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A statistical turbulent reacting flow model

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Abstract—A model of the turbulent mixing of reagents is presented which involves the coupled integrodifferential equations for the functions that describe the distribution of the turbulent energy and of the root-mean-square value of scalar field fluctuations over different length scales, and also for the characteristic function which represents the Fourier transform of the one-point probability density of scalar field fluctuations. The model is intended to calculate the mean rate of chemical reaction in a turbulent flow in the case of 'very fast chemistry'. A numerical solution is given for the system of equations for different conditions and comparison with experimental data is made. The possible way of extending the model to the case of a 'moderately fast chemistry' is suggested.

INTRODUCTION

WHEN studying the turbulent mixing of reacting gases it is important to distinguish between two aspects of the process: the dynamics of the length scales and the dynamics of the scalar field concentration scales of reagents. The length scale dynamics are determined by the turbulent microscopic motion of mixing gases. The concentration scale dynamics are connected with the effect of molecular diffusion. The interaction between these two aspects of turbulent mixing occurs due to the evolution of the spectrum of length scales creating steadily varying boundary conditions for molecular diffusion.

In the present paper the consideration will be limited to the following problem. Let two reagents, A and B, mix up in a turbulent flow and the chemical reaction produce the product P

$$\mathrm{A} + n\mathrm{B} \xrightarrow{w_r} \mathrm{P}. \tag{1}$$

Here n is the stoichiometric coefficient, w_r is the chemical reaction rate in the case when the reagents A and B are mixed up into a homogeneous molecular mixture. This quantity will be regarded as being much greater than the rate of turbulent mixing of reagents w_t, thus limiting the discussion to the case of large Damköhler numbers

$$Da = \frac{w_r}{w_t}. \tag{2}$$

As is known [1], in order to determine the mean rate of chemical reaction in a turbulent flow it is sufficient in this case to know the statistical properties of one passive scalar field determined by the formula

$$\hat{C}(\mathbf{x}, t) = nC_A(\mathbf{x}, t) - C_B(\mathbf{x}, t). \tag{3}$$

The scalar field $\hat{C}(\mathbf{x}, t)$ is described by the equation

$$\frac{\partial \hat{C}}{\partial t} + \mathbf{u} \cdot \nabla \hat{C} = D \Delta \hat{C}. \tag{4}$$

Here $\mathbf{u}$ is the velocity field, the equation for which will be given later; D is the diffusion coefficient which is taken to be the same for both reagents A and B.

In the case when there are chemical reactors into which each of the components A and B enter as one or more jets, then, by designating these jets by the numbers 1 and 2, respectively, it is possible to write the boundary conditions for the scalar field over the inlets to the reactor in the form

$$\hat{C}|_1 = nC_{A0} \tag{5}$$

where C_{A0} is the concentration of reagent A at the inlet to the reactor numbered 1

$$\hat{C}|_2 = -C_{B0} \tag{5'}$$

where C_{B0} is the concentration of reagent B at the inlet to the reactor numbered 2.

Thus, the passive scalar field $\hat{C}(\mathbf{x}, t)$, defined by equality (3), is described by equation (4) with boundary conditions (5) and (5′).

The mean concentration of reagent A can be calculated by the formula

$$\langle C_A(t) \rangle = \frac{1}{n} \int_{\beta - 1}^{\beta/\hat{\beta} + \beta} (C + 1 - \beta) f_t(C) \, \mathrm{d}C. \tag{6}$$

Here $f_t(C)$ is the probability density function of the scalar field fluctuations $c = \hat{C} - \langle \hat{C} \rangle$, which, in the case of an isotropic flow behind a grid, depends on the time variable t and, in the case of one-dimensional treatment of inhomogeneous flows, depends on the longitudinal coordinate x. The quantity $\hat{\beta}$ determines the relationship between the concentrations of reagents A and B prior to their mixing

NOMENCLATURE

$B^c(r, x)$	two-point second-order moment of the turbulent reagent scalar field
$c(\mathbf{x}, t)$	fluctuation of scalar field $\hat{C}(\mathbf{x}, t)$, $\hat{C}(\mathbf{x}, t) - \langle \hat{C}(\mathbf{x}, t) \rangle$
$\hat{C}(\mathbf{x}, t)$	passive scalar field determined by formula (3)
$d(x)$	root-mean-square value of scalar fluctuations, $\langle c^2(x) \rangle / \langle c^2(0) \rangle$
Da	Damköhler number
$f_x(C)$	probability density function of the scalar field fluctuations
$F(x)$	fractional conversion, $1 - [\langle \hat{C}(x) \rangle / \langle \hat{C}(0) \rangle]$
$N(x)$	rate of scalar fluctuation intensity dissipation
$N_p(x)$	rate of pumping of the scalar field turbulent fluctuation intensity
$P_x(r)$	distribution of the turbulent velocity fluctuation energy over different length scales
$P_x^c(r)$	distribution of the intensity of fluctuation $c(\mathbf{x}, t)$ over different length scales
$T_x(r)$	two-point, third-order moment of the turbulent reagent scalar field
$U(x)$	cross-section-mean flow velocity
w_r	chemical reaction rate
w_t	rate of turbulent mixing of reagents.
Greek symbols	
$\varphi_x(\eta)$	one-point characteristic function of scalar field $c(\mathbf{x}, t)$.

$$\beta = \frac{C_{B0}}{nC_{A0}}. \tag{7}$$

The quantity β is called the stoichiometric ratio, it determines the ratio of the mean concentrations of reagents B and A in the initial cross-section of the reactor

$$\beta = \frac{\langle C_B(0) \rangle}{n \langle C_A(0) \rangle}. \tag{8}$$

Note, that all the quantities in formula (6) are nondimensionalized through division by the quantity $n\langle C_A(0) \rangle$.

It is clear that the quantities $\langle C_B(0) \rangle$ and $\langle C_A(0) \rangle$ should be prescribed independently of the quantities C_{B0} and C_{A0} since their magnitudes are determined by the conditions of the supply of reagents to the reactor. The probability density function $f_0(C)$ in the initial cross-section, where the reagents A and B are in a completely segregated state, is determined by the expression

$$f_0(C) = \frac{1}{\beta + \hat{\beta}}[\beta\delta(C + 1 + \hat{\beta}) + \hat{\beta}\delta(C - \beta/\hat{\beta} - \beta)], \tag{9}$$

from which it is seen that for the nondimensionalized fluctuations of the field $\hat{C}$ the distribution function depends on two dimensionless parameters β and $\hat{\beta}$.

