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NUMERICAL SOLUTION OF THE EQUATION FOR THE SINGLE-POINT PROBABILITY DENSITY FUNCTION OF TURBULENT FLUCTUATIONS OF A SCALAR FIELD

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Consideration is given to the problem of turbulent mixing behinning with the state of total unmixing of a scalar field on the molecular level. It is implemented by numerical integration of the equation for the single-point probability density function (PDF) $f_t(\Gamma)$ of fluctuations of a passive scalar field using the tools of solution of retrospective problems. The obtained evolution of $f_t(\Gamma)$ agrees with the results of a number of theoretical and experimental works.

Introduction. In the theory of turbulent combustion, the probabilistic description of interaction of the events of turbulent mixing and chemical reactions based on the use of the formalism of the PDF of the turbulent fluctuations has gained wide acceptance. The advantage of this method lies in the fact that in the equations for the PDF the source terms related to the production of mass in chemical reactions are expressed in closed form. In this approach, the problem of closing arises only for the terms characterizing the turbulent transfer and dissipation of fluctuations on the molecular level.

In the present work, consideration is given to the equation for the single-point PDF of fluctuations of a passive scalar field. Formally, this equation has the form of the equation of transfer of the scalar with a negative diffusion coefficient, which makes the problem under consideration similar to the classical incorrect problems [1], in particular, to the retrospective problem (the problem with inverse time) [2]. Such a structure of the equation does not allow direct use of conventional calculational procedures in numerical integration.

The aim of the work is to investigate turbulent mixing beginning with the state of total unmixing of a scalar field on the molecular level. This problem is implemented by numerically solving the equation for the single-point PDF $f_t(\Gamma)$ of fluctuations of a passive scalar field, statistically homogeneous on large length scales, using the tools of solution of retrospective problems. In the work, we give a short review of the methods of numerical solution of such problems.

Single-Point PDF Equation. We will consider a random scalar reacting field $c(x_i, t)$ (fluctuations of a mixture component), whose change is determined by the equation of balance [3]:

$$\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} = D \frac{\partial^2 c}{\partial x_i \partial x_i} + \omega (c) . \tag{1}$$

The single-point PDF $f_t(\Gamma)$ of the scalar is determined by the formula $f_t(\Gamma) = \langle \delta(c(x_i, t) - \Gamma) \rangle$ [4]. In deriving the equation for the function $f_t(\Gamma)$, use is made of the so-called finely dispersed probability density $\Phi(\Gamma, x_i, t) = \delta(c(x_i, t) - \Gamma)$ [4]; it is a function of the variable Γ and the functional of the field $c(x_i, t)$ and possesses the property that $\Phi(\Gamma, x_i, t)d\Gamma$ is equal to the probability of the values of c being a quantity equal

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to Γ at thr point x_i and at the time t. Thus, $f_t(\Gamma) = \langle \Phi \rangle$. Differentiating the function $\Phi(\Gamma, x_i, t)$ with respect to time and using (1) and the relation $\frac{\partial \Phi}{\partial t} = \frac{\partial \Phi}{\partial c}\frac{\partial c}{\partial t} = -\frac{\partial c}{\partial t}\frac{\partial \Phi}{\partial \Gamma}$, we can obtain an equation for the finely dispersed distribution function. Further averaging yields an equation for the single-point PDF $f_t(\Gamma)$. For the case of homogeneous fields on large length scales in an incompressible fluid without the process of chemical reacting, we have [3]

$$\frac{\partial f_t(\Gamma)}{\partial t} = -\frac{\partial^2}{\partial \Gamma^2}[\chi_t(\Gamma) f_t(\Gamma)], \quad -1 \le \Gamma \le 1, \tag{2}$$

where $\chi_t(\Gamma) = D\langle \frac{\partial c}{\partial x_i}\frac{\partial c}{\partial x_i} | c = \Gamma \rangle$ is the conventional dissipation rate of the intensity of scalar fluctuations. The term on the right-hand side of Eq. (2) describes diffusion in the space of the considered scalar quantity. Its unclosed form (since $\chi_t(\Gamma)$ is an unknown function) creates the main difficulty in describing the processes of turbulent mixing on the basis of the PDF. For closing it different models are suggested. For instance, in [5] the expression for $\chi_t(\Gamma)$ was obtained using the method of mapping functions in the form

$$\chi_t(\Gamma) = A(t) \exp\left\{-2[\mathrm{erf}^{-1}|\Gamma|]^2\right\}, \tag{3}$$

where $A(t) = \chi(t) \cot\{\pi[\langle c^2(0)\rangle - \langle c^2(t)\rangle]\}$. The functions $\langle c^2 \rangle$ and χ are the solution of the external problem. Let us assume that their evolution is known.

