DESCRIPTION OF THE REAGENT TURBULENT MIXING PROCESS ON THE BASIS OF THE EQUATION OF THE SCALE PROBABILITY DENSITY

V. A. Sosinovich and V. A. Tsyganov

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A system of equations is derived and solved numerically that describes the process of turbulent mixing of reagents in terms of one of the mixing criteria, the degree of flow miscibility.

The process of turbulent mixing of reagents to a molecular level can be separated conditionally into three separate stages: large-scale mixing of large turbulent vortices; fine-scale mixing to the smallest turbulent scale because of fine-scale motion; mixing to the molecular level because of themolecular diffusion process [1].

Formation of the scale spectrum of the reagent concentration field occurs in the first stage, which corresponds to the large-scale vortex of the velocity field characteristic for this flow. The description of this stage can be made on the basis of a formalism using the separation of turbulent fields into components: mean, large-scale, and fine-scale [2]. A certain function $\hat{P}^c{}_t(r)$, the probability density of the concentration field scales, which can later be used as initial condition for description of the second mixing stage, is the result of the computation. In this stage the single-point probability density of the concentration field $f_t(\hat{c})$ varies slightly.

The fine-scale flow configuration plays the main role in the second mixing stage, which can be considered isotropic in a good approximation, and the formalism of isotropic turbulence is used in its description. In this stage a reduction in the size of the reagent concentration field occurs down to the smallest of turbulence scales. The probability density of the concentration field $f_c(\hat{c})$ varies slightly, but the scale probability density reaches the developed state. Molecular diffusion and the chemical reaction are still of low intensity in this mixing stage. Only at the end of the second stage, when a noticeable fraction of scales on the Kolmogorov order appears in the flow, does the effective operation of diffusion start, as thereby does the third, terminating mixing stage. Consequently, a homogeneous mixture appears in the flow, i.e., the reagents are mixed to the molecular level. The single-point probability density changes radically: if it can be approximated by the sum of two δ-functions at the beginning of the third mixing stage, indicating the separateness of the reagents in the flow, then at the end it is a smooth function reflecting the presence of a mixture with any relationship between the reagents in the flow [3]. The probability density of the scale distribution $\hat{P}^c{}_t(r)$ varies slightly in this stage. Termination of the third stage is accompanied by the beginning of an intensive chemical reaction and the appearance of the reaction product in a noticeable quantity in the flow.

There follows from this schematic representation of the turbulent mixing process that the probability density distribution of the scales $\hat{P}^c{}_t(r)$ and the single-point probability density of the concentration field $f_t(\hat{c})$ can be criteria for the mixing quality. Indeed, $\hat{P}^c{}_t(r)$ is a function sensitive to the degree of reduction of the scalar turbulent fields in size, and consequently it can be used to describe adequately the first and second mixing stages. The function $f_t(\hat{c})$ starts to change strongly in the last mixing stage and consequently can be a good indicator of the diffusion process.

The present paper is devoted to a description of the second stage in turbulent mixing of reagents. The evolution of the scale probability density of the concentration field of one of the reagents is studied on the basis of a numerical solution of the system of equations for this function. The initial state is here assumed known.

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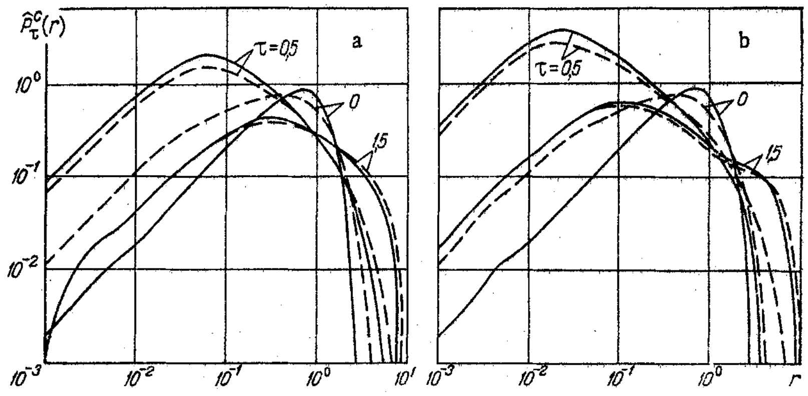

