



Modeling of turbulent reacting flows on the base of the equation for the scalar field correlation function

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ABSTRACT

A model based on an equation for the scalar correlation function is used for calculating the interaction between chemical reactions and micromixing in a turbulent flow of constant density. The Prandtl hypothesis for the terms responsible for turbulence affect the scalar field structure and the simplest approximation for the terms depending on chemical reactions are used to close the equation for the correlation function. The closure proposed is shown to be statistically reliable. To determine the effect of chemical reactions on the averaged field and the correlation function, the probability density function (PDF) is found in the presumed form which has allowed one to obtain the data on the averaged field and the correlation function. The admixture is assumed to be passive, i.e., it does not affect the parameters of turbulence and turbulent diffusivity, and the required parameters of the homogeneous turbulent field – to be known. The characteristic features of the transport phenomena in a 2D layer with a given value of a scalar at its boundaries are considered. Results on the effect of the chemical reaction on the distributions of an averaged scalar, a scalar fluctuation intensity, and a scalar dissipation rate are obtained. The process of developing a reaction zone is calculated.

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1. Introduction

The problem of determining the effect of turbulence on the statistical characteristics of a scalar field is the principal problem in analyzing turbulent reacting flows. Statistics of a fluctuating scalar field (temperature, concentration) should be known in many areas of modern physics. For example, the propagation of laser beams and radiowaves in the atmosphere is strongly affected by the distribution of a small scale temperature gradient. The parameters of the scalar field affected by turbulence determine the most important processes in engineering applications, including internal combustion engines, chemical reactors, power plants, mixing and destruction of contaminants in the atmosphere. The fluctuations of electric current in the probes used for diagnostics of turbulent flows of conducting fluids are also determined by the statistics of the distributions of conducting components.

The mixing mechanism in a turbulent flow is the following. The turbulent motion makes the isoscalar surfaces to be warped and stretched, thus causing the gradients and Laplacians of the scalar field to increase and the exchange processes to intensify. The molecular transport smoothes the scalar field, and a dynamic equilibrium occurs between the smoothing, and the warping and stretching.

Because of the stochastic nature of turbulent motions, the problem of determining the micromixing intensity reduces to determining the statistical characteristics of the scalar field Laplacians whose values allow finding the PDF required for calculation of averaged rates of chemical reactions.

It is reasonable to divide all the methods for micromixing into local or one-point and nonlocal ones among which the two-point methods are the simplest.

To correctly present the mixing of reacting flows, the description should include actual values of transport coefficients, that is possible only in two-point models.

The two-point approach is able to properly take into account actual values of diffusivities and thermal conductivity and to compute characteristic scales of the scalar field. In addition, the above approach permits one to divide the effect of turbulence into advection and micromixing. As a result, we can consider the unsteady processes such as the combustion zone formation and describe the dependence of the rate of premixed turbulent combustion on physical and chemical characteristics of a combustible mixture.

The two-point model can be constructed by several methods: on the basis of an equation for the two-point PDF of a scalar (PDF2); an equation for the joint PDF of a scalar and its gradient or an equation for a scalar correlation function (SCF). In any case, the derived equations need closing.

Our interest to the equation for the SCF arose in analyzing a capability of the PDF2 to describe turbulent combustion [1].

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Nomenclature

$B_{rr}(\mathbf{x})$	correlation function of the longitudinal component of turbulent velocity fluctuation	$P(\mathbf{z}, c)$	scalar PDF at point \mathbf{z}
$(c(\mathbf{x}_{1 2}, t))$	instantaneous scalar	$\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$	vector that joints points \mathbf{x}_1 and \mathbf{x}_2
$C(\mathbf{x}_{1 2})$	averaged scalar	r, θ, ϕ	spherical variables
$c'(\mathbf{x}_{1 2}, t) = c(\mathbf{x}_{1 2}, t) - C(\mathbf{x}_{1 2})$	instantaneous scalar fluctuation	$R(\mathbf{x}_1, \mathbf{x}_2, t)$	scalar correlation function
$D(\mathbf{x}_{1 2}, t)$	turbulent diffusivity	t	time
Da	Damköhler number (14)	$\mathbf{U}_{1 2}$	averaged velocity
$div_{r \eta}(\mathbf{u})$	divergence of the argument vector over the variable denoted by an index	$W(c)$	chemical reaction rate
$disp(\mathbf{z})$	variance of the scalar PDF $P(\mathbf{z}, c)$	$\langle W(c) \rangle$	averaged chemical reaction rate
D_m	molecular diffusivity	W'	chemical reaction rate fluctuation
$D_r(\mathbf{x}_{1 2}, t)$	eddy-diffusivity	$\mathbf{x}_{1 2}$	spatial coordinates of the considered pair of points
$F(\mathbf{z}, c) = \int_c^\infty P(\mathbf{z}, c') dc'$	scalar probability distribution at point \mathbf{z}	$\mathbf{z} \eta = (\mathbf{x}_1 + \mathbf{x}_2)/2$	coordinate pointed to the middle between the points \mathbf{x}_1 and \mathbf{x}_2
		λ	turbulent velocity field microscale