We choose the initial form of the function $f_t(\Gamma)$ in a form that corresponds to the state of total unmixing of a scalar field on the molecular level:

$$f_t(\Gamma)|_{t=0} = \frac{1}{2}[\delta(\Gamma + 1) + \delta(\Gamma - 1)]. \tag{4}$$

For the convenience of further numerical investigation, we introduce the integral distribution function $F_t(\Gamma) = \int_0^\Gamma f_t(\hat{\Gamma}) d\hat{\Gamma}$ and, taking into account symmetry of the function $\chi_t(\Gamma)$ and antisymmetry of $F_t(\Gamma)$, we write problem (2)–(4) for $0 \le \Gamma \le 1$ in terms of this function as

$$\frac{\partial F_t(\Gamma)}{\partial t} = -\frac{\partial}{\partial \Gamma}\left[\chi_t(\Gamma)\frac{\partial}{\partial \Gamma}F_t(\Gamma)\right] \tag{5}$$

with the corresponding initial

$$F_t(\Gamma)|_{t=0} = F_0 \tag{6}$$

and boundary conditions

$$F_t(\Gamma)|_{\Gamma=0} = 0, \quad F_t(\Gamma)|_{\Gamma=1} = 0.5. \tag{7}$$

Retrospective Problems and Some Methods of Their Numerical Solution. As has been mentioned in the Introduction, problem (2)–(4) (along with (5)–(7)) is similar to incorrect problems because the right-hand sides of the equations contain expressions having the form of the terms with a negative diffusion coef-

ficient in the phase space of the scalar values [1]. In particular, mathematically it can be considered as the retrospective problem of parametric identification according to the classification given in [2, 6–8], where an analysis is made of the state-of-the art and some prospects for the development of the methods of solution of such problems in thermophysical studies. This becomes completely clear if, for instance, in (5)–(7) we perform replacement of the time variable $\theta = T - t$:

$$\frac{\partial F_t}{\partial \theta} = \frac{\partial}{\partial \Gamma}\left[\chi_t (T - \theta, \Gamma) \frac{\partial F_t}{\partial \Gamma}\right], \tag{8}$$

$$\text{Boundary conditions: } F_t\big|_{\Gamma=0} = 0\,, \quad F_t\big|_{\Gamma=1} = 0.5\,. \tag{9}$$

Here, some additional information for $\theta = T$ is known, $F_t\big|_{\theta=T} = F_0$, and we seek the form of the function $F_t\big|_{\theta=0}$ at the initial time $\theta = 0$ that satisfies the measurement result at the end of the time interval $\theta = T$.

The general methodology of solution of incorrect problems is formulated in [1] based on the regularization theory and numerous methods and algorithms which implement the basic concepts of this theory. As applied to the formulation of the problem of the present work, we would like to note the methods with perturbation of the initial equation, namely, the quasi-inversion methods in different variants [9, 10]. Another class of methods is related to perturbation of the initial conditions and requires formulation of the problem as a problem of optimal control [11]. Based on the general results of the theory of construction and stability of difference schemes [12], algorithms are suggested to solve retrospective problems based on the regularization principle that allows one to obtain difference schemes of prescribed quality which approximate the retrospective problems and are uniformly stable in the initial data. Such an approach is described in [9]. For the type of inverse problems considered, completely stable difference schemes are constructed in [13, 14]. A particular case of them is the so-called superexplicit schemes representing standard schemes with weights [12] but with a negative choice of the weight parameter [15]. The iteration methods of solution of incorrect problems [16, 17], where the number of iterations consistent with the error of input data serves as the regularization parameter, and the gradient iteration methods with a variational formulation of the retrospective problem [2, 18] have found wide application.

