EFFECT OF TEMPERATURE FLUCTUATIONS ON HETEROGENEOUS PARTICLE COMBUSTION

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The effect of temperature pulsations in the surrounding medium on a steady-state chemically reacting system is analyzed using equations for the particle temperature probability distribution function. Single-mode and bimodal distributions, realized respectively at low and high chemical reaction rates, are considered.

A quite large number of studies have already investigated the effect of turbulent pulsations on homogeneous chemical reactions [1, 2]. At the same time, heterogeneous combustion of a solid fuel has usually been considered only in the quasi-laminar approximation [3]. The problem of heterogeneous reaction regimes in the presence of fluctuations in heat and mass liberation coefficients was considered in [4, 5]. In consequence of the significantly nonlinear dependence of heterogeneous reaction rate on temperature, the problem of the effect of temperature pulsations in an external turbulent medium upon combustion is no less important.

We will consider nonsteady combustion of a small isolated particle in the assumption that change in particle radius over the time required to achieve the steady state is negligible. The turbulent random temperature field of the external medium will be modeled by a Gaussian random process with specified autocorrelation function. The reverse effect of the heterogeneous combustion process on temperature change in the external medium may be neglected, since we are considering an isolated particle. This approximation describes combustion processes in a highly rarefied gas-dispersed flow with adequate accuracy.

Change in instantaneous particle temperature over time is described by the equation

$$\frac{d\vartheta_p}{d\tau} = \frac{t-\vartheta_p}{\tau_t} + q(\vartheta_p). \tag{1}$$

The first term on the right side of Eq. (1) defines heat exchange between the particle and surrounding medium, and the second is the result of heat liberation from the heterogeneous combustion. The temperature dependence of heat liberation (combustion rate) for sufficiently small particles, the combustion of which occurs in the kinetic regime, can be described by the Arrhenius law

$$q = k\exp(-E/R\vartheta_p), \quad k = \mathrm{const}. \tag{2}$$

Because of the random character of change in the temperature of the turbulent medium over time Eq. (1) is stochastic. The random process characterized by Eq. (1) can also be described by the Fokker–Planck equation for the probability density of particle temperature [6, 7]. The probability density can be obtained conveniently from Eq. (1) by the functional differentiation method [8].

We introduce the particle temperature probability density

$$P(\vartheta, \tau) = \langle \delta(\vartheta-\vartheta_p(\tau)) \rangle, \tag{3}$$

where averaging is performed over realizations of the turbulent medium temperature field. Differentiating Eq. (3) over time, with consideration of Eq. (1) we obtain

$$\frac{\partial P}{\partial \tau} = -\frac{\partial}{\partial \vartheta}\left\langle \delta(\vartheta-\vartheta_p)\frac{d\vartheta_p}{d\tau}\right\rangle = -\frac{\partial}{\partial \vartheta}\left\langle \delta(\vartheta-\vartheta_p)\left(\frac{t-\vartheta_p}{\tau_t}+q(\vartheta_p)\right)\right\rangle. \tag{4}$$

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The temperature of the surrounding medium can be written in the form of average and pulsation components

$$t = T + t', \quad T = \langle t \rangle, \quad \langle t' \rangle = 0.$$

Then, with consideration of the relationship

$$\langle \delta(\vartheta - \vartheta_p(\tau)) \vartheta_p(\tau) \rangle = \vartheta P(\vartheta, \tau)$$

from Eq. (4) we obtain the following expression for the particle temperature probability density:

$$\frac{\partial P}{\partial \tau} + \frac{\partial}{\partial \vartheta}\left(\frac{T - \vartheta}{\tau_t} + q(\vartheta)\right) P = -\frac{1}{\tau_t} \frac{\partial \langle t'P \rangle}{\partial \vartheta}. \tag{5}$$

In order to obtain a closed equation for P, it is necessary to determine the correlation $\langle t'P \rangle$. To do this we make use of the Furuts–Novikov expression [8], assuming that the random field of temperature pulsations t' is Gaussian:

$$\langle z(\tau) R[z(\tau)] \rangle = \int \langle z(\tau) z(\tau_1) \rangle \frac{\delta P[z(\tau)]}{\delta z(\tau_1)} d\tau_1, \tag{6}$$

where $z(\tau)$ is a random process, $R[z]$ is a functional dependent on the random process, and $\delta P/\delta z$ is the functional derivative. From Eq. (6) it follows that

$$\langle t'P \rangle = \int \langle t'(\tau) t'(\tau_1) \rangle \frac{\delta P(\vartheta, \tau)}{\delta t'(\tau_1)} d\tau_1, \tag{7}$$

where in accordance with Eq. (3)

$$\frac{\delta P(\vartheta, \tau)}{\delta t'(\tau_1)} = -\frac{\partial}{\partial \vartheta}\left\langle \delta(\vartheta - \vartheta_p(\tau)) \frac{\delta \vartheta_p(\tau)}{\delta t'(\tau_1)} \right\rangle. \tag{8}$$