Similar studies have been reported by O'Brien [2,3]. A common point is the understanding that the micromixing model for turbulent reacting flows should be improved, which is impossible within the framework of one-point approaches.

The method of closing the equations for the PDF2 and SCF in [2,3] was based on analyzing the motion of a pair of particles in the turbulent velocity field. The particles were involved in Brownian motion, which in author's opinion models the molecular mixing. For the homogeneous conditions this theory allowed the calculation of eddy-diffusivity from the energy spectrum of the turbulent velocity field. The authors of [3] used linear dependencies for the chemical reaction rates, which enabled them to pay no attention to the closure of the corresponding term in the equation for the SCF.

Previously in [4,5], we also used the theory of motion of two particles for micromixing analysis. In such a case, however, the calculated eddy-diffusivity was time-dependent (as in [2,3]), which is rather an undesirable feature. When we tried to find another method of closure of the PDF2 equation, we found surprising correlations between the equations for the PDF2 and SCF. Closing the equation for the PDF2 results in the appearance of the SCF derivatives. This means that the problem on closing the PDF2 can be reduced to the closure of the equation for the SCF [1]. Such a circumference holds true also in the other methods, e.g., in the approach based on the equations for the joint PDF of a scalar and its gradient [6].

Our attempts to avoid the time dependence of eddy-diffusivity were began, assuming that the eddy-diffusivity can be considered at zero time. The calculation with the equation for the SCF agreed well with DNS [8]. Later on the derived form of the equation was explained from physical considerations [1]. The resulting form of closing is similar to proposed by Hasselmann for correlation function of a field of velocity [7]. Preliminary SCF computations are presented in [1]. The SCF computations results were used for solving the PDF equation and for determining the averaged chemical reaction rate.

As in [1], here we consider a constant density turbulent flow in a 2D layer with fixed values of a scalar at the boundaries. Chemical processes are assumed to affect the SCF both directly and indirectly by varying the averaged scalar field. The direct effect of chemical reactions on the SCF is modeled by closing the equation for the SCF. The developed closure is exact for both the linear reaction rate and for points $r = 0$ and $r = \infty$. To simplify the calculations, turbulence is assumed homogeneous and isotropic, and the scalar dissipation is also isotropic. In the anisotropic case the Prandtl hypothesis for the closure of the SCF equation allows us to obtain the tensor of eddy-diffusivity and thus to estimate a possible effect of scalar dissipation anisotropy. To enhance the reliability of

calculations, in parallel with solving the PDF equation, we found the PDF of a scalar using the presumed distribution form, which is suitable for the intermittence absence. Below we will obtain the distributions of averaged scalar and variance of scalar fluctuations over the layer and those of the averaged chemical reaction rate and scalar dissipation. In addition, the regime of the reaction zone development will be calculated.

2. Basic assumptions

The scalar correlation function

$$R(\mathbf{x}_1, \mathbf{x}_2, t) = \langle c'(\mathbf{x}_1, t)c'(\mathbf{x}_2, t) \rangle \quad (1)$$

is a two-point characteristic. The equation for the SCF can be derived in a usual way by multiplying the transport equation for scalar fluctuations at one-point by the value of the scalar fluctuation at the second point and, vice versa, and then by adding the equations.

Having passed to new independent variables $\eta = (\mathbf{x}_1 + \mathbf{x}_2)/2$ and $\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$ and having averaged we have