Algorithm of Numerical Solution. One of the last mentioned approaches, i.e., the method of conjugate gradients [2, 18], was used in solving (5)–(7) for the integral distribution function $F_t(\Gamma)$ with the prescribed form (3) for the conventional rate of scalar dissipation $\chi_t(\Gamma)$. We reduce problem (8) and (9) to a form convenient for application of this method. We represent $F_t(\Gamma)$ as the sum $F_t(\Gamma) = F + F^*$, where $F(\Gamma, \theta)$ is the solution of the problem

$$\frac{\partial F}{\partial \theta} = \frac{\partial}{\partial \Gamma}\left[\chi_t (T - \theta, \Gamma) \frac{\partial F}{\partial \Gamma}\right], \tag{10}$$

$$\text{initial conditions: } F\big|_{\theta=0} = \xi(\Gamma) \text{ (in principle, this is the sought function),} \tag{11}$$

$$\text{boundary conditions: } F\big|_{\Gamma=0} = 0\,, \quad F\big|_{\Gamma=1} = 0\,. \tag{12}$$

It is known additionally that for $\theta = T$, $F\big|_{\theta=T} = F_0 - F^*\big|_{\theta=T} = \Psi(\Gamma)$. In turn, $F^*(\Gamma, \theta)$ is the solution of the following problem:

$$\frac{\partial F^*}{\partial \theta} = \frac{\partial}{\partial \Gamma}\left[\chi_t (T - \theta, \Gamma) \frac{\partial F^*}{\partial \Gamma}\right], \tag{13}$$

$$\text{initial conditions: } F^*\big|_{\theta=0} = F_0\,, \tag{14}$$

$$\text{boundary conditions: } F^*\big|_{\Gamma=0} = 0\,,\quad F^*\big|_{\Gamma=1} = 0.5\,. \tag{15}$$

The solution of (13)–(15) presents no difficulties, but that of (10)–(12) requires the use of the method of conjugate gradients [2, 18], whose idea consists of constructing an iteration algorithm that gives a sequence of approximations of $\{\xi^n\}$ beginning with some initial prescribed estimate ξ^0. A correction on each iteration is calculated from the condition of decrease in the objective functional in the form of the root-mean-square discrepancy

$$J(\xi) = \frac{1}{2}\int_0^1 (F(\xi, \Gamma, T) - \Psi(\Gamma))^2\, d\Gamma \to \min_{\xi}\,, \tag{16}$$

which determines the extent of deviation of the function $F(\xi^n, \Gamma, T)$ (the solution of (10)–(12) for $\xi = \xi^n$) from the known $\Psi(\Gamma)$. For this purpose, we introduce a function $\psi(\Gamma, \theta)$ such that $\psi(\Gamma, T) = F(\xi, \Gamma, T) - \Psi(\Gamma)$, and the gradient of functional (16) is found as the solution $\psi(\Gamma, 0)$ of the problem conjugate to 910)–(12):

$$\frac{\partial\psi}{\partial\theta} = -\frac{\partial}{\partial\Gamma}\left[\chi_t(T-\theta, \Gamma)\frac{\partial\psi}{\partial\Gamma}\right], \tag{17}$$

$$\text{initial condition: } \psi(\Gamma, T) = F(\xi, \Gamma, T) - \Psi(\Gamma)\,, \tag{18}$$

$$\text{boundary condition: } \psi\big|_{\Gamma=0} = 0\,,\quad \psi\big|_{\Gamma=1} = 0\,. \tag{19}$$

In terms of the conjugate function $\psi(\Gamma, \theta)$, a sequence of approximations of $\{\xi^n\}$ is constructed according to [2, 18]

$$\xi^{n+1} = \xi^n - \beta_n p_n\,,$$

where

$$\beta_n = \frac{(\psi_n(\Gamma, 0), p_n)}{(F(p_n, \Gamma, T), F(p_n, \Gamma, T))}\,,\quad p_n = \psi_n(\Gamma, 0) + \frac{(\psi_n(\Gamma, 0), \psi_n(\Gamma, 0))}{(\psi_{n-1}(\Gamma, 0), \psi_{n-1}(\Gamma, 0))}\,p_{n-1}\,,\quad p_0 = \psi_0(\Gamma, 0)\,,$$

(V, U) is the scalar product in the functional space L_2.

The algorithm of solving problem (10)–(12) involves the following steps:

1. Let ξ be an approximate value of ξ.
2. Next we solve problem (10)–(12) with the initial condition ξ^n.
3. We check the criterion of stop of the iteration process [2].
4. We solve problem (17)–(19) and find p_n.
5. We solve problem (10)–(12) with the initial condition p_n and calculate β_n.
6. We find ξ^{n+1} and pass to step 2.