To calculate the functional derivative $\delta\vartheta_p/\delta t'$ in Eq. (8) we will limit our examination to cases close to static equilibrium, where the deviation of the temperature from the average value $\Theta$ is small, and the scale of turbulent pulsations of medium parameters $T_L$ (the Lagrangian time scale of the turbulence) is much less than the characteristic combustion rate scale $\tau_q = 1/q'_\Theta$.

In this case the term describing heat liberation can be linearized and Eq. (1) written in the form

$$\frac{d\vartheta_p}{d\tau} = \frac{t - \vartheta_p}{\tau_t} + q(\Theta) + q'_\Theta(\vartheta_p - \Theta), \tag{9}$$

where $q'_\Theta = (dq/d\vartheta_p)_{\vartheta_p = \Theta}$.

The solution of Eq. (9) will be

$$\vartheta_p(\tau) = \vartheta_p(0) \exp(-\tau/\tau_{t*}) + \int_0^\tau \left[\frac{t(\tau_1)}{\tau_t} + q(\Theta(\tau_1)) + q'_\Theta(\tau_1)\Theta(\tau_1)\right] \exp\left(-\frac{\tau - \tau_1}{\tau_{t*}}\right) d\tau_1, \tag{10}$$

where $\tau_{t*} = \tau_t/(1 - \tau_t q'_\Theta)$ is the particle thermal relaxation time with consideration of combustion; then in order that the quantity $\tau_{t*}$ be positive, the condition $\tau_t q'_\Theta < 1$ must be fulfilled.

We apply the functional differentiation operator to Eq. (10), taking into consideration the causality principle $\delta R[z(\tau)]/\delta z(\tau_1) = 0$ for $\tau < \tau_1$ and the absence of dependence of the initial condition $\vartheta_p(0)$ on t'. As a result we obtain

$$\frac{\delta \vartheta_p(\tau)}{\delta t'(\tau_1)} = \frac{1}{\tau_t} \exp\left(-\frac{\tau - \tau_1}{\tau_{t*}}\right) \eta(\tau - \tau_1), \tag{11}$$

where $\eta(\tau) = 0,\ \tau < 0;\ \eta(\tau) = 1,\ \tau \geqslant 0.$

With consideration of Eqs. (8) and (11), Eq. (7) takes on the form

$$\langle t'P \rangle = -f_t \langle t'^2 \rangle \frac{\partial P}{\partial \Theta}, \tag{12}$$

where

$$f_t = \int_0^\infty \frac{\langle t'(\tau) t'(\tau+\xi) \rangle}{\langle t'^2(\tau) \rangle} \exp\left(-\frac{\xi}{\tau_{t*}}\right) \frac{d\xi}{\tau_{t*}} \tag{13}$$

Substituting Eq. (12) in Eq. (5), we obtain a closed equation for the particle temperature probability density in the turbulent medium

$$\frac{\partial P}{\partial \tau} + \frac{\partial}{\partial \vartheta}\left(\frac{T-\vartheta}{\tau_t} + q(\vartheta)\right) P = \frac{f_t \langle t'^2 \rangle}{\tau_t} \frac{\partial^2 P}{\partial \vartheta^2} \tag{14}$$

To determine the coefficient $f_t$, characterizing the intensity of particle temperature pulsations, we approximate the two-dimensional temperature pulsation autocorrelation function by a step function [9]

$$\frac{\langle t'(\tau) t'(\tau+\xi) \rangle}{\langle t'^2(\tau) \rangle} = 1 - \eta(\xi - T_L). \tag{15}$$

With consideration of Eq. (15), it follows from Eq. (13) that

$$f_t = \frac{\tau_{t*}}{\tau_t}\left[1 - \exp\left(-\frac{T_L}{\tau_{t*}}\right)\right] = \frac{1}{1-\beta\Omega}\left[1 - \exp\left(-\frac{1-\beta\Omega}{\Omega}\right)\right], \tag{16}$$

where $\beta = T_L/\tau_q$, $\Omega = \tau_t/T_L$ are parameters defining the ratios of the external flux temperature pulsation scale $T_L$ to the characteristic chemical reaction time $\tau_q$ and the particle thermal relaxation $\tau_t$.