Fig. 1

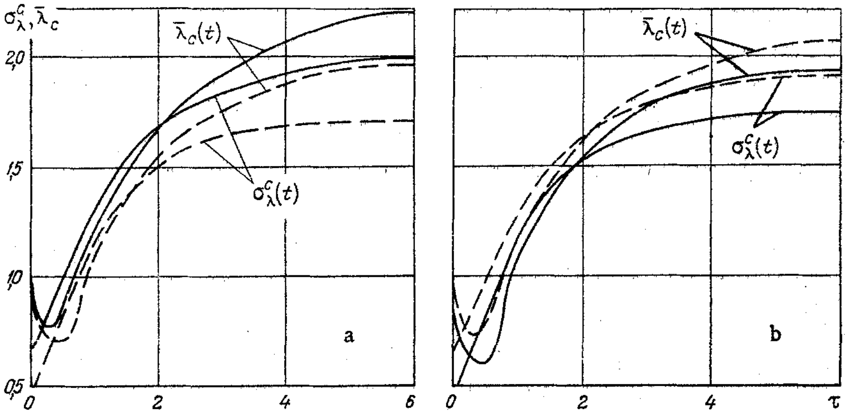

Fig. 2

Fig. 1. Scale probability density of a turbulent concentration field for Re = 200 (a) and Re = 1000 (b); solid curves — σ = 0; dashes — σ = 0.5.

Fig. 2. Mean scale and scale variance of turbulent concentration field for Re = 200 (a) and Re = 1000 (b); solid curves — σ = 0; dashes — σ = 0.5.

The scale probability density of the concentration field can be determined as follows:

$$\hat{P}_t^c(r) = P_t^c(r) / \int_0^\infty P_t^c(r)\,dr, \tag{1}$$

where

$$P_t^c(r) = \frac{1}{2} H_r'(r, t). \tag{2}$$

The function H(r, t) is a two-point structural function of second order of the turbulent scalar field. Its determination in terms of the difference in scalar field concentration at flow points separated by a distance r has the form [4]

$$H(r, t) = \langle \Delta c(r, t)^2 \rangle . \tag{3}$$

If the equation

$$\frac{\partial c}{\partial t} + \frac{\partial (v_i c)}{\partial x_i} = \chi \frac{\partial^2 c}{\partial x_i \partial x_i} - \omega(c), \tag{4}$$

where

$$\omega(c) = k(c - c^2), \tag{5}$$

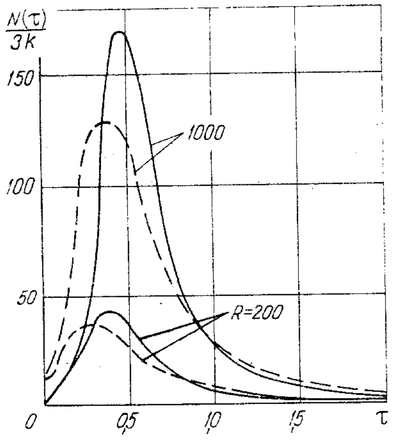

Fig. 3 The mean rate of dissipation of the turbulent scalar field fluctuation level: solid curves — $\sigma = 0$; dashes — $\sigma = 0.5$.

is taken as dynamic equation for the concentration field, then the following equation

$$\frac{\partial P_t^c(r)}{\partial t} = -\frac{1}{2}\left[L'(r,\ t) + \frac{2}{r}L(r,\ t)\right] + 2\chi\left[P_t^{c''}(r) + \frac{2}{r}P_t^{c'}(r) - \frac{2}{r^2}P_t^c(r)\right] - 2k(1 - 2\langle c\rangle)P_t^c(r) - 2kT'(r,\ t) \tag{6}$$

can be obtained for the function $\hat{P}^c{}_t(r)$. Here χ is the diffusion coefficent and k is the Arrhenius factor;

$$L(r,\ t) = \langle \Delta v(r,\ t)\Delta c^2(r,\ t)\rangle; \tag{7}$$

$$T(r,\ t) = \langle c^2(\vec{x},\ t)\,c(\vec{x} + \vec{r},\ t)\rangle. \tag{8}$$