To describe qualitatively and quantitatively the process of turbulent mixing of reagents it is convenient to have two functions which would characterize the field $c(x, t)$: the function $P_t^c(r)$, which describes the distribution of the intensity of fluctuations $c(\mathbf{x}, t)$ of the field $\hat{C}(\mathbf{x}, t)$ over different length scales, and the function $f_t(C)$, which describes the probability distribution of the fluctuations $c(\mathbf{x}, t)$ of the scalar field $\hat{C}(\mathbf{x}, t)$. Using these two functions for the description of the entire process of turbulent mixing to the molecular level, consider, for example, the mixing of the scalar field in an isotropic turbulent flow. On having introduced, into a gas flow behind a grid which produces the turbulent field of velocity fluctuations, the scalar field with the aid of another grid, the evolution of this field will provide a good example of the process of turbulent mixing. Over the initial stage of mixing there occurs the formation of the range of the scalar field length scales resulting in the evolution of the function $P_t^c(r)$ from the form, which corresponds to the presence of mainly large-scale scalar formations in the flow with the length scale of the order of the size of the grid mesh, up to a smooth function, which corresponds to the presence in the flow of scalar formations of all possible scales. The one-point probability density $f_t(C)$ remains nearly the same at this stage of mixing. Though the reagents are mixed, on average by large vortices, they do not come into contact yet and, therefore, each of them is in a pure form in the flow and there are no intermediate concentrations. The probability density $f_t(C)$ has the form of the sum of two δ-functions, equation (9). Next, the small-scale flow structure becomes operative in the mixing. A further intensive development of the ranges of scales takes place, and, consequently, of the form of the function $P_t^c(r)$. The probability density of concentrations $f_t(C)$ still varies insignificantly. Only when a noticeable fraction of the Kolmogorov order length scales appears in the flow and the boundary of contact between the two reagents becomes rather developed, does the culminating stage of the process of mixing begin. As a result, a large amount of a homogeneous mixture appears in the flow. The probability density of concentrations $f_t(C)$ undergoes a strong variation: when at the beginning it could be approximated by formula (9), then at the end this is a smooth function indicating the presence of concentrations of all the magnitudes in the flow. During this stage the function $P_t^c(r)$ varies slowly tending to zero at small values of r, because small length scales decay faster than large ones. Having further traced the process of mixing, it is possible to see that finally $f_t(C)$ acquires the form close to $\delta(C)$ indicating the presence of a homogeneous mixture in the flow and the absence of the fluctuations of concentrations. In this case the function $P_t^c(r)$ tends to zero at all values of r.

It follows from the aforegoing representation of turbulent mixing that the functions $P_t^c(r)$ and $f_t(C)$ are rather sensitive indicators of the process and are suited for its qualitative and quantitative description.

DETERMINATION OF THE FUNCTIONS $P_t^c(r)$, $f_t(C)$ AND $P_t(r)$

Thus, far, the functions $P_t^c(r)$ and $f_t(C)$ have been considered only qualitatively, leaving aside the problem of their formal determination in terms of the measured statistical characteristics of turbulence. As a function describing the scalar field fluctuation distribution intensity over different length scales it is possible to select the spectral function $E^c(k,t)$, the correlation function $B^c(r,t)$, the structural function $D^c(r,t)$, or the function $P_t^c(r)$ connected with the above functions by the following formulae

$$\begin{aligned} P_t^c(r) &= -\frac{\partial}{\partial r}B^c(r,t) \\ &= \frac{1}{2}\frac{\partial}{\partial r}D^c(r,t) \\ &= \int_0^\infty \left[\frac{\sin kr}{(kr)^2} - \frac{\cos kr}{kr}\right] kE^c(k,t)\,\mathrm{d}k. \end{aligned} \tag{10}$$

In all the designations the superscript 'c' is the symbol of the scalar field. The physical meaning of the function $P_t^c(r)$ as the turbulent scalar field fluctuation density is well illustrated by the following equality

$$\int_0^\infty P_t^c(r)\,\mathrm{d}r = B^c(0,t) = \langle c^2(t)\rangle \tag{10'}$$

where $\langle c^2(t)\rangle$ is the r.m.s. intensity of scalar field fluctuations.

When the function $P_t^c(r)$ is known, any of the functions $B^c(r,t)$, $D^c(r,t)$, $E^c(k,t)$ can be calculated from the following formulae:

$$\begin{aligned} B^c(r,t) &= \int_r^\infty P_t^c(r)\,\mathrm{d}r; \\ D^c(r,t) &= 2\int_0^r P_t^c(r)\,\mathrm{d}r; \\ E^c(k,t) &= \frac{2}{\pi k}\int_0^\infty (\sin kr - kr\cos kr)P_t^c(r)\,\mathrm{d}r. \end{aligned} \tag{11}$$

As a function which would describe the probability distribution of scalar field fluctuations $c(\mathbf{x},t)$, it is possible to take the probability density function $f_t(C)$ or the one-point characteristic function, coupled with the former through the Fourier transform,

$$\begin{aligned} \varphi_t(\eta) &= \int_{-(1+\hat{\beta})}^{\beta/\hat{\beta}+\beta} \mathrm{e}^{i\eta C} f_t(C)\,\mathrm{d}C; \\ f_t(C) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-i\eta C}\varphi_t(\eta)\,\mathrm{d}\eta. \end{aligned} \tag{12}$$

Here the variable C is nondimensionalized through the division by the quantity $n\langle C_A(0)\rangle$.

In the present paper the characteristic function $\varphi_t(\eta)$ will be used.