$$\begin{aligned} & \frac{\partial}{\partial t} R(\eta, \mathbf{r}, t) + ((\mathbf{U}_1 + \mathbf{U}_2)/2 \cdot \nabla_\eta) R(\eta, \mathbf{r}, t) \\ & + ((\mathbf{U}_1 - \mathbf{U}_2) \cdot \nabla_r) R(\eta, \mathbf{r}, t) + div_\eta \langle (\mathbf{u}'_1 + \mathbf{u}'_2)c'(\mathbf{x}_1, t)c'(\mathbf{x}_2, t) \rangle / 2 \\ & + 2div_r \langle (\mathbf{u}'_1 - \mathbf{u}'_2)c'(\mathbf{x}_1, t)c'(\mathbf{x}_2, t) \rangle \\ & = D_m \left(\frac{1}{2} \frac{\partial^2}{\partial \eta^2} R(\eta, \mathbf{r}, t) + 2 \frac{\partial^2}{\partial r^2} R(\eta, \mathbf{r}, t) \right) + (D(\mathbf{x}_1) \\ & + D(\mathbf{x}_2)) \frac{dC(\mathbf{x})}{dx} \Big|_{\mathbf{x}_1} \frac{dC(\mathbf{x})}{dx} \Big|_{\mathbf{x}_2} + \langle c'(\mathbf{x}_2, t)W' \Big|_{\mathbf{x}_1} \rangle + \langle c'(\mathbf{x}_1, t)W' \Big|_{\mathbf{x}_2} \rangle \quad (2) \end{aligned}$$

For this equation to be closed, we must find the terms with third moments and the chemical reaction rate.

Using the generalized Prandtl hypothesis, which relates the averaged flux of the scalar F to its gradient,

$$\langle (u'_i F(\mathbf{x}_1, \dots)) \rangle = \langle u'_i l \rangle \frac{\partial}{\partial x_i} F(\mathbf{x}_1, \dots) \quad (3)$$

(the dots denote the dependence at several space points, and subscript indicates to component), for the terms with third moments in Eq. (2)] it is obtained

$$div_\eta \langle (\mathbf{u}'_1 + \mathbf{u}'_2)c'(\mathbf{x}_1, t)c'(\mathbf{x}_2, t) \rangle / 2 = \frac{\partial}{\partial \eta_i} D(\mathbf{x}) \frac{\partial}{\partial \eta_i} R(\eta, \mathbf{r}, t) \quad (4)$$

and

$$2div_r \langle (\mathbf{u}'_1 - \mathbf{u}'_2)c'(\mathbf{x}_1, t)c'(\mathbf{x}_2, t) \rangle = \frac{\partial}{\partial r_i} (D_r(\mathbf{x}_1) + D_r(\mathbf{x}_2)) \frac{\partial}{\partial r_i} R(\eta, \mathbf{r}, t) \quad (5)$$

The closure of the SCF equation implies considerations of diffusion of a particle pair. The correlation function represents a “cloud” in fluid, and this cloud is deformed under the turbulence action like a real volume of fluid. Primary attention is paid to several characteristic points of the cloud, such as the cloud center. As a result, turbulent diffusivity appears in the description of the turbulent motion of this center in Eq. (4). The correlated endpoints of fragment \mathbf{x}_1 and \mathbf{x}_2 undergo diffusion. So, Eq. (5) contains the diffusion term with an unknown diffusivity that should be determined. This diffusivity can be expressed as a ratio of the turbulence intensity to the characteristic time. Instead of the intensity we can use the correlation function of the collinear to \mathbf{r} component of the velocity thus taking into account the stretching as the main effect of turbulence on the scalar field. The characteristic time can be found when considering an infinitely large distance between the two points. In such a case, the points are uncorrelated, and the diffusion intensity at each of them is the turbulent diffusivity. This allows us to write

$$D_r(\mathbf{x}_{1|2}) = D(\mathbf{x}_{1|2})(1 - B_{rr}(r)/B_{rr}(0)) \quad (6)$$

The terms for the effect of chemical reactions on the correlation function can be approximated by the following manner. When $r = 0$ both of these terms are the same, and they can be calculated from a known PDF. When $r \rightarrow \infty$, the terms are equal to zero. Taking into account the symmetry of the correlation function with respect to r we use the simplest interpolation

$$\langle c'(\mathbf{x}_2, t)W'_{|\mathbf{x}_1} \rangle + \langle c'(\mathbf{x}_1, t)W'_{|\mathbf{x}_2} \rangle = \left(\langle c'W' \rangle_{|\mathbf{x}_1} + \langle c'W' \rangle_{|\mathbf{x}_2} \right) \bar{R}(\boldsymbol{\eta}, \mathbf{r}, t) \quad (7)$$

Here $\bar{R}(\boldsymbol{\eta}, \mathbf{r}, t)$ is the normalized correlation function of a scalar. It is equal to unity at $r = 0$.

$$\bar{R}(\boldsymbol{\eta}, \mathbf{r}, t) = R(\boldsymbol{\eta}, \mathbf{r}, t)/R(\boldsymbol{\eta}, \mathbf{0}, t) \quad (8)$$

The obtained form is exact when the reaction rate linearly depends on the concentration [3].

