INFLUENCE OF COLORED NOISE ON PARTICLE COMBUSTION

M. V. Tret'yakov

UDC 536.46

The influence of external noise with nonzero correlation time (colored noise) on the combustion of a single particle is investigated. An equation for the steady-state thermal regimes of the reaction is derived. Spontaneous ignition of a particle is considered.

Introduction. In practice, particle combustion takes place in most cases in a highly fluctuating medium, i.e., turbulent flows, fluidized-bed reactors, etc. The kinetics of chemical reactions is very complicated and it is impossible to establish exactly from experiments on theoretical considerations how a process proceeds in a reactor. It is extremely difficult to describe the evolution of such a system and to allow for the majority of factors affecting it by using deterministic differential equations. Therefore we propose to use the idea of stochastic differential equations (SDE) to substitute a random force for uncertainties inherent in a nonequilibrium combustion process. In [1-3], the necessity of applying the stochastic methods for investigation of chemical reactions is argued at greater length.

Usually an external random force is approximated by delta-correlated random processes (white noises). This is explained, primarily, by the comparative mathematical simplicity of such objects. Nevertheless, any real process has a finite radius of correlation and from the physical viewpoint it is more correct to use colored noise.

In the present article we investigate the influence of colored noise on the steady-state condition of a heterogeneous reaction and stochastic ignition of a particle. It is shown that an account of the finite radius of correlations affecting the system of fluctuations yields the results qualitatively different from the case of white noise.

Model. We consider the model equation of thermal balance for particle combustion with additive noise [4, 5]:

$$C\frac{dT}{dt} = \frac{Qc_0\beta k(T)}{\beta + k(T)} - \alpha(T - T_0) + \xi(t),$$
$$k(T) = z\exp(-E/RT). \tag{1}$$

The system is influenced by a set of different factors; therefore a random force should be modeled by a Gaussian or Poisson random process [1, 6]. Here $\xi(t)$ is the Gaussian colored noise with the zero mean

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = S/t_c \exp(-|t - t'|/t_c). \tag{2}$$

The limiting transition $t_c \to 0$ in (2) leads to a delta-correlated Gaussian process.

Noise corresponds to temperature fluctuations of "a cooler" $T_0(t)$. They may be caused, for instance, by temperature nonuniformity in a fuel or oxidant flow. For the random time function $T_0(t)$:

$$\alpha^2 \langle T_0(t)T_0(t') \rangle = \langle \xi(t)\xi(t') \rangle.$$

A correlator of the temperature $T_0(t)$ may be evaluated experimentally. By T_c in (1) and henceforth is understood the mean value of the function $T_0(t)$. The rest of the symbols are the generally accepted ones [4, 5]. The noise $\xi(t)$ may be regarded as a random heat source caused by the nonuniformity of the temperature fields, the inhomogeneity of the fuel composition, the formation of random structures on a catalyst surface, etc.

A. M. Gor'kii Ural State University, Ekaterinburg. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 63, No. 2, pp. 156-160, August, 1992. Original article submitted August 13, 1991.

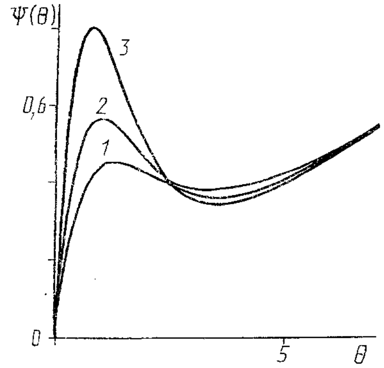

Fig. 1

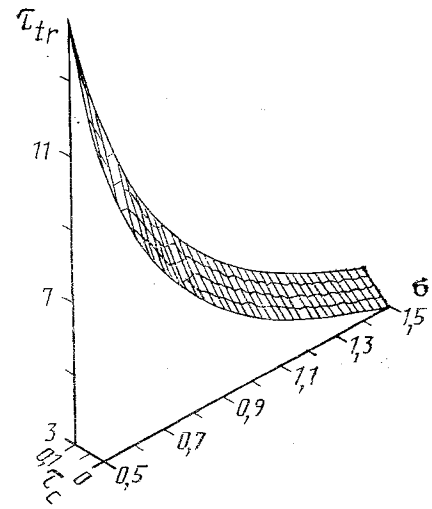

Fig. 2

Fig. 1. Function $\psi(\theta)$ versus temperature θ at $\mu = 0.08$ for different $\sigma\tau_c$: 1) $\sigma\tau_c = 0$; 2) 0.4; 3) 0.8.

Fig. 2. Mean time of transition τ_{tr} as a function of noise parameters σ and τ_c at $\mu = 0.05$, $\delta = 0.35$.

