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Thermal explosion problem with a stochastic boundary: quasi-stationary approximation and direct numerical modelling

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Abstract. This paper considers a stochastic modification of the Frank–Kamenetskiy problem of exothermic reaction dynamics in a plane-parallel layer with random temperature fluctuations at the outer boundary as a means of modeling the behavior of chemical reactors when operating under uncontrolled environment impacts. Unlike deterministic formulations, such approaches take into account the possibility of a thermal explosion whose probability depends on the noise intensity. Based on random process theory, the conditions for achieving ignition in the quasi-stationary approximation (i.e., when the thermal relaxation rate is much higher than the rate of temperature change) are estimated. The possibility of using such a formulation to obtain an approximate relationship between the parameters of the noise and the dynamic characteristics of ignition (expected thermal explosion time) is demonstrated. The equation of non-stationary heat transfer in the reacting medium is solved numerically for a large number of random temperature trajectories at the boundary of the region of interest using a scheme combining explicit approximation of the nonlinear source with implicit approximation of the temperature field. By comparing the two approaches, the main regularities of non-stationary development of a thermal explosion in a stochastic environment can be approximated with good accuracy. Such a comparison relies on dependencies obtained when solving the quasi-stationary problem, taking into account a small correction for the critical temperature (marking the stability boundary for the stationary problem). Distributions of ignition characteristics (ignition temperature, maximum ambient temperature, and ignition time) and their dependence on input parameters (reactivity and noise intensity) are discussed.

***Keywords*:** exothermic reaction, ignition, stochastic differential equations, numerical simulation

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ЭНЕРГЕТИКА

Научная статья
УДК 536.2:519.63

Задача теплового взрыва со стохастической границей: квазистационарное приближение и прямое численное моделирование

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Резюме. Цель работы состоит в численном исследовании стохастической модификации задачи Франка-Каменецкого о развитии экзотермической реакции в плоскопараллельном слое со случайными флуктуациями температуры на внешней границе. Изменение температуры задается случайным процессом (броуновским движением). Такая задача может моделировать поведение некоторых типов химических реакторов, например, при их работе в условиях неуправляемых внешних воздействий. Важное отличие рассмотренной постановки от детерминированной заключается в том, что наличие шума допускает достижение критических условий при любых начальных условиях. Методы, используемые в работе, включают математическую теорию случайных процессов, а также численные методы решения стохастических дифференциальных уравнений. С помощью известных результатов теории случайных процессов оценены условия достижения зажигания в квазистационарном приближении (т.е. когда скорость тепловой релаксации намного выше скорости изменения температуры).

Показано, что в такой постановке можно получить приближенную зависимость между параметрами случайного блуждания и динамическими характеристиками зажигания (ожидаемым временем достижения условий теплового взрыва). Кроме этого, уравнение нестационарного теплопереноса в реагирующей среде решается численно для большого количества случайных траекторий температуры на границе области. Для этого используется комбинированная схема с явной аппроксимацией нелинейного источника и неявной аппроксимацией температурного поля. Сравнение двух подходов показало, что основные закономерности нестационарного развития теплового взрыва в стохастической среде могут быть с хорошей точностью приближены зависимостями, которые получаются из решения квазистационарной задачи с учетом небольшой корректировки для критической температуры (отвечающей границе устойчивости для стационарной задачи). Получены распределения характеристик зажигания (температуры зажигания, максимальной температуры окружающей среды, времени зажигания) при разных значениях реакционной способности и интенсивности шума.

***Ключевые слова*:** экзотермическая реакция, зажигание, стохастические дифференциальные уравнения, численное моделирование

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INTRODUCTION

Chemical reactions often occur under conditions with dynamic variations of temperature, pressure, and concentrations. The average rate of a chemical reaction cannot always be estimated by the average values of the determining parameters. In the simplest cases, variations in conditions can be represented as noise with given spectral characteristics. However, the influence of these characteristics on the reaction rate (in particular) and the stability of the reaction system (in general) is an important task which requires special research for each individual set of chemical reactions and range of conditions.