It was shown that the approach (4) together with (5) is statistically reliable and satisfies the requirements of the known Khinchin theorem [1].

Thus we have

$$\begin{aligned} \frac{\partial}{\partial t} R(\boldsymbol{\eta}, \mathbf{r}, t) + \frac{1}{2} ((\mathbf{U}_1 + \mathbf{U}_2) \cdot \nabla_{\boldsymbol{\eta}}) R(\boldsymbol{\eta}, \mathbf{r}, t) \\ + ((\mathbf{U}_1 - \mathbf{U}_2) \cdot \nabla_r) R(\boldsymbol{\eta}, \mathbf{r}, t) = \frac{\partial}{\partial \eta_i} (D(\boldsymbol{\eta}) + D_m) \frac{\partial}{\partial \eta_i} R(\boldsymbol{\eta}, \mathbf{r}, t) \\ + \frac{\partial}{\partial r_i} (D_r(\mathbf{x}_1) + D_r(\mathbf{x}_2) + 2D_m) \frac{\partial}{\partial r_i} R(\boldsymbol{\eta}, \mathbf{r}, t) + (D(\mathbf{x}_1) \\ + D(\mathbf{x}_2)) \frac{dC(\mathbf{x})}{dX} \Big|_{\mathbf{x}_1} \frac{dC(\mathbf{x})}{dX} \Big|_{\mathbf{x}_2} + \left(\langle c'W' \rangle_{|\mathbf{x}_1} + \langle c'W' \rangle_{|\mathbf{x}_2} \right) \bar{R}(\boldsymbol{\eta}, \mathbf{r}, t) \quad (9) \end{aligned}$$

2.1. Equation for the averaged scalar field

With the assumptions adopted the equation for the averaged value takes the form

$$\frac{\partial}{\partial t} C(\mathbf{z}, t) + (\mathbf{U} \cdot \nabla_z) C(\mathbf{z}, t) = \text{grad}_z((D(\mathbf{z}, t) + D_m) \text{div}_z C(\mathbf{z}, t)) + \langle W(c) \rangle \quad (10)$$

2.2. Determination of the probability density function of a scalar

To calculate the averaged chemical reaction rate it is necessary to know the scalar PDF. In our previous studies the PDF equation closed by the simplest micromixing model was integrated. In the present work the PDF is determined using the presumed form of the distribution. This improvement is aided by the fact that we

consider so called strong mixing regimes, virtually without intermittence. It allows assuming the PDF to be close to the normal distribution taking into account that the independent variable ranges from 0 to 1. In such a case the normalized distribution function takes the form

$$F(\mathbf{z}, c) = \frac{\left(-\text{erf} \left(\frac{c-C(z)}{\sqrt{\text{disp}(z)}} \right) + \text{erf} \left(\frac{1-C(z)}{\sqrt{\text{disp}(z)}} \right) \right)}{\left(\text{erf} \left(\frac{C(z)}{\sqrt{\text{disp}(z)}} \right) + \text{erf} \left(\frac{1-C(z)}{\sqrt{\text{disp}(z)}} \right) \right)} \quad (11)$$

All required averaged values are determined by integrating the function $F(\mathbf{z}, c)$.

3. Formulation of the problem

One of the essential difficulties associated with the equation for the SCF is a large number of independent variables. In the general case the SCF depends on six spatial variables and time. Under the stationary homogeneous conditions and isotropy the number of variables reduces down to two. In the case of inhomogeneity the minimum number of variables can be obtained considering the 2D flow of constant width at the walls of which the values of a scalar are given, and inhomogeneity takes place only over one variable.

This case corresponds to the Couette flow between two infinite flat plates one of which moves with a constant velocity. The temperatures (scalars) of the plates are constant but different. If the molecular conductivity differs from zero, then a heat flux occurs. In the space between the walls turbulence exists, which results in initiating the turbulent transport. In order to divide the molecular and turbulent transports, the turbulent transport of a scalar from the walls is assumed to be equal to zero. It is natural as the normal fluid velocity at the wall equals zero.

Fig. 1 shows a schematic of independent variables. The vertical line represents the spatial coordinate corresponding to the variation of the location of the two-point center. The lines that end at the boundaries clarify the boundary conditions for the SCF. At the boundary the scalar fluctuation is equal to zero.