The expression for the source term $\omega(c)$ in the form of (5) describes the following situation. A reagent A goes into reaction with a reagent B and is consequently transformed into B. Only two reagents therefore exist in the flow. The expression (5) is convenient in the respect that it is determined by the field of just one scalar and at the same time its magnitude depends completely on the mixing quality: $\omega(c) = 0$ where $c = 0$ or $c = 1$, i.e., where pure components are present, while $\omega(c)$ is maximal for $c = 0.5$, i.e., where uniform mixing of the reagents occurred.

Equation (6) is not closed because of the presence of two additional unknown functions L(r, t) and T(r, t). The function T(r, t) is generated by the source term $\omega(c)$ in (4) and determines the dissimilar roles of the scales of different magnitude during the chemical reaction. We limit ourselves in this paper to considering the fast reaction case when it is sufficient to know just the statistics of the passive scalar [5] to calculate the reaction rate. Hence, terms associated with the chemical reaction rate in the equation for the function $P^c{}_t(r)$ are omitted.

The function L(r t) describes mixing of the reagents by an isotropic velocity field. Analogies with the molecular diffusion mechanism, just as was done in deriving the equation for the spectrum in the Heisenberg approximation [4], can be used to model it. The following equation for $P^c{}_t(r)$ can consequently be obtained:

$$\frac{\partial P_t^c(r)}{\partial t} = 2\beta\sqrt{P_t(r)r}\left[P_t^{c'}(r) + \frac{2}{r}P_t^c(r)\right] + 2\left[\chi + \beta\int_0^r\sqrt{P_t(r')r'}\,dr'\right]\left[P_t^{c''}(r) + \frac{2}{r}P_t^{c'}(r) - \frac{2}{r^2}P_t^c(r)\right]. \tag{9}$$

Here β is a constant whose value will be determined later, $P_t(r)$ is the energy distribution density of the turbulent velocity field in the different scales. This function is determined in terms of the structural two-point function D(r, t) from the formula

$$P_t(r) = \frac{1}{2}D'(r,\ t). \tag{10}$$

A closed equation can be obtained for the function (10) if (15) from [6] is used and the analogy with the molecular energy transfer mechanism relied upon for its closure. This equation has the form

$$\frac{\partial P_t(r)}{\partial t} = 2\gamma\sqrt{P_t(r)\,r}\left[P_t'(r) + \frac{4}{r}P_t(r)\right] + 2\left[\nu + \gamma\int\limits_0^r \sqrt{P_t(r')\,r'}\,dr'\right]\left[P_t''(r) + \frac{4}{r}P_t'(r) - \frac{4}{r^2}P_t(r)\right]. \quad (11)$$

The constants β and γ, which can be associated with the constants in the $^2/_3$ law for the inertial-convective and inertial intervals if these equations are solved in the intervals mentioned, enter into (9) and (11) [4]. The appropriate formulas have the form

$$\beta = \frac{2{,}4\sqrt{3}}{\sqrt{CS}}; \quad \gamma = \frac{12}{11\sqrt{3}C^{3/2}}, \quad (12)$$

where C is a constant in the $^2/_3$ law for the velocity structural function, and S is the same for the structural function of the concentration field. According to [4], these constants have the following magnitudes: C = 1.9 and S = 2.8. Therefore, we obtain for the constants β and γ

$$\beta = 1.08; \ \gamma = 0.24. \quad (13)$$

Equations (9) and (11) must be solved jointly by giving the functions $P^c_t(r)$ and $P_t(r)$ at the initial time.

The function

$$P_0(r) = 2B(0)\frac{r}{\lambda^2}\exp\left\{-\frac{r^2}{\lambda^2}\right\} \quad (14)$$

can be used as initial conditions for $P^c_t(r)$ and $P_t(r)$. Here λ in the distribution parameter or the characteristic scale, B(0) is the rms value of the concentration fluctuations in the case of a scalar reagent concentration field, and the rms energy of the velocity fluctuation in the case of the velocity field.