In dimensionless variables

$$\tau = \frac{\alpha}{C} t, \; \theta = \frac{E}{RT_0^2}(T - T_0), \; \sigma = \left(\frac{E}{RT_0^2}\right)^2 \frac{1}{C\alpha} S,$$
$$\delta = \frac{Qk(T_0)c_0 E}{\alpha R T_0^2}, \quad \mu = k(T_0)/\beta, \; \tau_c = \frac{\alpha}{C} t_c \tag{3}$$

Eq. (1) has the form

$$\frac{d\theta}{d\tau} = \delta \exp(\theta)/[1 + \mu \exp(\theta)] - \theta + \xi(\tau). \tag{4}$$

The Governing Equation. In the majority of real situations the correlation time is much less than the other characteristic times of a process. Therefore, we have investigated weak Gaussian noise: the correlation time is small, $\tau_c << 1$, but differs from zero. Then SDE (4) corresponds to an approximate governing equation for the density function $\rho(\tau, \theta)$ of temperature θ [7]

$$\frac{\partial \rho(\tau, \theta)}{\partial \tau} = -\frac{\partial}{\partial \theta} f(\theta)\rho(\tau, \theta) + \frac{\partial^2}{\partial \theta^2} D(\theta)\rho(\tau, \theta), \tag{5}$$

where

$$f(\theta) = \delta \exp(\theta)/[1 + \mu \exp(\theta)] - \theta; \quad D(\theta) = \sigma[1 + \tau_c df/d\theta].$$

In Eq. (5), there is a dimensionless temperature dependent coefficient θ at the diffusion addend and in the case of the additive Gaussian delta-correlated process the diffusion coefficient is constant. Mathematically, this is the difference between the approximations of white and colored noise. Colored noise, even additive, influences the system in a multiplicative manner [3].

Steady-State Regimes. In deterministic theory, steady states are defined from a solution of the algebraic equation $f(\theta) = 0$ [4]. In the case of stochastic differential equations, steady states are extremum points of the stationary probability density $\rho_s(\theta)$ [1, 7]

$$\rho_s(\theta) = \lim_{\tau \to \infty} \rho(\tau, \theta) = N/D(\theta) \exp\left\{\int_0^\theta dx\, [f(x)/D(x)]\right\}, \tag{6}$$

where N is the normalization constant. Taking into consideration that $\tau_c << 1$, formula (6) acquires the form

$$\rho_s(\theta) = N/D(\theta)\exp\left[\frac{1}{2\sigma}\left\{\tau_c\left(\frac{\delta^2}{[1+\mu]^2} - f(\theta)^2\right) - \theta^2\right\}\right](1 + \mu\exp(\theta))^{\delta/\sigma\mu}. \tag{7}$$

From (5), the equation for the steady state of a heterogeneous reaction in the presence of fluctuations follows

$$\delta = \theta[\exp(-\theta) + \mu]\{1 - \sigma\tau_c[1 - \mu\exp(\theta)]/[1 + \mu\exp(\theta)]^2\}^{-1} \equiv \psi(\theta). \tag{8}$$

Figure 1 shows the plots of the function $\psi(\theta)$ for different $\sigma\tau_c$. At $\sigma\tau_c = 0$ (curve 1), Eq. (8) is consistent with the classical theory [4] and with the case of additive white Gaussian noise [5]. With increasing $\sigma\tau_c$ (curves 2 and 3), the critical temperature of ignition increases, while that of extinction decreases. The region in which both the lower and upper temperature regimes are possible enlarges. Within the region of parameters where only the kinetic regime is implemented according to deterministic theory, with the noise or the correlation time increased, the particle combustion may proceed also in the diffusion regime. If deterministic theory forecasts the diffusion regime, then in the presence of colored noise the reaction may proceed in the kinetic regime. Such a situation is impossible in the case of additive white noise.

Stochastic Ignition. Let dimensionless parameters μ and δ of a reaction be such that the equation $f(\theta) = 0$ has three solutions. Consequently, three stationary regimes are possible, two of which, namely, the kinetic (θ_1) and the diffusion ones (θ_2) are stable, while the third regime (θ_n) is unstable [4]. Equation (8) may have somewhat different roots – θ_{c1}, θ_{c2}, and θ_{cn}, respectively. It is assumed that at the initial moment a particle has a temperature θ from the range $(0, \theta_n)$. In this case, according to deterministic theory [4], the particle attains the stationary temperature θ_1 of the kinetic regime within a short period of time and burns up in this regime for the characteristic dimensionless time $\tau_k = \alpha/k(T_1)C$.

From the stochastic point of view, it looks differently [6, 8]. The temperature $\theta(\tau)$ fluctuates like a Brownian particle. There always exists the nonzero probability of temperature transition from one stable condition to another, i.e., a thermal regime of particle combustion may spontaneously turn from the kinetic to the diffusion regime (stochastic ignition). The mean time τ_{tr} for which such a transition may occur is calculated as the mean time of transition through the barrier $\theta = \theta_{cn}$ [6, 7]:

$$\tau_{tr} = 2\int_{\theta_{c1}}^{\theta_{cn}}\left[\int_0^x \rho_s(z)\,dz\right]\frac{dx}{D(x)\rho_s(x)}. \tag{9}$$

It is easy to show that the following asymptotic behavior is satisfied: at $\sigma \to 0$, $\tau_{tr} \to \infty$, at $\sigma \to \infty$ $\tau_{tr} \to 0$ and at $\theta_{c1} \to \theta_{cn}$ it corresponds to an increase of δ and a decrease of μ, $\tau_{tr} \to 0$. The limit $\tau_c \to 0$ in (9) gives an expression for the mean transition time in the case of Gaussian white noise [5, 8]. With increasing the correlation time τ_c, the induction time τ_{tr} increases. Figure 2 shows the mean transition time τ_{tr} as a function of noise parameters σ and τ_c.