For the steady-state regime the SCF should contain three independent variables: the center position across the layer z , the segment length r , and the direction angle θ . The variables r and θ represent a polar coordinate system when there is no dependence

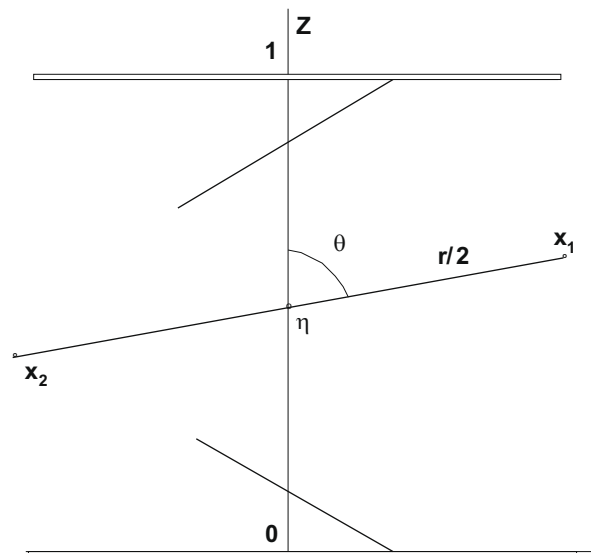


Fig. 1. Computational domain and independent variables.

on third variable ϕ . To reduce the number of independent variables the SCF is assumed to be independent of the direction angle θ . This is a very strong assumption but permissible for illustration of the method proposed (see the estimates made in [1]).

Thus we have

$$\frac{1}{2} \frac{\partial}{\partial z} (D(z) + D_m) \frac{\partial}{\partial z} R + \frac{1}{r^2} \frac{\partial}{\partial r} r^2 D_m \frac{\partial}{\partial r} R + (D(x_1) + D(x_2)) \frac{dC(z)}{dz} \Big|_{x_1} \frac{dC(z)}{dz} \Big|_{x_2} + \langle c'W(c) \rangle \bar{R} = 0 \quad (12)$$

Here, D_m is the coefficient that includes the eddy-diffusivity and molecular transport

$$D_m = 2D_m + (D(z + r/2) + D(z - r/2)) \cdot \left(1 - \frac{B_{LL}(r)}{B_{LL}(0)}\right) \quad (13)$$

and velocity correlation function was approximated as [1]: $B_{LL}(r)/B_{LL}(0) = \exp(-r^2/(4\lambda^2))$.

The chemical reaction rate is expressed:

$$W(c) = Da \cdot (c - c_{min}) \cdot (c_{max} - c) \text{ when } c_{min} < c < c_{max} \text{ and it is zero in other cases.} \quad (14)$$

The problem depends on the following dimensional parameters: the turbulent diffusivity at the layer center D_0 , the boundary layer thickness δ , the internal scale of the turbulent velocity field λ , and the molecular diffusivity D_m .

The value of the turbulent diffusivity is given as [1],

$$D(z) = D_0 D_1(z) D_1(1 - z) \quad (15)$$

where $D_1(z) = \frac{z^2/\delta^3}{D_{1m}(1+z^2/\delta^3)}$ and D_{1m} is the value of $D_1(z)$ at the center of the layer.

According to (15) the turbulent diffusivity is zero at the boundaries. Only in this case we can separate the effects of turbulent and molecular transports on the distribution of the averaged scalar. The third power in the expression for D_1 is chosen according to the conditions applied to the normal velocity component and the scale at the wall.

In our homogeneous case the balance equation for the averaged scalar $C(z)$ (10) takes the form

$$\frac{\partial}{\partial z} (D(z) + D_m) \frac{\partial}{\partial z} C(z) + \langle W(c) \rangle = 0 \quad (16)$$

3.1. Dimensionless variables

To bring the problem to a dimensionless view we used the layer width and the turbulent diffusivity D_0 . This yields the value of D_m to be a combination of the Reynolds and Prandtl or Schmidt numbers $D_m = k/(PrRe)$, where the Reynolds number is calculated by the fluctuation velocity u' and the layer width, whereas the value of k depends on the ratio of the integral scale of turbulence l to the width of the layer and the coefficient k_T in the relation $D = k_T u' l$. For $D_m = 0.0005$ and $Pr = 0.7$, characteristic for further calculations, the Reynolds number is equal to about 70,000.