In what follows a function will be needed which would describe the turbulent velocity fluctuation energy distribution over different length scales. For this function it is possible to take the energy spectral density $E(k,t)$, the correlational function $B(r,t)$, the structural function $D(r,t)$ or their related function $P_t(r)$:

$$\begin{aligned} P_t(r) &= -\frac{\partial}{\partial r}B(r,t) = \frac{1}{2}\frac{\partial}{\partial r}D(r,t) \\ &= 2\int_0^\infty \left\{\left[\frac{3}{(kr)^4} - \frac{1}{(kr)^2}\right]\sin kr \right. \\ &\qquad \left. - \frac{3}{(kr)^3}\cos kr\right\} kE(k,t)\,\mathrm{d}k. \end{aligned} \tag{13}$$

The physical meaning of the function $P_t(r)$ as the turbulent fluctuational energy density in the space of length scales is seen from the following equality

$$\int_0^\infty P_t(r)\,\mathrm{d}r = B(0,t) = \frac{2}{3}q \tag{14}$$

where q is the r.m.s. energy of turbulent velocity fluctuations.

As shown earlier [2], the function $P_t(r)$ has some advantages over the other listed functions in the theoretical description of turbulence. The main argument for the selection of the function $P_t(r)$ is its decaying form in the inertial range of scales thus admitting the assignment of this function at any r without reference to the system size. The other functions, for example $D(r)$ and $E(k)$, do not possess this property. Moreover, the function $P_t(r)$ is directly connected with the correlational function of the velocity field vorticity $\omega = \operatorname{rot}\mathbf{u}$ [2]

$$\langle \omega_1' \omega_1'' \rangle = \left(\frac{\partial}{\partial r} + \frac{4}{r}\right)P_t(r).$$

The vorticity approach to the turbulence theory seems to be intuitively more substantiated than that based on the velocity field. In the present paper, the functions $P_t(r)$ and $P_t^c(r)$ will be used to describe the spectral state of the flow.

When the function $P_t(r)$ is known, then any of the functions $B(r, t)$ and $D(r, t)$ can be calculated from the formulae similar to formula (11). The function $E(k, t)$ can be calculated from the formula

$$E(k,t) = \frac{1}{\pi k} \int_0^\infty [(3 - k^2r^2)\sin kr - 3kr\cos kr]P_t(r)\,\mathrm{d}r. \quad (15)$$

A CLOSED EQUATION FOR *Pt(r)*

Since the field $\hat{C}(\mathbf{x}, t)$, defined by formula (3), is the field of the passive scalar, the following equation can be used as the initial equation for the fluctuations $c = \hat{C} - \langle \hat{C} \rangle$

$$\frac{\partial c}{\partial t} + \frac{\partial (u_i' c)}{\partial x_i} = D\Delta c + \varphi(\mathbf{x}, t). \quad (16)$$

Here $\varphi(\mathbf{x}, t)$ is the external casual force with the prescribed statistical properties: normal distribution of probabilities and the δ-correlativeness in time [3]. The parameters of this distribution will be so selected that this term could model the influence of the change in the scalar field mean characteristics on the field of fluctuations.

The field of velocity fluctuations u_i' in equation (16) will be described by the following equation

$$\frac{\partial u_i'}{\partial t} = -\frac{\partial u_i' u_k'}{\partial x_k} - \frac{1}{\langle \rho \rangle}\frac{\partial P'}{\partial x_i} + v\frac{\partial^2 u_i'}{\partial x_k \partial x_k} - \langle u_k \rangle \frac{\partial u_i'}{\partial x_k} - u_k' \frac{\partial \langle u_i \rangle}{\partial x_k} + f_i(\mathbf{x}, t). \quad (17)$$

Here $\langle u_k \rangle$ is the mean velocity determined by the homogeneous deformation rate which will be considered as given; $\langle \rho \rangle$ is the mean medium density which is also a given function; $f_i(\mathbf{x}, t)$ is the external casual force in terms of which the interaction between the velocity fluctuations and the mean flow will be taken into account.

Equation (17) is valid in the coordinate system moving with the velocity $U(x)$. It differs from the equation of isotropic turbulence with a time-varying density [4] by the presence of the term $f_i(\mathbf{x}, t)$. This term in equation (17) is taken to be the external casual force with the prescribed statistical properties: the normal distribution of probabilities and δ-correlativeness in time. In this case, the distribution parameters are so selected that this term could model the transport of energy from the mean velocity field to the fluctuational velocity field. The model, represented by equation (17), can be used to describe the fluctuational velocity field in the inhomogeneous turbulent flow field. The main aspects of the interaction between the fluctuational field and the inhomogeneous turbulent flow will be taken into account by the last three terms on the RHS of equation (17).

By resorting to the familiar technique of the correlational function derivation from the equation for fluctuations and also by using the results of work [4], representing the variation of $\langle u_k \rangle$ in terms of the flow deformation parameters, the definition of equation (10) and the analogy between the turbulent and molecular diffusion to bring about the closure, then it is possible to obtain a closed equation for the function $P_t^c(\mathrm{r})$ [10]. Then, converting to the fixed coordinate system and limiting the discussion to the case stationary in time, the following form of the closed equation for the function $P_x^c(r)$ can be obtained:

$$U(x)\frac{\partial P_x^c(r)}{\partial x} = 2\beta\sqrt{rP_x(r)}\left(\frac{\partial}{\partial x} + \frac{2}{r}\right)P_x^c(r) + 2\left[D(x) + \beta\int_0^r \sqrt{r'P_x(r')}\,\mathrm{d}r'\right]\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{2}{r^2}\right)P_x^c(r) - \Phi(x)\left(1 + r\frac{\partial}{\partial r}\right)P_x^c(r) + 4N_\mathrm{p}(x)\frac{\mathrm{r}}{L_\mathrm{c}^2(x)}\exp\left[-\frac{r^2}{L_\mathrm{c}^2(x)}\right]. \quad (18)$$

Here $D(x)$ is the kinematic diffusion coefficient which can depend on the longitudinal coordinate because of the change in the mean temperature

$$\Phi(x) = \frac{1}{\lambda}\frac{\mathrm{d}\lambda}{\mathrm{d}x}; \qquad \lambda = \sqrt[3]{\langle \rho(0) \rangle / \langle \rho(x) \rangle} \quad (19)$$

$N_\mathrm{p}(x)$ is the rate of pumping of the scalar field turbulent fluctuation intensity, $L_\mathrm{c}(x)$ is the scalar field macroscale; the pumping of the scalar fluctuation intensity takes place over the scale of the order of $L_\mathrm{c}(x)$. The functions $U(x)$, $\Phi(x)$, $N_\mathrm{p}(x)$ and $L_\mathrm{c}(x)$ are the prescribed parameters within the framework of the present approach and can be obtained experimentally or calculated from the solution of a one-point momentum model.