According to Eq. (16), the coefficient $f_t$ takes on positive values over the entire range of change of the parameters $\Omega$ and $\beta$, not only for $\beta \ll 1$. Consequently, for all values of $\Omega$ and $\beta$, Eq. (14) is a parabolic type equation, i.e., it describes diffusion-type processes. By solving Eq. (14) we can calculate the mean particle temperature $\Theta = \int \vartheta P d\vartheta$ and the temperature pulsation dispersion $\langle \vartheta'^2 \rangle = \int (\vartheta - \Theta)^2 P d\vartheta$. It should be noted that Eq. (14) is integrodifferential, since it contains the quantity $\Theta$, which appears in $\beta$ and correspondingly in $f_t$.

In the steady state it follows from Eq. (14) that the probability density satisfies the equation

$$\left[\frac{T-\vartheta}{\tau_t} + q(\vartheta)\right] P_s = \frac{f_t \langle t'^2 \rangle}{\tau_t} \frac{\partial P_s}{\partial \vartheta},$$

the solution of which with consideration of Eq. (2) for the combustion rate has the form

$$P_s(\vartheta) = C \exp(-U), \quad C = \mathrm{const}, \tag{17}$$

where U is the potential defined by the expression

$$U(\vartheta) = \begin{cases} -\dfrac{\tau_t}{f_t \langle t'^2 \rangle}\left[\vartheta \dfrac{\left(T - \frac{1}{2}\vartheta\right)}{\tau_t} + k\vartheta E_2(1/\vartheta)\right], & \vartheta > 0, \\[2ex] -\dfrac{\tau_t}{f_t \langle t'^2 \rangle} \vartheta \dfrac{\left(T - \frac{1}{2}\vartheta\right)}{\tau_t}, & \vartheta \leq 0. \end{cases}$$

Here $E_2(x) = \int_1^\infty e^{-x\tau} \tau^{-2} d\tau$ is an integral exponential function.

It is evident from Eq. (17) that the function $P_s(\vartheta)$ takes on extremal values at those points where the relationship

$$T = \vartheta - \tau_t q(\vartheta) \tag{18}$$

is satisfied.

With consideration of Eq. (2), condition (18) coincides with the expression for determining the steady-state particle temperature in the absence of medium temperature fluctuations. According to Eq. (18), the steady-state probability density has a single maximum when Eq. (18) has a single root, or two maxima and a minima when Eq. (18) has three roots.

Upon imposition of the additional limitation $\tau_t q'_\theta \ll 1$, when, according to Eq. (18), the steady-state probability density has one maximum and a crisis-free combustion regime is realized, the approximate solution of Eq. (14) can be written as a Gaussian distribution [6]

$$P(\vartheta, \tau) = \frac{1}{\sqrt{2\pi \langle \vartheta'^2(\tau) \rangle}} \exp\left\{-\frac{[\vartheta - \Theta(\tau)]^2}{2\langle \vartheta'^2(\tau) \rangle}\right\}. \tag{19}$$

The time dependence of Eq. (19) is parametric and manifested through the quantities $\Theta$ and $\langle\vartheta'^2\rangle$, which are defined by the equations

$$\frac{d\Theta}{d\tau} = \frac{T - \Theta}{\tau_t} + q(\Theta) + \frac{1}{2} q''_\theta \langle \vartheta'^2 \rangle, \tag{20}$$

$$\frac{d\langle \vartheta'^2 \rangle}{d\tau} = \frac{2f_t}{\tau_t} \langle t'^2 \rangle - \frac{2(1 - \tau_t q'_\theta)}{\tau_t} \langle \vartheta'^2 \rangle, \tag{21}$$

where $q''_\theta = (d^2q/d\vartheta_p^2)_{\vartheta_p=\Theta}$.

Equation (20) can be obtained directly by averaging Eq. (1). In the quasi-steady approximation it follows from Eq. (21) that

$$\langle \vartheta'^2 \rangle = \frac{f_t}{1 - \tau_t q'_\theta} \langle t'^2 \rangle. \tag{22}$$

An argument in favor of use of Eq. (22) is the fact that at $\tau_t q'_\theta \ll 1$ the temperature pulsation relaxation time in accordance with Eq. (21) is almost twice as small as the mean temperature relaxation time according to Eq. (20), i.e., the quasi-steady-state with respect to $\langle\vartheta'^2\rangle$ is established almost twice as rapidly as with respect to $\Theta$.

It follows from Eq. (20) that temperature pulsations may lead to both increase (for $\Theta < E/2R$, when $q''_\theta > 0$) or decrease (for $\Theta > E/2R$, when $q''_\theta < 0$) of particle steady-state temperature.