3.2. Boundary conditions and calculation scheme

The fact that we have to calculate simultaneously the system of equations with a different set of independent variables results in dividing the boundary conditions into groups. The first group of the boundary conditions is used for the averaged field and the distribution function

$$\begin{aligned} z = 0 : \quad C(0) = 0, \quad F(0, c) &\equiv 0 \\ z = 1 : \quad C(1) = 1, \quad F(1, c) &\equiv 1 \end{aligned} \quad (17)$$

Additionally for the distribution function

$$\begin{aligned} c = 0 : \quad F(z, 0) &\equiv 1 \\ c = 1 : \quad F(z, 1) &\equiv 0 \end{aligned} \quad (18)$$

and finally for the SCF

$$\begin{aligned} z + r/2 = 1 : \quad R(z, r/2) &= 0 \\ z - r/2 = 0 : \quad R(z, r/2) &= 0 \end{aligned} \quad (19)$$

The relation between the equations is the following. The averaged field determines the boundary condition for the SCF when one of the points lies at the boundary of the computational domain. The correlation function determines the distribution of the variance and the micromixing rate (scalar dissipation). The variance is used for finding the PDF that is applied for averaging the terms depending on the reaction rate in Eqs. (16) and (12).

The averaged field was calculated using the DBVPFD subroutine from IMSL. It uses the Newtonian procedure involving automatic generation of a grid. Depending on the parameters Da and D_m , the number of nodes varied from 50 to 2000. The parameter determining the convergence of the equation for the averaged value was set to 10^{-9} . The SCF was calculated by means of the DLSLXG (IMSL) subroutine. The procedure enables solving a linear set of equations on the basis of the LU factorization and the Markovitz symmetric strategy for rarified matrices. The calculations were performed with a variable grid density (from 8×8 to 256×256). The SCF was calculated in a rectangular domain $0 < z < 1, 0 < |r| < z$ for $z < 0.5$ and $0 < |r| < 1 - z$ for $0.5 < z < 1$ under the zero boundary conditions.

4. Calculation results

4.1. Variation of scalar dissipation caused by variation of mean scalar field

The effect of chemical reactions on micromixing is characterized by the distribution of scalar dissipation. The scalar dissipation changes, first, due to varying averaged scalar field and related source term in the SCF equation and, second, due to a direct effect of chemical reactions on the equation for the SCF. An analysis of the latter effect is the main goal of the present study. In the present section we discuss the effect of variation of the averaged field on the scalar dissipation distribution. For this purpose the term including $\langle c'W(c) \rangle$ in the SCF equation is omitted.

The effect of the Damköhler number on the distribution of the averaged scalar (Fig. 2) is strongly pronounced in the vicinity of the boundaries where the averaged scalar gradients vary violently. Near the surface $z = 0$ the gradient grows, which can be explained by an increase of the averaged scalar in the layer. The scalar flux from the boundary also grows. Near the boundary $z = 1$ the scalar gradient decreases in comparison with a nonreacting case due to the disappearance of one chemical reaction component. The iteration process diverges when the Damköhler number exceeds 2.5. The calculations performed by the relaxation method reveal that such a behavior is attributed to the instability of the method for seeking a stationary solution.

The calculation of the averaged scalar field by the relaxation method was performed using the DMOLCH procedure (IMSL). The initial condition was the linear distribution over the layer width, which corresponds to the absence of turbulence and chemical reactions. The equation for the SCF was solved in the quasi-static formulation. This is consistent to the assumption that the variance of the scalar field reaches the stationary condition much faster than the averaged field itself.

Fig. 3 shows the process of reaching the stationary regime for $Da = 5$. This process can be divided into three stages: initial stage

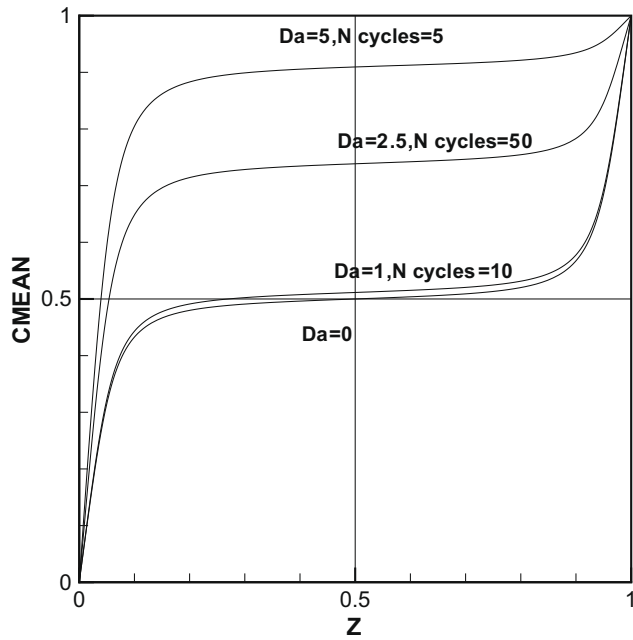


Fig. 2. Averaged scalar field for various Damköhler numbers. $c_{min} = 0.6, c_{max} = 0.9$.

up to the characteristic time $T = 0.8$, the main stage up $T = 10$, and the final stage. At the initial stage when the turbulent field with a appreciable level of variance develops, there is no reaction effect. At the main stage, the reaction zone is formed. The final stage is characterized by a stationary reaction regime corresponding to all previous examples for which the iteration method was used. As can be seen from Fig. 3, the maximum averaged reaction rate is first observed in the vicinity of the boundary $z = 1$, and then the maximum shifts to the opposite boundary in spite of the used dependence for the reaction rate, implying that the maximum reaction rate reaches the scalar value equal to 0.75.

