_t(\hat{\Gamma}) = \chi(t)\kappa(\hat{\Gamma}) / 6D\sqrt{\overline{c^2(t)}} \quad (6)$$

$$\kappa(\hat{\Gamma}) = N(n)(2n+1)\left(\hat{\Gamma}/N(n)\right)^{\frac{2n-1}{2n+1}} \times \left[2n - (2n+1)\left(\hat{\Gamma}/N(n)\right)^{\frac{2}{2n+1}}\right] \quad (7)$$

$$N(n) = \sqrt{\pi}\,\Gamma(2n+2)/\Gamma(2n+3/2) \quad (8)$$

$\Gamma(x)$ is gamma-function and parameter $n \geq 0$ is of the order of unity.

The fifth term in (1) explains action of chemical reaction rate on the JPDF. One can make an effort to solve equation (1) numerically if calculating evolution of the functions $S_{UC}(t)$, $D_{CC}^{(IV)}(0,t)$, $\varepsilon(t)$, $\chi(t)$, and $\overline{c^2(t)}$ from any auxiliary system. At the moment, this problem has not been solved because of difficulties related to multi-dimensionality of this function.

There are two closely related with the JPDF but more simple statistical functions applicable to wide class of turbulent combustion problems. The first one is the conditional scalar dissipation rate (CSDR), which means the scalar fluctuation intensity dissipation rate averaged under the definite value of the scalar field $C(x,t) = \Gamma$ in the same point. The second one is the surface density function (SDF), which represents the specific area of isoscalar surface $C(x,t) = \Gamma$ per unit of volume.

The CSDR and SDF functions are of wide use in intensively developed over the last years flamelet approach to turbulent reacting flows, (Peters, 1986), which allows to separate effectively the complexities of chemical reactions from the problem of turbulent mixing modeling. Information on the CSDR and SDF functions is critically important for the success of different flamelet models of turbulent reacting flows. The equations of flamelet models for the average species mass fraction and temperature, those bearing the responsibility for turbulence information, involve the conditional scalar dissipation rate of a passive scalar (mixture fraction), calculated on the stoichiometric surface, $\chi_t(\Gamma)$. On the other hand, a number of flamelet models is connected with the balance equation for the SDF function, $\Sigma_t(\Gamma)$, in a flame (see, for instance, (Vervich et al., 1995), (Candel, Poinsot, 1990)).

An analytical expression for the CSDR has been derived in O'Brien, Jiang (1991), Girimaji (1992) by mapping closure approach. According to this approach the form of the CSDR turns out to be time-independent. Meanwhile, the results of computation of the CSDR based on DNS show the form of this function to undergo essential changes during turbulent mixing (Eswaran, Pope, 1988). This fact was confirmed by studying this function experimentally in various turbulent flows (Kailasnath et al., 1993). In Sosinovich et al. (1995), the complex transformation of the CSDR was explained by changing characteristic modes of the turbulent scalar field during evolution. The equation for the SDF was derived in Vervich et al. (1995) through the JPDF of a scalar and its gradient. In this balance equation the various terms and mechanisms were considered using the results of DNS from Trouve, Poinsot (1994).

Up to now the most achievements in studying the CSDR and SDF were obtained by DNS or experimentally. Traditional statistical approaches for these functions have not been developed. It complicates the application of new flamelet models and their further development. So, the main purpose of this work is to derive closed equations for the CSDR and SDF on statistical ground.

CLOSED EQUATIONS FOR THE SDF AND PDF

Note, that the SDF and CSDR functions represent the first and second order moments of the function $P_t(W,\Gamma)$, correspondingly. In isotropic case the relation for $\Sigma_t(\Gamma)$ can be presented through the JPDF of scalar and the value of scalar gradient with the formula

$$\Sigma_t(\Gamma) = \int_0^\infty W P_t(W,\Gamma)\,dW \quad (9)$$

Using this definition and equation for the JPDF, we can obtain the equation for $\Sigma_t(\Gamma)$