Fluctuation processes are particularly important in relation to problems related to the thermal stability of exothermic chemical reactors and other heat-generating devices, for example, in the study of emergency modes of electrochemical elements and methods for preventing them [1, 2].

The classic Frank-Kamenetskiy problem involves determining the conditions for thermal explosion (thermal ignition) in a sample with competition between heat release due to a chemical reaction and heat removal due to thermal conductivity. If we neglect reagent conversion, then the problem is reduced to solving the following equation [3]:

$$\frac{\partial\theta}{\partial t} = \frac{\partial^2\theta}{\partial\xi^2} + Fk\ exp\left(\frac{\theta}{1+Ar\ \theta}\right). \qquad (1)$$

Here, θ is the nondimensional temperature, t is the time (in Fourier number units), ξ is the spatial coordinate, Ar is the Arrhenius number (usually a small parameter), and Fk is Frank-Kamenetskiy number, which is a critical parameter of the problem. The initial condition is the uniform distribution of the temperature $\theta(0, \xi) = 0$. The boundary conditions are as follows:

$$\frac{\partial\theta}{\partial\xi}(t,0) = 0\,; \frac{\partial\theta}{\partial\xi}(t,1) = Bi[\theta_b - \theta(t,1)]. \qquad (2)$$

If $\theta_b = 0$, $Ar = 0$ and $Bi = \infty$, then the critical value of Fk_0 is about of 0.88. If Fk is greater than Fk_0, then the problem (1)–(2) does not have a stationary solution, and the temperature tends to infinity (thermal explosion occurs). Naturally, the unbound increase in the sample temperature is a result of an accepted approximation, namely, conversion neglect: in this case, we study ignition conditions, not the development of a process after ignition.

Often, ignition occurs in environments with stochastic perturbations of external parameters, for example, those associated with natural causes (noise, flow instability). In this regard, it is important to estimate the probability of ignition for a known range of such variations.

The influence of fluctuations on the development of a thermal explosion in adiabatic systems was investigated in [4–6], where the different nature of fluctuation dynamics in sub- and supercritical conditions was established. Simpler models (for complex chemical reactions under isothermal conditions) were considered in [7–9], including stochastic

chain termination reaction [10]. Small reacting systems were investigated in [11–13]. Linear heat losses (Semenov's problem) were studied by the authors of [14, 15]; fluctuations of the mass transfer coefficient for a heterogeneous exothermic reaction – in [16].

As was pointed out in [17], there is mutual influence of a chemical reaction and transport processes at the fluctuation level even despite the different tensor dimensions of the corresponding flows. In [18, 19], the mutual influence of a chemical reaction and transport coefficients was considered; in [20], the fluctuation-dissipation relations for mass transfer and chemical reactions were derived (in the absence of mass transfer, such relations are given in [21, 22]). Markov approximations for linear equations of chemical kinetics were considered in [23, 24], and in [25, 26], numerical algorithms based on the Monte Carlo method were proposed for their implementation (including those based on splitting methods [27]). Bistable potentials for reaction-diffusion equations were used to study thermal stability in [28, 29]. The problem of thermal explosion with temperature fluctuations was considered in [30, 31]; the influence of reaction rate fluctuations on the stability of flat samples was investigated in [32] using the Lyapunov method.

In relation to the topic of the present work, the works of Derevich and coauthors are of interest, in which statistics of the behavior of reacting particles in stochastic media were studied [33, 34], as well as the influence of the stochastic distribution of active centers in porous catalytic granules [35] (a similar formulation was also considered in [36] for simpler symmetry). In [37] a one-dimensional problem of a thermal explosion with temperature fluctuations at the spherical symmetry boundary was considered.