It is obvious that a change of the thermal regime of combustion due to fluctuations is possible only provided that τ_{tr} is less than the time τ_k of particle combustion in the kinetic regime. For this, it is necessary, as a rule, that

$$\int_0^{\theta_{cn}} \rho_s(x)\,dx < \int_{\theta_{cn}}^{\infty} \rho_s(x)\,dx.$$

i.e., the inverse transition (extinction) be hardly probable.

The problem on stochastic particle extinction may be treated analogously.

Conclusions. Colored as well as white noise [5, 8] may lead to spontaneous particle ignition and, therefore, deterministic theory gives an underestimated combustion time. Indeed, let the characteristic dimensionless time of particle combustion τ_k in the kinetic regime be ~150 and in the diffusion regime, ~20. In the presence of noise, for the situation under consideration (see Fig. 2) the mean time τ_{tr} of stochastic ignition may be ~5-10. According to the deterministic theory, a particle whose initial temperature is within the interval $(0, \theta_1)$ will burn up for the dimensionless time ~150. From the stochastic considerations it follows that the thermal regime of a reaction may change, on average, in the time τ_{tr} and a particle will burn up for the characteristic time ~30. Note that the inverse transition time (the characteristic time of stochastic extinction) in the situation considered is about 250-300, i.e., particle extinction is hardly probable.

In the case of colored, unlike white, noise the region of parameters where three combustion regimes are possible expands. When deterministic theory [4] or SDE with inclusion of white noise [5, 8] predicts implementation of only the kinetic (only the diffusion) regime, in the assumption of colored noise the low- and high-temperature regimes are also possible. From the consideration of unsteady-state thermal regimes and stochastic ignition, it follows that an increase in the correlation time τ_c results in an increase of the time of possible transition from the kinetic to the diffusion regime. The reason for the different behaviors of the system in the case of white and colored noise lies in the fact that the correlated process is the process "with memory" that gives rise to "inertia properties" of an object.

Statistical characteristics of colored noise (2) are, undoubtedly, more physical and more understandable to experimentalists than analogous quantities for white noise [5, 8]. The characteristic stochastic ignition time τ_{tr} is an experimentally measured quantity. Therefore, we hope that this work will attract the attention of experimentalists and results will be obtained to confirm or disprove the theory developed.

NOTATION

C, heat capacity of a particle; T, temperature of particle surface; t, t', moments of time; Q, thermal effect of the reaction; c_0, concentration of a limiting substance in a volume; β, mass transfer coefficient; z, preexponential factor; E, activation energy; R, gas constant; α, heat-transfer coefficient; T_0, temperature of the surrounding medium to which heat is transferred to; $\xi(t)$, a random process; t_c, correlation time; S, noise level; τ, dimensionless time; θ, dimensionless temperature; σ, dimensionless noise level; δ, μ, dimensionless parameters of the reaction; $\rho(\tau, \theta)$, density function of temperature θ at the moment of time τ; $\rho_s(\theta)$, stationary density function; θ_1, θ_2, θ_n, temperature of steady states; θ_{c1}, θ_{c2}, θ_{cn}, the same for colored noise; θ_0, initial temperature of a particle; τ_k, characteristic combustion time in the kinetic regime; τ_{tr}, mean time of spontaneous transition from the kinetic to the diffusion regime.

LITERATURE CITED

1. V. Khorstkhemke and E. Lefevr, Noise-Induced Transitions [Russian translation], Moscow (1986).
2. L. K. Doraiswamy and B. D. Kulkarny, The Analysis of Chemically Reacting Systems. A Stochastic Approach, New York–London–Paris–Montreux–Tokyo, Gordon and Breach (1987).
3. Yu. A. Buevich and S. P. Fedotov, Inzh.-Fiz. Zh., **53**, No. 5, 902-805 (1987).
4. D. A. Frank-Kamenetskii, Diffusion and Heat Transfer in Chemical Kinetics [in Russian], Moscow (1987).
5. S. P. Fedotov and M. V. Tret'yakov, Khim. Fiz., **10**, No. 2. 238-241 (1991).
6. K. V. Gardiner, Stochastic Methods in Natural Sciences [in Russian], Moscow (1986).
7. J. Masoliver, B. J. West, and K. Lindenberg, Phys. Rev. A. **35**, No. 7, 3086-3094 (1987).
8. S. P. Fedotov and M. V. Tret'yakov, Combust. Sci. Technol., **78**, Nos. 1-3, 1-6 (1991).