The solution of the SCF equation is affected by the variance distribution $\langle c^2 \rangle$. Fig. 4 shows the appropriate distributions. Comparing them with those in Fig. 2 one can conclude that the higher values of the variance are observed in the regions of stronger gradients of the averaged field. The variance decrease due to that of gradients is much distinguished for large z and the Damköhler numbers. It is natural, since only the distribution of averaged values affects the solution of the SCF equation by varying the source term. These distributions are the starting ones for finding the PDF.

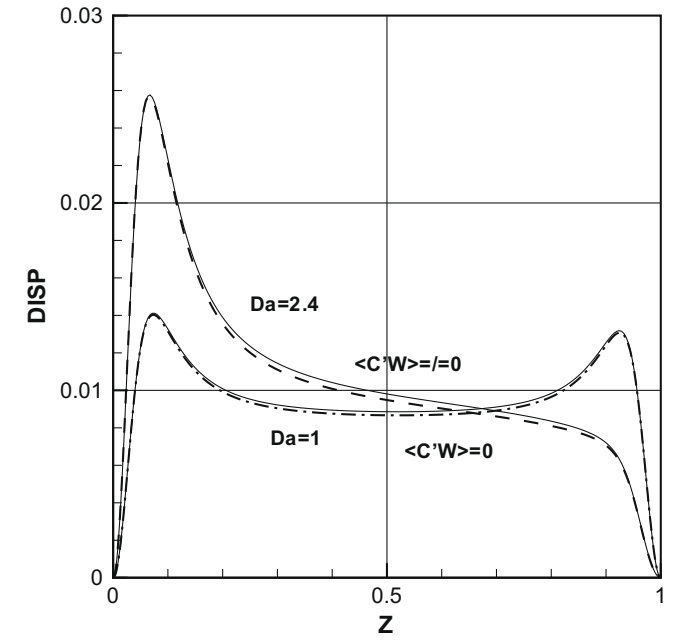


Fig. 4. Distribution of the scalar fluctuation for various Da with (solid lines) and without regard to the terms with $\langle cW \rangle$ in Eq. (9).

The main goal of our study on the modeling of turbulent reacting flows is to calculate the scalar dissipation. Fig. 5 shows the distributions of the scalar dissipation for various Damköhler numbers. The case under consideration is characterized by the dissipation concentration in the near-wall regions where the gradients of averaged values prevail.

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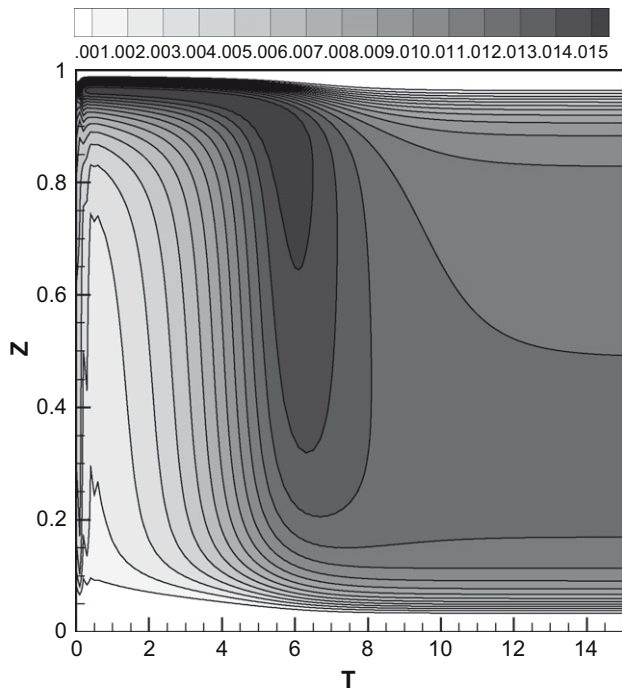


Fig. 3. Development of the reaction zone for $Da = 5$. Time variation of the averaged reaction rate distribution.