Equation (22), which establishes a relationship between the temperature pulsations of the particle and those of the surrounding medium, can be obtained directly from Eq. (1). To a linearized Eq. (1) there corresponds the following expression which in the quasi-steady approximation relates the two-dimensional correlation moments of particle temperature pulsations $\phi = \langle\vartheta'(\tau)\vartheta'(\tau + \xi)\rangle$ and those of the surrounding medium $\Psi = \langle t'(\tau)t'(\tau + \xi)\rangle$:

$$\frac{d^2\varphi}{d\xi^2} - \frac{\varphi}{\tau_{t*}} = -\frac{\Psi}{\tau_t}. \tag{23}$$

Its solution, satisfying the boundary conditions

$$\xi = 0 \quad \frac{d\varphi}{d\xi} = 0, \quad \xi \to \infty \quad \varphi \to 0,$$

has the form

$$\varphi(\xi) = \frac{\tau_{t*}}{2\tau_t^2}\left\{\exp\left(\frac{\xi}{\tau_{t*}}\right)\int_\xi^\infty \exp\left(-\frac{\xi_1}{\tau_{t*}}\right)\Psi(\xi_1)\,d\xi_1 + \exp\left(-\frac{\xi}{\tau_{t*}}\right)\left[\int_\xi^\infty \exp\left(-\frac{\xi_1}{\tau_{t*}}\right)\Psi(\xi_1)\,d\xi_1 + \int_0^\xi \exp\left(\frac{\xi_1}{\tau_{t*}}\right)\Psi(\xi_1)\,d\xi_1\right]\right\}.$$

Hence, since $\langle\vartheta'^2\rangle = \phi(0)$, Eq. (22) follows.

In the absence of combustion Eq. (22) transforms to the expression obtained in [9]. In the presence of combustion, since $dq/d\vartheta_p > 0$, positive feedback exists: particle temperature fluctuations produce pulsations in the combustion rate, which in turn increase the intensity of the former.

When the condition $\tau_t q'_\theta \ll 1$ is disrupted, the steady-state distribution of Eq. (17) becomes bimodal and is characterized by two minima of the potential U in the region of low temperatures $\vartheta_1$ and high $\vartheta_2$ (Fig. 1). In this case the Gaussian distribution of Eq. (19) becomes invalid and cannot describe possible transitions of the system through the potential barrier from one steady state to the other under the influence of pulsations in the temperature of the surrounding medium. The value of the potential barrier $|U(\vartheta_*) - U(\vartheta_i)|$ increases with increase in combustion rate. The minimum of the probability density, located at $\vartheta = \vartheta_*$, where $\vartheta_*$ is defined from the condition $\partial^2U/\partial\vartheta^2 = 0$, corresponds to an unstable stationary state of the system.

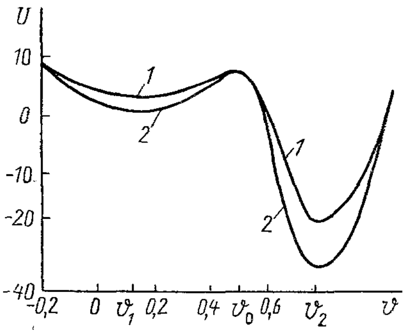


Fig. 1

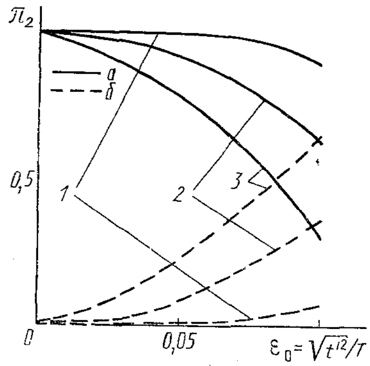


Fig. 2

Fig. 1. Overall form of bistable potential for various combustion rates: 1) $k\tau_t$ = 2.2; 2) 2.5.

Fig. 2. Probability of situation in high temperature state $\vartheta_2$ for various initial particle temperature values: a) $\vartheta_0 < \vartheta_*$, b) $\vartheta_0 > \vartheta_*$; 1) $\Omega$ = 0.1; 2) 1.0; 3) 10.0.