$$
\begin{aligned}
\frac{\partial \Sigma_t(\Gamma)}{\partial t} &= -2D(t)\sqrt{c^2(t)}\frac{\partial^2 \Sigma_t(\Gamma)}{\partial \Gamma^3} - \\
&- A(t)\left[\frac{\Sigma_t(\Gamma)}{2} - \frac{8\sqrt{\mathrm{Pe}}}{3\sqrt{6\pi}}\chi(t)^{1/2} f_t(\Gamma)\right] + \\
&+ \frac{2C(t)\sqrt{\mathrm{Pe}}}{\sqrt{6\pi}}\tilde{N}_t(\Gamma)\frac{f_t(\Gamma)}{\chi(t)^{1/2}} + \\
&+ \frac{D(t)}{2}\frac{\partial}{\partial \Gamma}\left[X_t(\Gamma)\Sigma_t(\Gamma)\right] - \mathrm{Da}\,\Gamma\frac{\partial \Sigma_t(\Gamma)}{\partial \Gamma}
\end{aligned}
\qquad (10)
$$

where

$$
A(t)=\sqrt{\frac{\mathrm{Re}}{15}}\varepsilon(t)S_{uc}(t),\ C(t)=-\frac{D_{CC}^{(IV)}(0,t)}{\mathrm{Pe}^2},D(t)=\frac{2\chi(t)}{3\sqrt{c^2(t)}} \qquad (11)
$$

$$
\mathrm{Re}=\frac{\sqrt{q(0)}L}{\nu},\mathrm{Pe}=\frac{\sqrt{q(0)}L}{D},\mathrm{Da}=\frac{\tau_{chem}q(0)}{L} \qquad (12)
$$

These equations contain the time-dependent coefficients (dispersion, dissipation rate, asymmetry of velocity and scalar field) which are found using the distributions of turbulence energy and intensity of the scalar fluctuation field in different length scales. For these functions the closed system has been written in Sosinovich et al. (1987).

As follows from (10), the equation for $\Sigma_t(\Gamma)$ contains the one-point PDF $f_t(\Gamma)$. So, it is necessary to write separate equation for the latter function. This one can be deduced from equation (1) using the definition of $f_t(\Gamma)$

$$
f_t(\Gamma) = \int_0^\infty P_t(W,\Gamma)dW \qquad (13)
$$

As can be seen from (13), the one-point PDF is the zero order moment of the JPDF $P_t(W,\Gamma)$. Integrating equation (1) results in the known equation for $f_t(\Gamma)$, (O'Brien, 1980).

$$
\frac{\partial}{\partial t}f_t(\Gamma) = -\frac{\partial^2}{\partial \Gamma^2}\left[\chi_t(\Gamma)f_t(\Gamma)\right] - \mathrm{Da}\frac{\partial}{\partial \Gamma}\left[\dot{\omega}(\Gamma)f_t(\Gamma)\right] \qquad (14)
$$

As indicated by (14), the function CSDR appears in the expression for the one-point PDF. For this function one have to derive separate equation.

CLOSED EQUATION FOR $\chi_t(\Gamma)$

The CSDR is related to the JPDF $P_t(W,\Gamma)$ by formula

$$
\chi_t(\Gamma) = D\int_0^\infty W^2 P_t(W,\Gamma)dW / f_t(\Gamma) \qquad (15)
$$

As follows from this definition, the function $\chi_t(\Gamma)$ is actually the second order moment of the function $P_t(W,\Gamma)$. Multiplying equation (1) by DW^2 and integrating over W from 0 to ∞, and using the equation for the function $f_t(\Gamma)$, we obtain the following equation for $\chi_t(\Gamma)$

$$
\begin{aligned}
\frac{\partial \chi_t(\Gamma)}{\partial t} &= k_1 A(t)\left(1 - k_2\frac{\chi_t(\Gamma)}{\chi(t)}\right)\chi(t) - \\
&- C(t)\tilde{N}_t(\Gamma)\chi_t(\Gamma)\frac{\partial^2 \chi_t(\Gamma)}{\partial \Gamma^2} - \\
&- 2f_t^{-1}(\Gamma)\frac{\partial \chi_t}{\partial \Gamma}\frac{\partial}{\partial \Gamma}\left[\chi_t(\Gamma)f_t(\Gamma)\right] + \\
&+ \frac{D(t)}{f_t(\Gamma)}\frac{\partial}{\partial \Gamma}\left\{\Gamma\exp\left[-\alpha(T)\hat{\Gamma}^2\right]\chi_t(\Gamma)f_t(\Gamma)\right\} - \\
&- \mathrm{Da}\left(2\chi_t(\Gamma) - \Gamma\frac{\partial \chi_t(\Gamma)}{\partial \Gamma}\right)
\end{aligned}
\qquad (16)
$$

The coefficients k_1 and k_2 were used for adjusting.