In the present work, a non-stationary one-dimensional problem of heat conduction with a nonlinear source and stochastic fluctuations in the ambient temperature is numerically solved for cylindrical symmetry. The subject of interest is the dependence of the expected ignition characteristics (time, ambient temperature, and heat fluxes on the particle surface) on the intensity of fluctuations, which are represented by white noise. We study the influence of temperature fluctuations on the thermal ignition conditions of a flat sample (layer). Unlike previous works, this article focuses on the environmental parameters that lead to thermal explosion and the patterns of the simulated ignition dynamics.

QUASI-STATIONARY THEORY

Quasi-stationary approximation is based on a time-scale splitting: thermal relaxation is considered fast enough to adapt to environmental disturbances. This assumption is not valid for high-amplitude impacts and near-explosion conditions, but it is quite reasonable for subcritical modes with moderate noise intensity. Using the quasi-stationary approximation, we can solve the dynamic problem for boundary temperature only.

Let us consider the Frank-Kamenetskiy problem with temperature fluctuations at the outer boundary (in the environment). We will assume that these fluctuations follow a Wiener process:

$$d\theta_b = \sigma\, \delta W. \tag{3}$$

Then, we can write the diffusion equation (Fokker-Planck equation) for the probability density function of the environmental temperature:

$$\frac{\partial P_\theta}{\partial t} = \frac{\sigma^2}{2}\frac{\partial^2 P_\theta}{\partial \theta_b^2}. \tag{4}$$

We assume that the conditions in the sample are such that the Frank-Kamenetskiy number is below its critical value ($Fk_0 = 0.88$). From dimensional analysis, it follows that the critical boundary temperature for the quasi-stationary problem can be found by the following formula:

$$\frac{Fk_0}{Fk} = \frac{1}{(1+Ar\theta_b^*)^2}\exp\left(\frac{\theta_b^*}{1+Ar\theta_b^*}\right) \approx \approx \exp(\theta_b^*). \tag{5}$$

From here, we obtain:

$$\theta_b^* \approx \ln\left(\frac{Fk_0}{Fk}\right). \tag{6}$$

If at the initial moment, the temperature at the boundary is zero, then the solu-

tion to the diffusion equation (4) is the fundamental solution to the heat equation as long as the distribution is concentrated near zero (which results in $\mathrm{Var}[\theta_b(t)] = \sigma^2 t$). At later times, it is necessary to consider that specific random trajectories do not have physical meaning after ignition conditions are reached. Therefore, let us change the boundary conditions and consider the diffusion equation with an absorbing boundary:

$$P(t,-\infty) = 0;\ P(t,\theta_b^*) = 0. \tag{7}$$

It can be shown that for the integral of $P(t, \theta)$ to be finite over the entire state space, it is also necessary that:

$$\frac{\partial P}{\partial \theta_b}(t,-\infty) = 0. \tag{8}$$

We integrate equation (4) over the state space (possible boundary temperature values):

$$\int_{-\infty}^{\theta_b^*} \frac{\partial P(t,y)}{\partial t} dy = \frac{\sigma^2}{2} \int_{-\infty}^{\theta_b^*} \frac{\partial^2 P(t,y)}{\partial y^2} dy = \\ = \frac{\sigma^2}{2} \frac{\partial P}{\partial \theta_b}(t,\theta_b^*). \tag{9}$$

The resulting equation shows that the number of realizations corresponding to different random trajectories decreases in time due to absorption at the right boundary (i.e., systems that have reached a critical temperature do not evolve further). At low critical temperatures, we can present the equation for the distribution function in difference form (we assume that most of the distribution is close to zero):

$$\frac{d\Phi}{dt} \approx \frac{\sigma^2}{2} \frac{\Phi}{(\theta_b^*)^2}. \tag{10}$$

Here $\Phi(t) = \int_{-\infty}^{\theta_b^*} P(t,y)dy$ is the survival probability, i.e., the probability that the system has not reached critical conditions for thermal ignition (has not drifted beyond the right boundary). Then we can introduce a characteristic non-dimensional diffusion parameter:

$$\frac{\sigma^2 \tau}{2(\theta_b^*)^2} = O(1). \tag{11}$$

This gives us an estimate of the half-life:

$$\tau = O\left[\frac{2(\theta_b^*)^2}{\sigma^2}\right]. \tag{12}$$

According to this equation, as the critical temperature increases, the expected ignition time also increases (in this case, the dependence $t \sim \theta^2$, which is expected for diffusion processes, is observed). With increasing noise intensity, the expected ignition time decreases [32], a similar dependence is found.