The boundary condition for the function $P_x^c(r)$ at $x = 0$ can be taken in the form

$$P_0^c(r) = \frac{2B^c(0)r}{L_\mathrm{c}^2(0)}\exp\left[-\frac{r^2}{L_\mathrm{c}^2(0)}\right]. \quad (20)$$

Formula (20) may prove useful in the case of a scalar turbulent field with one characteristic scale $L_\mathrm{c}(0)$. If in the initial cross-section there is a developed range of length scales, then it is possible to make an attempt to approximate the initial function by the following formula

$$P_0^c(r) = 2B^c(0)r\int_0^\infty \frac{\mathrm{d}}{\lambda^2}\exp\left(-\frac{r^2}{\lambda^2}\right)f(\lambda; L_\mathrm{c}; \sigma_\mathrm{c}) \quad (21)$$

where $f(\lambda;\ L_\mathrm{c};\ \sigma_\mathrm{c})$ is the scale probability density function which depends on both the mean scale and variance of scales. The distribution of the probabilities $f(\lambda, L_c, \sigma_c)$ can be selected differently. For example, it is possible to select the uniform, the Poisson, or any other distribution. By varying the parameters of the selected distribution, it is possible to choose the form of the function $P_0^c(r)$ close to the experimental one. The constant β in equation (18) can be coupled with the constant s in the '2/3 law' for the structural function $D^c(r, t)$ by solving this equation in the inertia-convective range of scales. The corresponding formula has the form [10]:

$$\beta = \frac{2.4\sqrt{3}}{\sqrt{cs}}. \qquad (22)$$

Here c is the constant in the '2/3 law' for the velocity structural function. Since $s = 2.8$ and $c = 1.9$ [3], $\beta = 1.08$.

Equation (18) involves the function $P_x(r)$ for which a separate equation should be written. In the same approximation as for equation (18), the following closed equation can be obtained for the function $P_x(r)$ [10]:

$$U(x)\frac{\partial P_x(r)}{\partial x} = 2\gamma\sqrt{rP_x(r)}\left(\frac{\partial}{\partial r} + \frac{4}{r}\right)P_x(r)$$
$$+ 2\left[v(x) + \gamma\int_0^r \sqrt{r'P_x(r')}\,\mathrm{d}r'\right]$$
$$\left(\frac{\partial^2}{\partial r^2} + \frac{4}{r}\frac{\partial}{\partial r} - \frac{4}{r^2}\right)P_x(r) - \Phi(x)\left(3 + r\frac{\partial}{\partial r}\right)P_x(r)$$
$$+ \frac{4}{3}\varepsilon_p(x)\frac{r}{L^2(x)}\exp\left[-\frac{r^2}{L^2(x)}\right]. \qquad (23)$$

Here $v(x)$ is the kinematic viscosity coefficient; $\varepsilon_p(x)$ is the rate of turbulent energy pumping from the side of the mean velocity field; $L(x)$ the macroscale of the fluctuational velocity field; the pumping of the turbulent energy is made over the scale of order $L(x)$. Just as in the case of equation (18), the functions $U(x)$, $\Phi(x)$, $\varepsilon_p(x)$ and $L(x)$ should be given. The boundary condition for the function $P_x(r)$ can be taken in the form of equation (20) or (21) with the replacement $L_c(0) \to L(0)$, $B^c(0) \to B(0)$, $\sigma_c \to \sigma$, where σ is the variance of length scales for the velocity field in the initial cross-section. The constant γ in equation (23) can be expressed in terms of the constant c from the '2/3 law' for the structural velocity field function by solving this equation in the inertia range of scales. The corresponding formula has the form [10]:

$$\gamma = \frac{12}{11\sqrt{3}\,c^{3/2}}. \qquad (24)$$

Since $c = 1.9$, then $\gamma = 0.24$.

The system of equations (18) and (23) with the corresponding boundary conditions and familiar background functions $U(x)$, $\Phi(x)$, $N_p(x)$, $\varepsilon_p(x)$, $L_c(x)$, and $L(x)$ can be solved numerically to obtain the evolution of the functions $P_x(r)$ and $P_x^c(r)$ along the axis x. By solving the system of equations (18) and (23) it is possible to calculate the evolution of some of the parameters of these functions which more clearly illustrate the process of turbulent mixing. The rate of scalar fluctuation intensity dissipation is calculated by the formula

$$N(x) = 3D\lim_{r\to 0}\frac{\partial}{\partial r}P_x^c(r). \qquad (25)$$

The intensity of scalar fluctuations is determined from formula (10′). Of certain interest are the mean scale evolution and the variance of the scalar fluctuational field scales

$$\langle\lambda(x)\rangle = \frac{1}{B^c(x)}\int_0^\infty rP_x^c(r)\,\mathrm{d}r \qquad (26)$$

$$\sigma(x) = \sqrt{\langle\lambda^2(x)\rangle - \langle\lambda(x)\rangle^2}. \qquad (27)$$

Some of these characteristics are required to solve the equation for the one-point characteristic function.

A CLOSED EQUATION FOR THE PROBABILITY DISTRIBUTION OF SCALAR FIELD VALUES

The problem of the derivation of a closed equation for the function $f_x(C)$ which describes the distribution of the scalar field probabilities turns to be rather involved [5]. It is possible to state that as yet there is no wholly satisfactory form of the closed equation for $f_x(C)$. Most interesting solutions of this problem are suggested in works [6, 7] on whose basis a number of practical calculations were carried out.

In the present work a closed equation is suggested for the characteristic function $\varphi_x(\eta)$, which is connected with the function $f_x(C)$ by formulae (12).

The process of turbulent mixing in terms of the characteristic function $\varphi_x(\eta)$ for the fluctuational field $c = \hat{C} - \langle\hat{C}\rangle$ in the simplest case of $\beta = \hat{\beta} = 1$ is as follows. At the initial time instant, to the entirely non-mixed field (nondimensionalized through division by the quantity $n\langle C_A(0)\rangle$) there corresponds the function

$$\varphi_x(\eta) = \cos 2\eta. \qquad (28)$$

To the sinusoidal, i.e. slightly mixed, field $c(x, t)$ there corresponds the function

$$\varphi_x(\eta) = J_0(2\eta), \qquad (29)$$

where $J_0(x)$ is the zero-order Bessel function.