As has been shown in a number of studies on nonequilibrium phase transitions under the action of external noise [6, 7, 10, 11], the problem of determining the highest possible value of the temperature of a particle which had an initial temperature in the region of the unstable steady-state can be solved using split probabilities

$$\pi_1(\vartheta_0) = \Big[\int_{\vartheta_0}^{\vartheta_2} P_s^{-1}(\vartheta)\,d\vartheta\Big]\Big/\Big[\int_{\vartheta_1}^{\vartheta_2} P_s^{-1}(\vartheta)\,d\vartheta\Big],$$

$$\pi_2(\vartheta_0) = \Big[\int_{\vartheta_1}^{\vartheta_0} P_s^{-1}(\vartheta)\,d\vartheta\Big]\Big/\Big[\int_{\vartheta_1}^{\vartheta_2} P_s^{-1}(\vartheta)\,d\vartheta\Big] = 1 - \pi_1(\vartheta_0). \tag{24}$$

The values of $\pi_1$ and $\pi_2$ characterize the probability of transition of a particle having an initial temperature $\vartheta_0$, to a stable temperature state $\vartheta_1$ or $\vartheta_2$.

In the case of small values of the diffusion coefficient $f_t\langle t'^2\rangle/\tau_t$ Eq. (24) admits the asymptotic representation [7]

$$\pi_1 = \frac{1}{U'(\vartheta_0)}\sqrt{\frac{|U''(\vartheta_*)|\,\dfrac{f_t\langle t'^2\rangle}{\tau_t}}{2\pi}}\,\exp\left[\frac{U(\vartheta_0)-U(\vartheta_*)}{f_t\langle t'^2\rangle/\tau_t}\right], \quad \vartheta_0<\vartheta_*,$$

$$\pi_2 = 1+\frac{1}{U'(\vartheta_0)}\sqrt{\frac{|U''(\vartheta_*)|\,\dfrac{f_t\langle t'^2\rangle}{\tau_t}}{2\pi}}\,\exp\left[\frac{U(\vartheta_0)-U(\vartheta_*)}{f_t\langle t'^2\rangle/\tau_t}\right], \quad \vartheta_0>\vartheta_*.$$

Figure 2 shows the change in probability of finding a particle in the steady-state characterized by the high temperature $\vartheta_2$ with increase in intensity of pulsations of the surrounding medium temperature $\vartheta_2$ and various values of the initial temperature $\vartheta_0$. Calculations show that fine particles ($\Omega$ = 0.1) will practically always have a steady-state temperature corresponding to the value of the minimum in the potential U closest to $\vartheta_0$. However, with growth in thermal inertia of the particle ($\Omega$ = 1) the probability of jumping through the potential barrier increases. The fact indicates the possibility of extinction or ignition of large particles due to pulsation of surrounding medium temperature. With increase in combustion rate the probability of such transitions decreases, because of increase in the height of the potential barrier between the two stable steady states.

Thus, the proposed model permits determination of the most probable values of burning particle temperature in the presence of fluctuations in the temperature of the surrounding medium.

NOTATION

$\tau$, time; $\vartheta(\Theta)$, actual (average) particle temperature; t(T), actual (average) temperature of surrounding medium; P, probability density of particle temperature distribution; $\tau_t$, particle thermal relaxation time; E, activation energy; R, universal gas constant; U, potential; $\delta(x)$, delta-function; q, heterogeneous reaction rate; $\pi$, split probability. Subscripts: o, initial state; 1, 2, parameters of two stable states; p, particle.

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# PERCOLATION AND DIFFUSION IN FRACTAL TURBULENCE


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Experimental data on passive-impurity diffusion in fractal turbulence are interpreted on the basis of a percolational model.


## INTRODUCTION

The geometry of the eddy field in turbulized fluid is extremely fragmentary. Fragments of fluid with high vorticity are interspersed with fragments with low vorticity. Taking into account that in steady turbulent motion there is practically no transfer of passive impurity from the turbulent fragments to laminar fragments, but simply motion of the impurity with (and within) the turbulent fragments, fractal theory may be used to describe turbulent diffusion [1, 2]. The fact is that the problem of passive-impurity diffusion in homogeneous turbulence is still far from solution. Experiments with hydrodynamic lattices to model homogeneous turbulence give inconsistent data, and remain to be interpreted [3, 4]. In large-scale experiments in the ocean, which may also model homogeneous turbulence, the well-known Richardson 4/3 law for the effective diffusion coefficient is also found to be nonuniversal [5]. The reason for this is unclear. Could it be that the assumption of statistical homogeneity [6] is too limiting? Recently, this hypothesis has been weakened, substituting the less restrictive requirement of geometric self-similarity within some range of scales (e.g., see [1, 2]). This fractal approach may allow some of the features of impurity transport noted above to be taken into account and yield a theory which approximates the experimental effects.

Several fractal models of turbulence now exist (e.g., see [1, 2, 7]) and more will certainly appear in the future, since the approach to self-similar motion may take different forms, converging asymptotically on similar quasi-stable states [8]. The choice of a particular model of this process is largely dictated by considerations of convenience. In the

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