The following hypothesis was used when deriving equation (16)

$$
\overline{\chi_t^2(\Gamma)} = \chi_t(\Gamma)\chi_t(\Gamma) \qquad (17)
$$

It means insignificant influence of CSDR fluctuation on this function evolution.

THE NUMERICAL SOLUTION OF EQUATIONS FOR $\Sigma_t(\Gamma)$, $\chi_t(\Gamma)$ AND $f_t(\Gamma)$

The system being solved consists of non-dimensional equations (10) for the SDF, (14) the for one-point PDF, and (16) for the CSDR. To certain terms with chemical reaction rate in (10), (14), (16), it was necessary to determine the function $\dot{\omega}(\Gamma)$ and Damkohler number Da. For simplicity reason we assumed that expression for $\dot{\omega}(\Gamma)$ was specified by the first order reaction rate

$$\dot{\omega}(\Gamma) = \Gamma \tag{18}$$

This formula refers to binary chemical reaction, when one of the reactants is of great demand (Trouve, Poinsot, 1994).

The presence of "anti-diffusion" terms makes problem (10), (14), (16) similar to classic ill-posed inverse problems. Trying to integrate this system in normal time direction we faced with a strong numerical instability. So, the problem was solved in backward time direction, e.a. from some "start" time moment $t = t_s$ to $t = 0$.

When integrating system (10), (14), (16) in backward time direction, some numerical problems were also presented, especially in the regions where solution looked like a combination of δ -functions.

Solution of ill-posed problems in backward time direction is accessible in case of a) distributions of desired function are approximately known at $t = t_s$, b) no definite distributions at initial time $t = 0$ are specified, c) the solution itself is to some extent independent to small variation of "start" distributions.

Fortunately, in our case there are enough reasons to build "start" distributions at the end of mixing process, e.a. at a moment $t = t_s >> 1$. The choice of model analytical form of "start" profiles for the one-point distribution functions $\chi_t(t_s, \Gamma)$ and $f_t(t_s, \Gamma)$ was based on the fact that at the end of mixing the one-point distribution function $f_t(t_s, \Gamma)$ is Gaussian. As known, tending the one-point JPDF to Gaussian form is related to statistical independence of the CSDR function on a scalar value at this stage of mixing. Taking this fact into consideration, one can specify the "start" profile for the one-point PDF as being of Gaussian form and the CSDR function as independent on scalar field.

At this stage the "start" distributions of the function $f_t(\Gamma)$ was specified according to model analytical expression:

$$f_{t_s}(\Gamma) = \frac{\beta}{\alpha^2 + \Gamma^2} \tag{19}$$

where parameters α and $\beta(\alpha)$ control the sharpness of the distribution. The parameter β was chosen to satisfy boundary condition, which causes the value of α to be found from the transcendental equation: $\mathrm{arctg}(1/\alpha) - \alpha/(2\beta) = 0$. The parameter β was found by the known value of scalar dispersion $\overline{c_s^2}$ at the "start" moment, $\beta = \left(\overline{c_s^2} + \alpha^2\right)/2$.

Start distribution for conditional dissipation rate at $t = t_s$ models Π -like distribution of this value at the final stage of mixing:

$$\chi_{ts} = 2\frac{\overline{\chi_{ts}}}{\pi}\mathrm{arctg}((1 - \Gamma)/\gamma) \tag{20}$$

where γ is a small parameter, controlling the sharpness of graduated distribution (20). The value of γ was varied in the range $\gamma \sim 0.01 - 0.003$ during computation.