When the field $c(x, t)$ is rather well mixed and the distribution of the probabilities of fluctuations becomes uniform, then to this state there corresponds the characteristic function

$$\varphi_x(\eta) = \frac{\sin 2\eta}{2\eta}. \qquad (30)$$

Passing through a number of intermediate forms, the function $\varphi_x(\eta)$ for the flow, mixed up to the molecular level, acquires the form

$$\varphi_x(\eta) = 1. \tag{31}$$

The use of the characteristic function instead of the probability density gives some advantages. Thus, it makes the introduction of δ-functions unnecessary and this is of importance for numerical solutions of equations. The region for the determination of the function $\varphi_x(\eta)$ represents an infinite interval which poses certain difficulties in solving equations and computing integrals.

Using equation (16) as a dynamic equation for the scalar field fluctuations $C(x, t)$ and assuming that the field of velocity fluctuations varies in conformity with equation (17), it is possible to obtain a closed equation for the function $\varphi_x(\eta)$ [8,9]. In a fixed coordinate system it can be written as

$$\begin{aligned} U(x)\frac{\partial\varphi_x(\eta)}{\partial x} &= \frac{1}{2}\eta^2\tilde{N}(x)[1-(\alpha+1)d^{\alpha}(x)]\varphi_x(\eta) \\ &\quad - \frac{(\alpha+1)[\varphi_x(\eta)-\varphi_x^0(\eta)]}{\tau_r(x)}. \end{aligned} \tag{32}$$

Here the function $\tilde{N}(x)$ is determined by the following formula

$$\tilde{N}(x) = N(x) - N_p(x) \tag{33}$$

where $N(x)$ is determined by formula (25).

The function $N(x)$ designates the rate of scalar fluctuation intensity dissipation. The function $N_p(x)$ determines the rate of this intensity pumping from the side of the mean field and, within the framework of the present approach, is a given parameter which can be calculated by solving a one-point turbulent model or measured experimentally.

The function $d(x)$ is determined by the formula

$$d(x) = \frac{\langle c^2(x)\rangle}{\langle c^2(x)\rangle}. \tag{34}$$

The value of the parameter α satisfies the condition $\alpha < 0.2$ which follows from the requirement that the moments calculated from the function $\varphi_x(\eta)$ should vary monotonously. The specific value $\alpha = 0.18$ was selected by comparing the predicted results with the experimental data of work [1].

The characteristic relaxation time $\tau_r(x)$ is prescribed by the formula

$$\tau_r(x) = \frac{\langle c^2(x)\rangle}{\hat{N}(x)}. \tag{35}$$

The function $\varphi_x^0(\eta)$ is determined as follows

$$\varphi_x^0(\eta) = \exp\left\{-\frac{1}{2}\eta^2\langle c^2(x)\rangle[1-\alpha(x)]\right\}. \tag{36}$$

As the boundary condition along x for the function $\varphi_x(\eta)$ one may take to be the function in the form of equation (28) which corresponds to a fully segregated state of the scalar field.

SOLUTION OF THE SYSTEM OF EQUATIONS

Thus, the proposed statistical model of turbulent mixing involves three equations: (18), (23), (32). This system was solved numerically for the case when the pumping of turbulence energy and of scalar fluctuation intensities is equal to zero and the entire process of evolution is governed by the damping of the magnitudes of these quantities prescribed in the initial cross-section. As the boundary condition for $P_x^c(r)$ at $x = 0$ use was made of the function in the form of equation (21) with $f_x(\lambda, L_c, \sigma_c)$ in the form of uniform distribution

$$\begin{aligned} f(\lambda, L_c, \sigma_c) = \frac{1}{\sigma_c}\Bigg\{\theta\left[r-\left(L_c-\frac{\sigma_c}{2}\right)\right] \\ - \theta\left[r-\left(L_c+\frac{\sigma_c}{2}\right)\right]\Bigg\} \end{aligned} \tag{37}$$

where $\theta(x)$ is the Heavyside function.

In this case the function $P_0^c(r)$ has the form

$$\begin{aligned} P_0^c(r) = \frac{\sqrt{\pi}B^c(0)}{\sigma_c}\Bigg[\mathrm{erf}\left(\frac{r}{L_c-\sigma_c/2}\right) \\ - \mathrm{erf}\left(\frac{r}{L_c+\sigma_c/2}\right)\Bigg]. \end{aligned} \tag{38}$$

The boundary condition for the function $P_x(r)$ was selected in the form similar to that of equation (38) with the replacement $B^c(0) \rightarrow B(0)$, $L_c \rightarrow L$, $\sigma_c \rightarrow \sigma$, where $B(0)$, L, σ are the r.m.s. energy, mean scale and variance of velocity field scales.

The initial condition for the characteristic function $\varphi_x(\eta)$ was selected in the form

$$\begin{aligned} \varphi_0(\eta) = \frac{1}{\beta+\hat{\beta}}\Bigg\{\Bigg[\beta\cos(\eta(1+\hat{\beta})) \\ + \hat{\beta}\cos\left(\eta\left(\frac{\beta}{\hat{\beta}}+\beta\right)\right)\Bigg] + i\Bigg[-\beta\sin(\eta(1+\hat{\beta})) \\ + \hat{\beta}\sin\left(\eta\left(\frac{\beta}{\hat{\beta}}+\beta\right)\right)\Bigg]\Bigg\} \end{aligned} \tag{39}$$

which represents the Fourier transform of the function $f_0(C)$ in the form of equation (9) and describes the one-point statistics of completely segregated scalar field fluctuations $\hat{C}(\mathbf{x}, t)$ determined by formula (3).

Since the characteristic function is generally a complex one, then equation (32) is split up into two equations for the the real and imaginary parts of the function $\varphi_x(\eta)$.