Fig. 1 presents the result of the numerical solution of the diffusion equation in a semi-infinite region with an absorbing boundary, namely, the dependence of the ignition probability on time. There is an exponential decrease in the survival probability Φ_{surv} (correspondingly, an increase in the ignition probability $\Phi_{ign} = 1 - \Phi_{surv}$); soon after this, the curve tends to zero (or, correspondingly, one) as $t^{-1/2}$ (such a slowdown is associated with trajectories that move towards low temperatures and rarely return). The half-life appears to be quite close to the above estimate. The plotted markers are discussed below.

Upon closer examination, it turns out that the boundary condition in the form of an absorbing boundary is a fairly rough approximation. It is necessary to solve the heat transfer equation for a stochastic reacting medium in a nonstationary form. The stochastic equation for environmental temperature is complemented by the thermal conductivity equation in the medium. Then, the ignition conditions are determined not only by the possibility of achieving a critical environmental temperature but also by the propagation of thermal disturbances in the medium. As direct numerical modelling shows below, situations are possible when exceeding the critical temperature at the sample boundary does not lead to the development of a thermal explosion in a stochastic environment. The stochastic dynamics of the environmental temperature lead, to the residence time

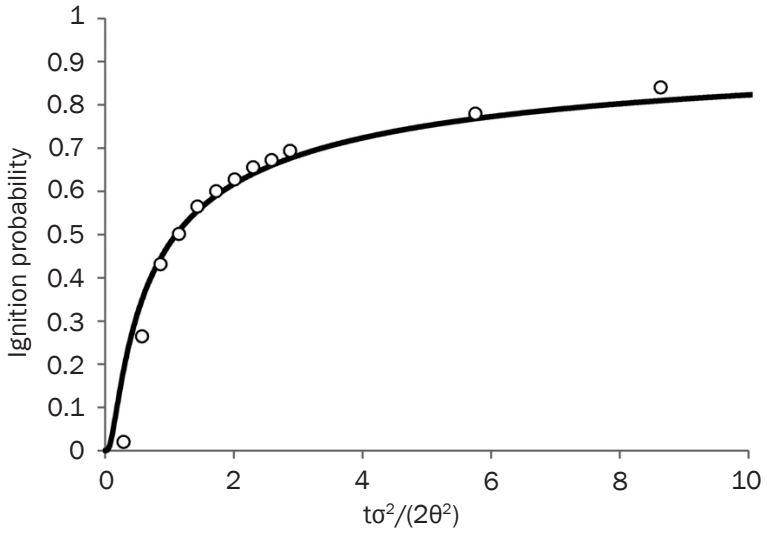

Fig. 1. *Solution of the diffusion equation with an absorbing boundary (the markers are the results of calculations using the Monte Carlo method with correction)*
Рис. 1. *Решение уравнения диффузии с поглощающей границей (маркеры – результаты расчетов с использованием метода Монте-Карло с поправкой)*

in the supercritical region possibly being too short for temperature disturbances to develop. Thus, the only way to study the stochastic problem of thermal explosion is direct numerical simulation.