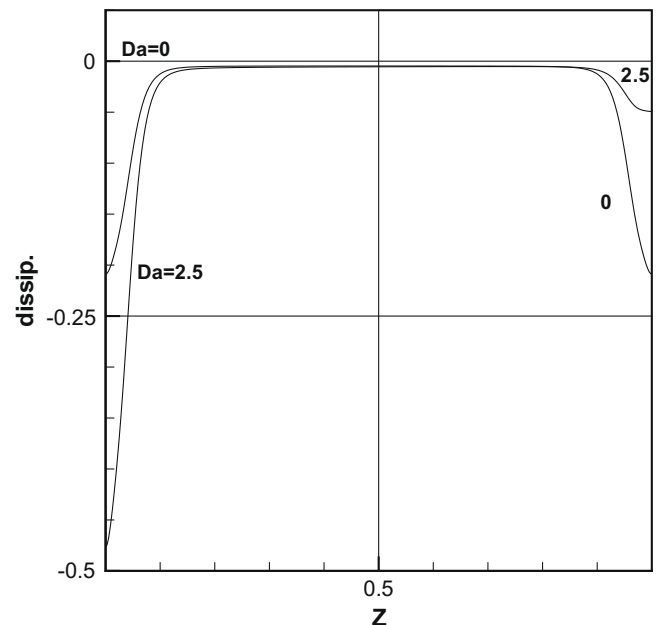


Fig. 5. Distribution of scalar dissipation for various Damköhler numbers.

4.2. Variation of scalar dissipation with regard to the direct effect of chemical reactions on the scalar correlation function

To clarify a direct effect of the chemical reaction on the scalar field structure we performed the calculations with the use of Eq. (9). Fig. 4 shows the fluctuation intensity distributions obtained with and without regard to the terms that directly depend on chemical reactions. It is surprising that the difference in the results is small. It can be explained by the fact that the regimes under consideration are characterized by thin zones of strong averaged gradients. In such zones the source terms in the equation for the SCF are very large, and their effect on the solution masks the direct effect of chemical reactions.

5. Conclusions

The micromixing model based on the equation for the scalar correlation function was used to describe the scalar field decay and the characteristic features of the mixing process in the 2D layer. To apply the proposed method for turbulent reacting flows the equation for the SCF is supplemented with a procedure of finding the PDF. This allows us to calculate the terms depending on the averaged chemical reaction rate. We are also able to describe the effect of the intensity of chemical reactions (the Damköhler number) on the distribution of the averaged scalar, variance, and scalar dissipation. Particular attention was paid to taking into account the direct effect of the chemical reactions in the equation for the SCF.

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References

- [1] V.P. Krasitskii, V.A. Frost, Molecular transfer in turbulent flows, *Izv. Ross. Akad. Nauk Mekhanika Zhidkosti i Gaza* 42 (2) (2007) 46–58 (in Russian), *Fluid Dyn.* 42 (2) (2007) 190–200.
- [2] V. Eswaran, E.E. O'Brien, A. Deckert, The modeling of the two-point probability density function of a reacting scalar in isotropic turbulence, *Combust. Sci. Technol.* 65 (1) (1989) 1–18.
- [3] K. Tsai, E.E. O'Brien, A hybrid one- and two-point approach for isothermal reacting flows in homogeneous turbulence, *Phys. Fluids A5* (11) (1993) 2901–2910.
- [4] V.A. Frost, The acceleration of molecular transfer in turbulent flows, *Dokl. Acad. Sci. USSR* 176 (4) (1967) 794–796 (in Russian).
- [5] V.P. Krasitskii, Approximate calculation of lagrangian statistic functions of fluid particle pairs in isotropic turbulence, *Boundary-Layer Meteorol.* 54 (1991) 231–247.
- [6] V.A. Sosinovich, V.A. Babenko, J.V. Zhukova, The closed equations for the joint PDF of fluctuations of turbulent reacting scalar and its gradient, *JEPTEP* 71 (5) (1998) 827–849.
- [7] K. Hasselmann, Zur Deutung der dreifachen Geschwindigkeitskorrelationen der isotropen Trbulenz, *Deutsch. Hydrogr. Z. B.11* (H.5) (1958) S.207–S.210.
- [8] V.A. Frost, V.P. Krasitskii, J. Hierro, Description of molecular mixing, in: S. Frolov, V. Frost, D. Roekaerts (Eds.), *Micromixing in Turbulent Reactive Flows in Turbulent Flows Based on Twopoint PDF Equation for Passive Scalar*, Torus Press, Moscow, 2004, pp. 57–63.