The mean reagent concentration at an arbitrary point x is calculated by the formula

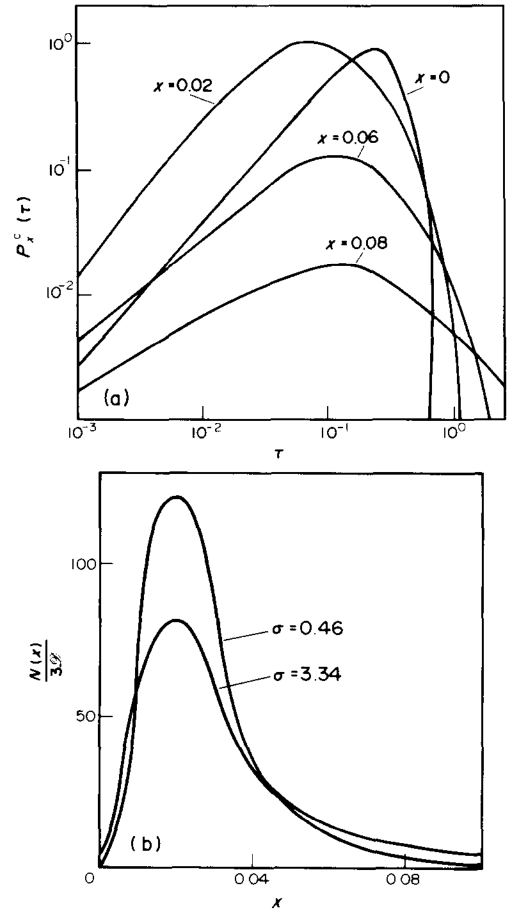

FIG. 1. (a) Evolution of the function $P_x^c(r)$ for the case of a 'fast chemical reaction'. (b) Variation of the mean rate of scalar fluctuation intensity dissipation.

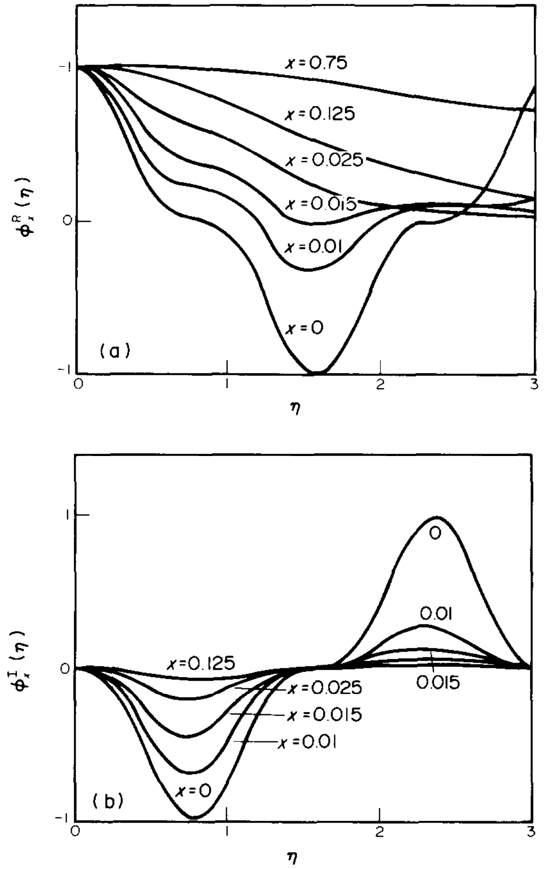

FIG. 2. Evolution of the real (a) and imaginary (b) parts of the characteristic function $\varphi_x(\eta)$ in the case of a 'fast chemical reaction' at $\beta = 2$ and $Sc \sim 10^3$.

$$\langle C_A(x)\rangle = \frac{1}{\pi}\int_0^\infty \Bigg\{\varphi_x^R(\eta)\ \frac{(1+\beta/\hat{\beta})\sin(\eta_{(+)}(\beta/\hat{\beta}+\beta))}{\eta} + \frac{\cos(\eta_{(+)}(\beta/\hat{\beta}+\beta)) - \cos(\eta(\beta-1))}{\eta^2} + \varphi_x^I(\eta)\Bigg[-\frac{(1+\beta/\hat{\beta})\cos(\eta_{(+)}(\beta/\hat{\beta}+\beta))}{\eta} + \frac{\sin(\eta_{(+)}(\beta/\hat{\beta}+\beta)) - \sin(\eta(\beta-1))}{\eta^2}\Bigg]\Bigg\}d\eta. \qquad (40)$$

Here $\eta_{(+)} = (1+\delta)$, $\delta \to 0$, $\delta > 0$; $\varphi_x^R(\eta)$, $\varphi_x^I(\eta)$ are the real and imaginary parts of the characteristic function $\varphi_x(\eta)$.

Formula (40) can be obtained from expression (6) with the aid of formulae (12).

It is seen from the predicted results for the function $P_x^c(r)$, which are given in Figs. 1(a) and (b), that in the initial stage the evolution of this function reduces to its extension to the side of smaller scales. Here the mean scale decreases sharply, the dissipation rate $N(x)$ increases [Fig. 1(b)] being indicative of the small-scale turbulent mixing in the flow. Starting from $x \sim 0.03$, the fast stage of mixing terminates and a slow evolution of the function $P_x^c(r)$ begins. The mean scale starts to increase and the rate of dissipation to decrease. In this stage the form of the function $P_x^c(r)$ becomes less sensitive to a change in the scalar field structure. However, a more intensive evolution of the characteristic function $\varphi_x(\eta)$ begins in this case. It is seen from Figs. 2(a) and (b) that equation (32) qualitatively models the behaviour of this function, indicating the formation of a homogeneous mixing from formerly separate reagents.

Figure 3 presents the results of calculation of the dependence of the mean reaction rate of the r.m.s. fluctuations at different values of the stoichiometric ratio β and gives a comparison with the experimental data from work [1]. It is seen that the proposed model gives an adequate description of the experimental results in the case of a very fast chemical reaction.

THE CASE OF A MODERATELY FAST CHEMICAL REACTION

The proposed statistical model of the mixing of reagents, somewhat improved, can also be used to estimate the mean time of chemical reaction in the

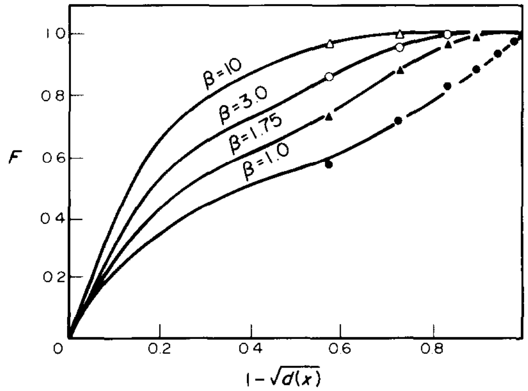

FIG. 3. Comparison of experimental data [1] with the results predicted on the basis of the 'fast chemical reaction' model for different values of β.

case of comparable characteristic times of reaction and turbulent mixing, i.e. for the case of moderate Damköhler numbers. Then, the mean concentration of reagent A should be determined from the equation

$$U(x)\frac{\mathrm{d}\langle C_A(x)\rangle}{\mathrm{d}x} = \langle w_A(x)\rangle \tag{41}$$

where $w_A(x)$ is the source term.