If the initial distribution is characterized by a broad scale spectrum, then an attempt can be made to approximate it by the expression

$$P_0(r) = \frac{2B(0)\,r}{\sqrt{2\pi}\sigma}\int\limits_0^\infty \frac{d\lambda}{\lambda^2}\exp\left\{-\frac{r^2}{\lambda^2} - \frac{(\lambda-\lambda_0)^2}{2\sigma^2}\right\}, \quad (15)$$

which is obtained by taking the average of (14) under the assumption that the scale λ in (14) is a random variable with normal probability distribution. The quantities λ_0 and σ are the mean scale and the scale variance, respectively. The form of the function $P_0(r)$ is shown in Fig. 1 for $\sigma = 0.5$ and $\sigma = 0$. The case $\sigma = 0$ corresponds to (14).

The system (9) and (11) with initial conditions in the form (15) was solved numerically. For convenience in the calculations, all the variables were made dimensionless by using the following relations

$$r = \lambda_0\bar{r}; \ t = \frac{\lambda_0}{\sqrt{B(0)}}\tau; \ \mathrm{Re} = \frac{\lambda_0\sqrt{B(0)}}{\nu}; \ \mathrm{Pe} = \frac{\lambda_0\sqrt{B(0)}}{\chi}. \quad (16)$$

The formula (15) for $\sigma = 0, \sigma = 0.5$ was used as initial conditons in the computation. The integrals in the right side of the equations were computed by the trapezoid formula. A nonuniform step in r was used. The size of the step was increased as r increased. The initial values of Re and Pe = Re were selected equal to 200 and 1000. The time to compute one version in σ, Re and $\tau = 15$ was 10 min.

Results of computing the scale probability densities for different initial conditions are presented in Fig. 1a and b. Certain moments of these functions were also calculated, which illustrate the turbulent mixing process more graphically. The mean scale is

$$\langle\lambda(t)\rangle = \frac{1}{B(t)}\int\limits_0^\infty rP^c_t(r)\,dr, \quad (17)$$

where

$$B(t) = \int\limits_0^\infty P^c_t(r)\,dr. \quad (18)$$

The variance of the scales is

$$\sigma_\lambda(t) = \sqrt{\langle\lambda^2(t)\rangle - \langle\lambda(t)\rangle^2}, \quad (19)$$

where

$$\langle \lambda^2(t) \rangle = \frac{1}{B(t)} \int_0^\infty r^2 P_t^c(r)\,dr. \tag{20}$$

These quantities are represented in Fig. 2a and b.

The rate of dissipation of the turbulent scalar field fluctuation level

$$N(t) = 3\chi P_t^{c'}(r)|_{r=0} \tag{21}$$

is shown in Fig. 3.

It is seen from the results presented for the computation that in the initial evolution stage the probability density $\hat{P}^c{}_t(r)$ reduces to stretching the function towards smaller scales. In this stage the mean scale drops abruptly, the variance of the scales grows because of the increase in the contribution of the small scales, which is a reflection of the fine-scale turbulent mixing in the flow. Starting with $\tau = 0.5$-1 the fast mixing stage terminates and the slow evolution of the probability density starts. The scale starts to grow. If we were to try to assess the degree of miscibility by just the mean scale, then we could arrive at a false deduction that small scales vanish in the flow. But this is not so, as is seen well from the graph of the probability density of the reagent field scales. The growth of $<\lambda(t)>$ is related to a relative increase in the role of the large scales, but small scales are also present in the flow. It is seen from Figs. 2a and b that for $\tau = 0$ and $\tau = 0.8$ the mean scale is practically identical. However, the probability density function $\hat{P}^c{}_t(r)$ and hence the structure of the reagent field also are completely different. The characteristic reflecting this difference is the variance of the scales (see Figs. 2a and b) which constantly grows.

As is seen from Fig. 1, the difference between the variants with different initial variances diminishes with time. It is seen from Fig. 3 that in the case of a large reduction in the flow size, the maximum of the dissipation rate is reached earlier. However, the magnitude of the dissipation at the point of the maximum turns out to be greater in the case of a smaller initial reduction in the flow size.