Start profile for the function $\Sigma_t(\Gamma)$ is prescribed by the formula $\Sigma_{t_s}(\Gamma) = f_{t_s}(\Gamma)\chi_{t_s}(\Gamma)$, expressing statistical independence of a scalar and scalar gradient at a final stage of mixing (Dopazo, 1994):

$$\Sigma_{t_s}(\Gamma) = \frac{\beta}{\alpha^2 + \Gamma^2}\frac{2\sqrt{\chi_{t_s}}}{\pi}\mathrm{arctg}((1 - \Gamma)/\gamma) \tag{21}$$

Integration of equations in backward direction was routinely begun at the moment $t_s = 25 \div 30$. It relates to nearly complete mixing state. This corresponds to sharp maximum of the function $f_t(\Gamma)$ at $\Gamma = 0$ and nearly zero $f_t(\Gamma)$ at $\Gamma > 0$.

In test numerical runs the sensibility of solution to specified start conditions was checked. In particular, the same conditions (19) - (21) were assigned at different time moments t_s selected from the range $t_s \in (15 \div 30)$.

RESULTS

As it is seen from fig. 1, the initial form of the one-point PDF $f_t(\Gamma)$ (curve 1) looks as a sum of two delta-functions, reflecting a nearly non-premixed state of scalar field at the beginning of mixing process. The content of mixed fluid is further increased (curve 2), but, the form of the one-point PDF at this initial stage remains principally the same, characteristic for sine wave realization of a scalar field. This form of PDF is connected (Eswaran, Pope, 1988) with the presence of diffusion layers in turbulent flow. Curves 3 - 6 demonstrates growing maximum at $\Gamma = 0$, thus showing two-mode form of the PDF and reflecting the presence in a flow of non-mixed and mixed up to a molecular level fragments of fluid. Such behavior of the PDF is not reproduced by known DNS results, possibly because of too small Reynolds and Peclet numbers used.

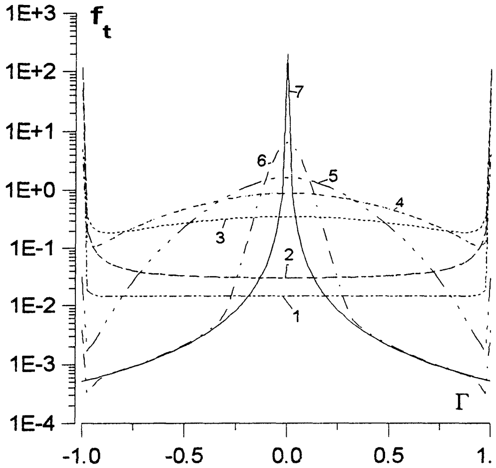

Fig. 1. The evolution of the PDF form: 1-t =0, 2-t =0.2, 3-t =1., 4-t =2.5, 5-t =5, 6-t =15, 7-t =25.

This feature does not also present in the majority of models based on mean turbulence characteristics. On the other hand, two-mode character of the PDF was marked in experimental work Kennedy, Kent (1979) and some theoretical papers Cremer et al. (1994) and Sosinovich et al. (1995). Figures 2 and 3 exhibit the CSDR function at various stages of turbulent mixing. A parabolic initial form of the CSDR corresponds to

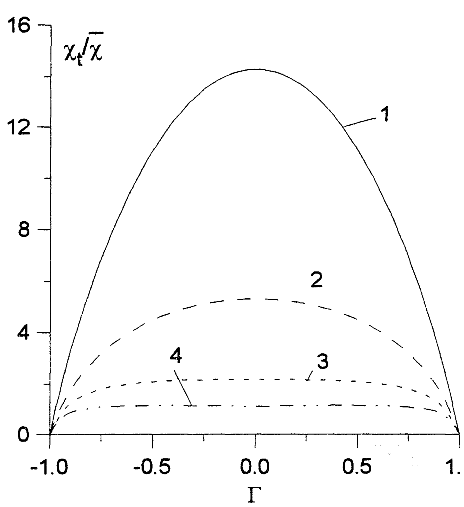

Fig. 2. The evolution of conditional dissipation rate $\chi_t(\Gamma)/\bar{\chi}(t)$: 1-$t$ =0, 2-t =0.5, 3-t =1, 4-t =2.5