DIRECT NUMERICAL SIMULATION

For calculations, we use the following semi-implicit difference scheme:

$$\frac{\theta_i - \theta_i^0}{\Delta t} = \frac{\theta_{i-1} - 2\theta_i + \theta_{i+1}}{h^2} + Fk \exp\left(\frac{\theta_i^0}{1 + Ar\,\theta_i^0}\right). \quad (13)$$

The boundary conditions for this system of difference equations are written as follows:

$$\theta_1 - \theta_2 = 0;\ \theta_N - \theta_{N-1} = h\,Bi\,(\theta_b - \theta_N). \quad (14)$$

We use the following parameter values for calculations: spatial grid step 2×10^{-3}; time grid step 1×10^{-3} (adaptation of the grid step is needed, as a rule, only near the explosion time; in this work, a time grid step is constant, so the ignition time is determined up to its value). Using explicit approximation for the heat source in (13), we obtain a system of linear equations that is solved by the tridiagonal matrix algorithm (the numerical solution is described in more detail in [36, 38]). The stochastic equation for the boundary temperature has the following difference approximation (Euler-Maruyama method [39]):

$$\theta_b = \theta_b^0 + \varepsilon\sigma\sqrt{\Delta t}\,. \quad (15)$$

Here, ε is a normally distributed random number with unit variance.

Let us consider ignition under conditions where the initial state and parameters of the problem at $\sigma = 0$ correspond to subcritical conditions. As mentioned above, the critical number Fk_0 is 0.88 for $Bi = \infty$ and $Ar = 0$. Under $Bi = 1000$ and $Ar = 0.02$, the critical number Fk_0 slightly increases to approximately 0.897 (a time period of approximately 80 Fourier numbers is considered). The value $Fk = 0.8$ was chosen as the deliberately subcritical mode. Numerical calculations show that at this Fk, a stationary solution is established with a maximum temperature of approximately 0.73. According to several papers [32, 33], the onset of a thermal explosion in a stochastic system is inevitable, although the expected ignition time increases sharply with distance from the stability limit [3]. For $Fk = 0.8$, the critical ignition temperature is 0.118; the numerical calculation is shown in Fig. 2, confirming the validity of formula (6). The ignition criterion in the calculations is the achievement of a high temperature in the centre of the sample ($\theta(\tau_{ign}, 0) > 10$).

Note that even at a value of *Fk* above the critical value, there are random trajectories leading to the region of low temperatures, so the onset of a thermal explosion, in the general case, is not guaranteed even for samples with high reactivity (this effect can be seen even for the quasi-stationary approximation in (Fig. 1). Calculations show that for *Fk* = 1, the probability of ignition after 40 temporal units is 0.87 (for *Fk* = 2, it is already 0.98 but still less than 1).

The overall calculation time for all the cases is 40 temporal units (in this case, the time unit corresponds to the Fourier number). The ignition time, as mentioned above, increases sharply when approaching the critical value *Fk*, so calculating the exact limit is practically impossible. The graph in Fig. 3 shows that the ignition probability expectedly increases with the time span. The behaviours of the curves in Fig. 1 and 3a qualitatively coincide (up to the time scale).

We solve a system of equations with the initial condition $\theta(0, \xi) = 0$ for different random trajectories $\theta_b(t)$ (a total of 1000 trajectories for each value of σ) and study the distribution of the resulting solutions. Note that the histograms presented below contain only solutions with successful ignition. The probability of ignition Φ_{ign}, calculated as the ratio of the number of calculations with successful ignition to the total number of calculations, is shown in Fig. 3: this value does not exceed 0.87 for all considered parameter values. In this case, however, only the ignition probability in a given time interval is considered: as the previous analysis shows, the ignition probability increases slowly over large periods of time. The equipment of multi-access center “High-temperature circuit” was used for computations.