Problems (10)–(12), (13)–(15), and (17)–(19) were solved numerically using an implicit difference scheme. We used a nonuniform grid for the space variable Γ and a uniform grid for the time variable. At the next time step, the values of the functions were found using the elimination algorithm [12].

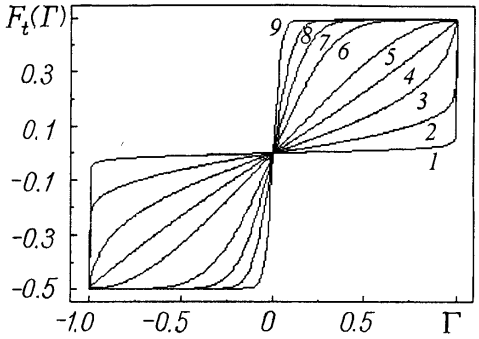

Fig. 1. Evolution of the integral distribution function $F_t(\Gamma)$: 1) t = 0; 2) 0.5; 3) 0.9; 4) 1.07; 5) 1.17; 6) 1.24; 7) 1.26; 8) 1.2685; 9) 1.27.

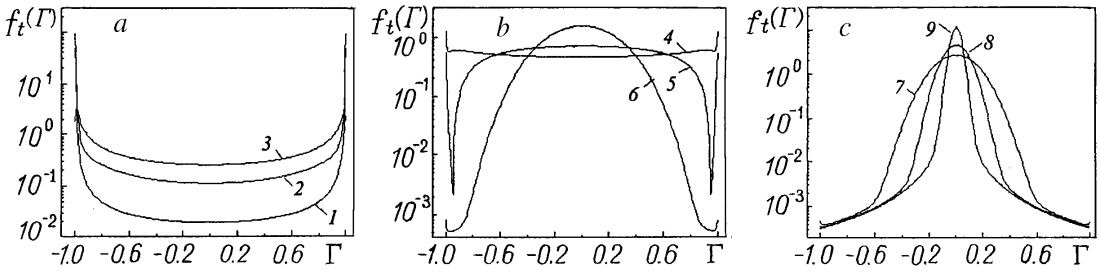

Fig. 2. Evolution of the single-point probability density function $f_t(\Gamma)$ in the initial (a), intermediate (b), and final (a) stages of mixing (notation is the same as in Fig. 1).

Results Obtained and Conclusions. The use of this algorithm has allowed integration of the equation for the function $F_t(\Gamma)$ with the prescribed conventional rate of scalar dissipation $\chi_t(\Gamma)$ at desired time intervals (Fig. 1). The evolution of the single-point PDF $f_t(\Gamma)$ of fluctuations of the scalar field in the initial stages of mixing is of a single-mode nature (Fig. 2a). Next, in the intermediate stages $f_t(\Gamma)$ acquires a double-mode form (Fig. 2b), which is indicative of the presence, in the flow, of unmixed components and those mixed to a molecular level simultaneously. As a result, $f_t(\Gamma)$ tends to the state corresponding to total mixing (Fig. 2c). Such behavior of this function was noted in a number of experimental and theoretical works [19–22].

In considering problems of evolution of the single-point PDF, the conventional rate of scalar dissipation of fluctuations of the scalar field, and the joint PDF of fluctuations of an isotropic turbulent scalar field and its gradient [20, 23] for the processes of turbulent mixing with chemical reactions, taking into account the multiscale nature of turbulent mixing [19], some computational features arise which are similar to those considered in the present work. Therefore, the results of the conducted computational experiment allow us to hope that the algorithms of solution of retrospective problems that we used can find further successful application in the indicated investigations.

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NOTATION

x_i, Cartesian coordinates; u_i, components of rate fluctuations; t and θ, time variables; T, bound of the time interval; D, diffusion coefficient; $\omega(c)$, function describing the rate fluctuations of a chemical reaction; $\langle\ \rangle$, operator of averaging over the ensemble of implementations; δ, Dirac function; Γ, independent PDF variable; $\mathrm{erf}^{-1}|\Gamma|$, function reciprocal of the integral of errors; $\langle c^2(t)\rangle$, variance of scalar fluctuations; $\chi(t)$, mean

dissipation rate of scalar fluctuations; $\hat{\Gamma}$, integration variable; J^n, functional on the nth iteration. Subscripts and superscripts: t, dependence on time; i = 1, 2, 3, number of the component; n, iteration number.

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