A conventional expression for the source term has the form

$$w_A(x) = k(T)C_A C_B. \tag{42}$$

Even with the temperature fluctuations ignored, a two-dimensional probability distribution function is required to obtain the mean value $\langle w_A(x)\rangle$. To remain at the level of one-dimensional distribution, it will be assumed that the concentrations of reagents A and B are coupled through the relation

$$C_A(x,t) + C_B(x,t) = C_0,$$

where C_0 is the maximum concentration of reagents.

With regard to this coupling, the expression for $w_A(x)$ will have the form

$$w_A(x) = k(T)C_A(C_0 - C_A). \tag{43}$$

The introduction of new variables

$$\hat{C} = \frac{C_A}{C_0}; \qquad k = k(T)C_0; \qquad w = \frac{wA}{C_0} \tag{44}$$

will yield the following expression for w

$$w = k\hat{C}(1 - \hat{C}). \tag{45}$$

Expression (45) is convenient as it is determined by the concentration field of only one scalar with its value depending entirely on the quality of mixing. The value of w is indeed close to zero at those points where $\hat{C} = 0$ or $\hat{C} = 1$, i.e. where there are pure reagents; the quantity w has the maximum at the points where $\hat{C} = 0.5$, i.e. where uniform mixing of reagents is attained [10].

The equation for the mean concentration $\langle\hat{C}\rangle$ with the source term in the form of equation (45) acquires the form

$$U(x)\frac{\mathrm{d}\langle\hat{C}\rangle}{\mathrm{d}x} = -k[\langle\hat{C}\rangle(1 - \langle\hat{C}\rangle) - \langle c^2\rangle]. \tag{46}$$

Here $c = \hat{C} - \langle\hat{C}\rangle$.

The r.m.s. value of the fluctuations of reagent $\langle c^2\rangle$ can be calculated from the formula

$$\langle c^2\rangle = -\frac{\partial^2}{\partial\eta^2}\varphi_x^R(\eta)|_{\eta=0} \tag{47}$$

where $\varphi_x^R(\eta)$ is the real part of the characteristic function of the reagent A field.

The equation for the characteristic function $\varphi_x(\eta)$ will have the same form as that of equation (32), with the RHS having only the source term $\hat{W}_\Phi$ in the form

$$\hat{W}_\varphi = -k\eta\left[i\langle c^2\rangle + (1 - 2\langle\hat{C}\rangle)\frac{\partial}{\partial\eta} + i\frac{\partial^2}{\partial\eta^2}\right]\varphi_x(\eta). \tag{48}$$

The initial condition for the function $\varphi_x(\eta)$ is

$$\begin{aligned}\varphi_0(\eta) = {} & [(1 - \langle\hat{C}_0\rangle)\cos\eta\langle\hat{C}_0\rangle \\ & + \langle\hat{C}_0\rangle\cos(\eta(1 - \langle\hat{C}_0\rangle))] \\ & + i[-(1 - \langle\hat{C}_0\rangle)\sin\eta\langle\hat{C}_0\rangle \\ & + \langle\hat{C}_0\rangle\sin(\eta(1 - \langle C_0\rangle))].\end{aligned} \tag{49}$$

The value of $\langle\hat{C}_0\rangle$ can be taken between 0 and 1.

To solve the equation for the characteristic function, it is necessary to know the functions $N(x)$ and $d(x)$ which are calculated from the function $P_x^c(r)$ by formulae (33), (34), (35) and (10′). The equation for $P_x^c(r)$ will differ then from equation (18) by the presence of the source term on its RHS

$$\hat{W}_p = -2k(1 - 2\langle\hat{C}\rangle)P_x^c(r) - 2k\frac{\partial}{\partial r}T_x(r). \tag{50}$$

Here the function $T_x(r)$ is the two-point, third-order moment of the turbulent reagent scalar field

$$T_x(r) = \langle c^2(x)c(x + r)\rangle. \tag{51}$$

For this function the following approximation was used

$$T_x(r) = T_x(0)\frac{B^c(r,x)}{B^c(0,x)}. \tag{52}$$

Here $T_x(0)$ is the one-point, third-order moment of the field $c(\mathbf{x},t)$. It can be calculated from the characteristic function by the following formula

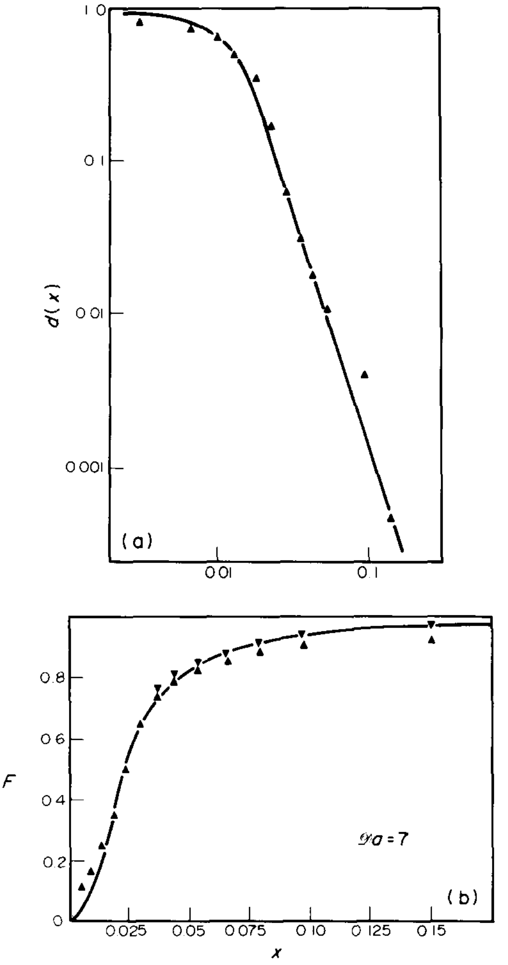

FIG. 4. (a, b) Comparison of experimental data [1] with the results predicted on the basis of the 'moderately fast chemical reaction' model for $Da = 7$ and $Sc \sim 10^3$.