The difference between Re = 200 and Re = 1000 is that for larger Re number the scale probability density is large for small values of the scale, i.e., the scalar field turns out to be reduced to a large extent.

The results obtained in this paper refer to modeling the second stage of the mixing and the beginning of the third stage. The first stage is substantially anisotropic. Consequently its description should be based on examination of the evolution of large-scale coherent flow structure. This question is not examined in this paper. On the basis of the results obtained the deduction can be made that the second stage of turbulent mixing is modelled well by the evolution of the scale probability density $\hat{P}^c{}_t(r)$. Moments of this function will enter as coefficients into the equation for the probability density of values of the turbulent scalar field $f_t(\hat{c})$, whose study is needed for modeling the third stage of turbulent mixing of reagents and for computation of the chemical reaction rate.

NOTATION

$\hat{P}^c{}_t(r)$ scale probability density of a turbulent isotropic concentration filed; $f_t(\hat{c})$ a single-point probability density of values of the turbulent concentration field; $H(r, t)$ a two-point structural, second-order function of a turbulent scalar field; $\Delta c(r, t)$, difference in concentrations of a scalar turbulent field at points separated by a distance r at a time t; ν, χ, molecular viscosity and diffusion coefficients; $\hat{P}_t(r)$ function describing the energy distribution in different scales of the turbulent velocity field; $D(r, t)$ two-point structural second-order function of the turbulent velocity field; $<\lambda(t)>$, mean scale of the concentration field; $\sigma_\lambda(t)$, scale variance; $N(t)$ rate of dissipation of the turbulent scalar field fluctuations level.

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MODELING THE DELAY IN MIXING TO THE MOLECULAR LEVEL IN CALCULATING THE THERMAL RADIATION OF TURBULENT FLOWS

A. I. Bril'

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An appropriate method is proposed for taking account of the delay in mixing to the molecular level in turbulent flows of jet type; the method is intended for the calculation of the thermal radiation.

In calculating the physical and chemical processes occurring in free jets and wakes with the decay of tangential disturbances, with a nonlinear dependence on the thermodynamic parameters, there arises the problem of taking correct account of the problem of turbulent mixing, which influences the structure of the concentration and temperature fields [1-3]. One of the most important manifestations of the flow turbulence is the delay in mixing to the molecular level, i.e., the retention of the individual characteristics (temperature, chemical composition, etc.) of the volume of material penetrating into the turbulized region for a finite interval of time. In [3], it was shown that the problem of taking turbulence into account in calculating the chemical-reaction rates in peripheral regions of turbulent jets may be successfully solved by direct modeling of the mixing delay.

Such modeling may also be required in calculating the thermal radiation of a high-temperature jet issuing into a medium at a lower temperature and also in developing optical methods of turbulent-flow diagnostics. This is associated with the fact that finite volumes of unmixed hot gas penetrate from the potential core of the flow into the peripheral regions of the jet, with a certain probability. Neglecting this phenomenon may significantly affect estimates of the transverse dimensions of the jet with respect to the thermal radiation or the calculation of the brightness-temperature fields. Quantitative estimates are required for more definite assertions regarding the influence of the mixing delay on the thermal radiation. A corresponding method for numerical investigations will be constructed, following [3], on the basis of a two-parameter model of the turbulent viscosity.

Numerous variations of the two-parameter model of turbulent viscosity (i.e., models in which the turbulent viscosity is determined by two characteristic parameters of the turbulence field) are based on the kinetic-energy balance equation of the pulsations, to which is added the differential equation determining the scale of the pulsations. The basis of the two-parameter model, its fundamental equations, and also some examples of its use may be found in [4], for example. Critical analysis of the principal modifications of the model based on a comparison of experimental and theoretical data may be found in [5].

So as to be specific, isobaric axisymmetric jets will be considered below. The so-called <kε2> model of turbulent viscosity will be used for their calculation [5]. One of the advantages of this model is that, in selecting the empirical coefficients, much attention is given to the description of sections of the flow remote from the axis, which is important in calculating the radiation in peripheral regions of the jet. Within the framework of the <kε2> model, the dissipation of the kinetic energy of the pulsations ε is used as the function determining the characteristic scale of the pulsations. The turbulent viscosity is

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