sine wave realizations of turbulent scalar field. At subsequent stages of mixing, when $5 < t < 15$, (curves 3, 4) the profile of the CSDR function in the middle part becomes nearly flat. It's probably caused by the typical realizations of scalar turbulent field becoming saw-tooth, so scalar and its gradient are in a weak correlation. Later on, when $t > 15$ (fig. 3), the CSDR profile repeatedly takes a parabolic form. It is possible to assume, that such a form of the CSDR is connected to an aggravation of typical realizations of scalar field in such a manner that the maximum gradient is observed at large values of scalar, that results in strong correlation of a scalar and its gradient. The further evolution of the CSDR ($t \geq 25$) results in nearly flat distribution again. At this final stage of evolution the form of PDF is like Gaussian curve.

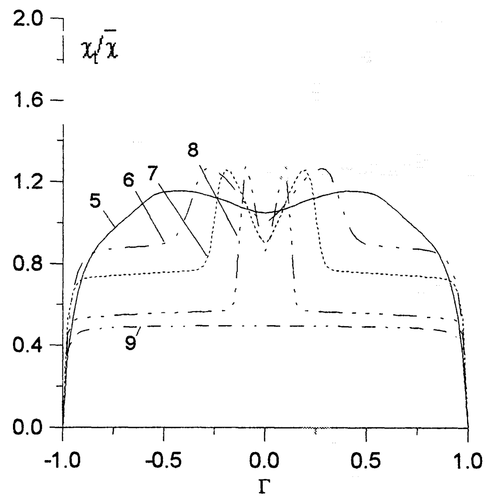

Fig. 3. The evolution of conditional dissipation rate $\chi_t(\Gamma)/\bar{\chi}(t)$: 5-$t$ =5, 6-t =10, 7-t =15, 8-t =20, 9-t >25 (asymptotic state).

The form of calculated surface density function divided at integral surface area

$$\bar{\Sigma}_t = \int \Sigma_t d\Gamma \tag{22}$$

is shown at fig 4. As this figure shows, evolution of the SDF is in sharpening of its form. Initially, it has a parabolic form, but after $t > 0$ the SDF looks like a δ-function, which becomes more and more narrow.

This kind of evolution at large t is probably related to the loss of statistical correlation between fluctuation of scalar field and its gradient.

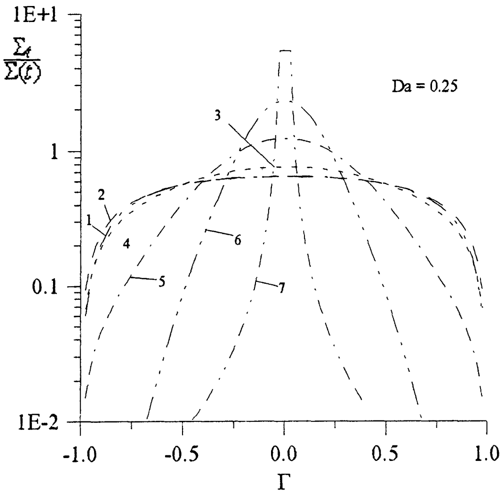

Fig. 4. Form evolution of the conditional surface density function at Da=0.25: 1-t =0, 2-t =0.5, 3 - t =1, 4-t =2.5, 5 - t =5, 6 - t =15, 7 - t =20.

CONCLUSION

The developed in the given work closed model for evaluation of the functions $\chi_t(\Gamma)$, $f_t(\Gamma)$, and $\Sigma_t(\Gamma)$ can be used at modeling the chemical reactions in turbulent streams within frameworks of flamelet approach. The calculated evolution of the one-point PDF $f_t(\Gamma)$ demonstrates two-mode form at intermediate stages of turbulent mixing. This outcome is in the qualitative correspondence with experiment, but theoretically it was obtained for the first time. The sequence of the CSDR forms agrees well with the DNS results, (Eswaran, Pope, 1988), and experiment (Kailasnath et al., 1993). The evolution of desired functions $\chi_t(\Gamma)$ and $\Sigma_t(\Gamma)$ was tabulated. It enables to use them in other researches.

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