$$T_x(0) = -\frac{\partial^3}{\partial \eta^3}\varphi_x^1(\eta)_{\eta=0}. \qquad (53)$$

Taking into account formula (52) and also formulae (9) and (10), the equation for $\hat{W}_p$ can be rewritten in the form

$$\hat{W}_p = -2k\left[1 - 2\langle \hat{C}(x)\rangle - \frac{T_x(0)}{\langle c^2(x)\rangle}\right]P_x^c(r). \qquad (54)$$

The function $P_x(r)$, required to solve the equation for $P_x^c(r)$, can be found from equation (23). The initial conditions for the functions $P_x^c(r)$ and $P_x(r)$ can be selected to be the same, as in the case of the passive scalar, i.e. in the form of equation (38).

Thus, besides equation (46) for $\langle \hat{C}(x)\rangle$, the model of the mixing of reagents in the case of moderately fast chemistry includes equation (32) for $\varphi_x(\eta)$, augmented on the RHS with the source term (48); equation (18), augmented on the RHS with term (54); and equation (23) for $P_x(r)$. The results of calculations, presented in Figs. 4(a) and (b), indicate that the model can be used to estimate the chemical reaction mean rate depending on the conditions of the problem.

REFERENCES

1. H. L. Toor, The non-premixed reaction A + B products. In *Turbulence in Mixing Operations* (Edited by R. S. Brodkey). Academic Press, New York (1975).
2. S. Chandrasekhar, The theory of turbulence, *J. Madras Univ.* **B6**, 27(1), 251–275 (1957).
3. A. S. Monin and A. M. Yaglom, *Statistical Hydrodynamics*, part 2. Nauka, Moscow (1967).
4. V. M. Ievlev, *Turbulent Motion of High-temperature Continua*. Nauka, Moscow (1975).
5. E. E. O'Brien, The probability density function (pdf) approach to reacting turbulent flows. In *Topics in Applied Physics*. Vol. 44, *Turbulent Reacting Flows*. Springer-Verlag, Berlin (1980).
6. V. R. Kuznetsov, A. B. Lebedev, A. N. Sekundov and I. P. Smirnova, Investigation of the quasi-homogeneous turbulent diffusion combustion with the use of the equation for the function of the concentration probability density distribution, *Izv. Akad. Nauk SSSR, Mekh. Zhidk. Gaza* No. 4, 3–11 (1981).
7. V. A. Sabelnikov, Model equation for the velocity and concentration probability distribution in turbulent mixing and diffusion combustion of gases, *Fiz. Gor. Vzryva* No. 2, 37–46 (1983).
8. V. Sosinovich and C. Meola, A statistical model for the turbulent mixing of reactants, *IX Convegno Annuale della Sezione Italiana del Combustion Institute* (27–28 guigno 1984), 3.6–3.7. Instituto di Ricerche sulla Combustione—C.N.R., Napoli (1984).
9. B. A. Kolovandin, V. A. Sosinovich and V. A. Tsyganov, A system of equations for the calculation of the mean rate of chemical reaction in an isotropic turbulent flow, *Proc. All-Union Meeting on the Structure of Gas-phase Flames*, Novosibirsk (1983).
10. V. A. Sosinovich and V. A. Tsyganov, Description of the process of turbulent mixing of reagents based on the equation of the probability density of scales, *J. Engng Phys.* **16**(2), 219–225 (1984).

UN MODELE D'ECOULEMENT STATISTIQUEMENT TURBULENT AVEC REACTION

Résumé—On présente un modèle du mélange turbulent de réactants qui utilise les équations couplées intégrodifférentielles pour les fonctions qui décrivent la distribution de l'énergie turbulente et de l'écart-type des fluctuations scalaires sur différentes échelles de longueur, et aussi pour la fonction caractéristique qui représente la transformée de Fourier de la densité de probabilité des fluctuations scalaires. Le modèle permet le calcul de la vitesse moyenne de la réaction chimique dans un écoulement turbulent pour une "chimie très rapide". Une solution numérique est donnée pour le système d'équations avec différentes conditions et une comparaison est faite avec des données expérimentales. On suggère la voie possible d'extension du modèle dans le cas d'une "chimie modérément rapide".

EIN STATISTISCHES MODELL TURBULENTER REAGIERENDER STRÖMUNG

Zusammenfassung—Es wird ein Modell der turbulenten Vermischung von Reaktanden vorgestellt, welches die gekoppelten Integro-Differential-Gleichungen für die Verteilung der turbulenten Energie und des Effektivwertes der skalaren Schwankungen über unterschiedliche Längen und für die Fourier-Transformation der punktuellen Wahrscheinlichkeitsdichte der Schwankungen des Skalarfeldes enthält. Das Modell ist für die Berechnung der mittleren Reaktionsgeschwindigkeit in turbulenten Strömungen im Bereich der "schnellen Chemie" vorgesehen. Es wird eine numerische Lösung des Gleichungssystems für unterschiedliche Bedingungen angegeben, ein Vergleich mit experimentellen Daten wurde durchgeführt. Die Möglichkeit einer Erweiterung des Modells für den Fall der "mittel-schnellen Chemie" wird vorgeschlagen.

СТАТИСТИЧЕСКАЯ МОДЕЛЬ ТУРБУЛЕНТНОГО РЕАГИРУЮЩЕГО ПОТОКА

Аннотация—Представлена модель турбулентного смешения реагентов, включающая три связанных интегродифференциальных уравнения для функций, описывающих распределение энергии турбулентности, среднеквадратичной величины флуктуаций скалярного поля по различным масштабам длины и для характеристической функции, являющейся преобразованием Фурье одноточечной плотности вероятности значений флуктуаций скалярного поля. Эта модель предназначена для вычисления средней скорости химической реакции в турбулентном потоке в случае «очень быстрой химии». Приведено численное решение системы уравнений для различных условий и дано сравнение с экспериментальными данными. Указан возможный способ обобщения представленной модели на случай «умеренно быстрой химии».