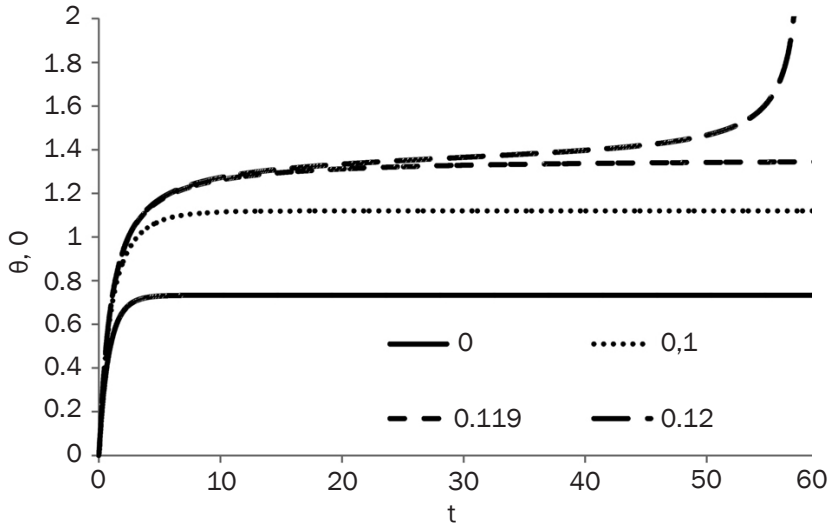

Fig. 2. *Temperature dynamics in the centre of the sample for a deterministic problem for Fk = 0.8 and different values of the environment temperature*

Рис. 2. *Динамика температуры в центре образца для детерминированной задачи при Fk = 0,8 и при различных значениях температуры окружающей среды*

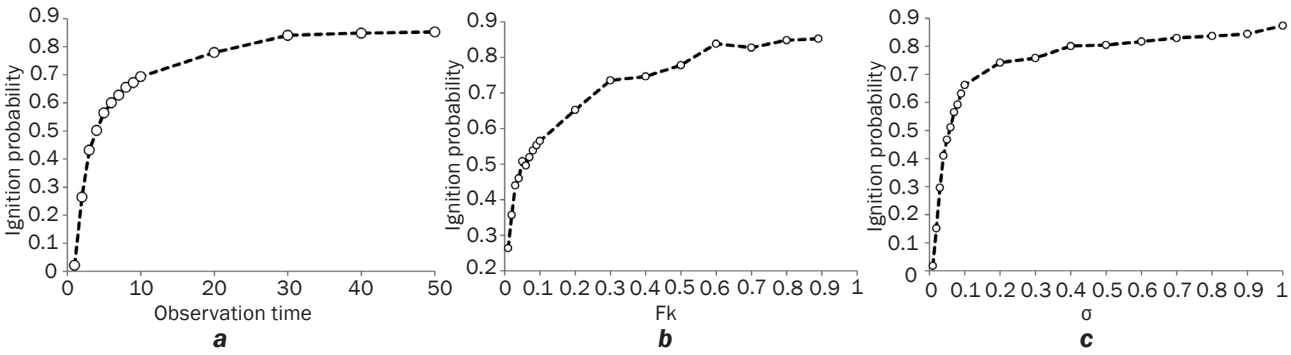

Fig. 3. *Ignition probability vs calculation time, Fk number and noise intensity σ*

Рис. 3. *Зависимость вероятности воспламенения от времени расчета, числа Fk и шага случайного блуждания σ*

CALCULATION RESULTS AND DISCUSSION

The results are presented in two types of figures: histograms showing the distributions from computational experiments (probability is interpreted as relative frequency, Figs. 4–9); and moments of these distributions (mean and variance, Figs. 10 and 11).

As the step of the noise intensity σ increases, the variance of the temperature at which ignition occurs also increases (Fig. 4). The maximum of the distributions in all the cases is shifted toward positive values of the dimensionless temperature. At $\sigma = 0.1$, the distribution is concentrated near $\theta_{ign} = 0$, while at $\sigma > 0.7$, the maximum of the distribution is at $\theta_{ign} > 1$$. Since the critical temperature in this case is low, ignition requires that the environment temperature remained in the region $\theta_b > \theta_b^*$ long enough for the thermal disturbance to propagate throughout the sample. With a small σ, the θ_b values stay longer within the ignition range after entering it, while with larger variances, the temperature will change more significantly. With increasing σ, the fraction of solutions with successful ignition increases when the environmental temperature is lower than the critical value. That is, if "no return" conditions are achieved (i.e., thermal disturbances developed enough), then the environmental temperature decrease caused by the noise cannot prevent ignition. Fig. 5 shows the values of the

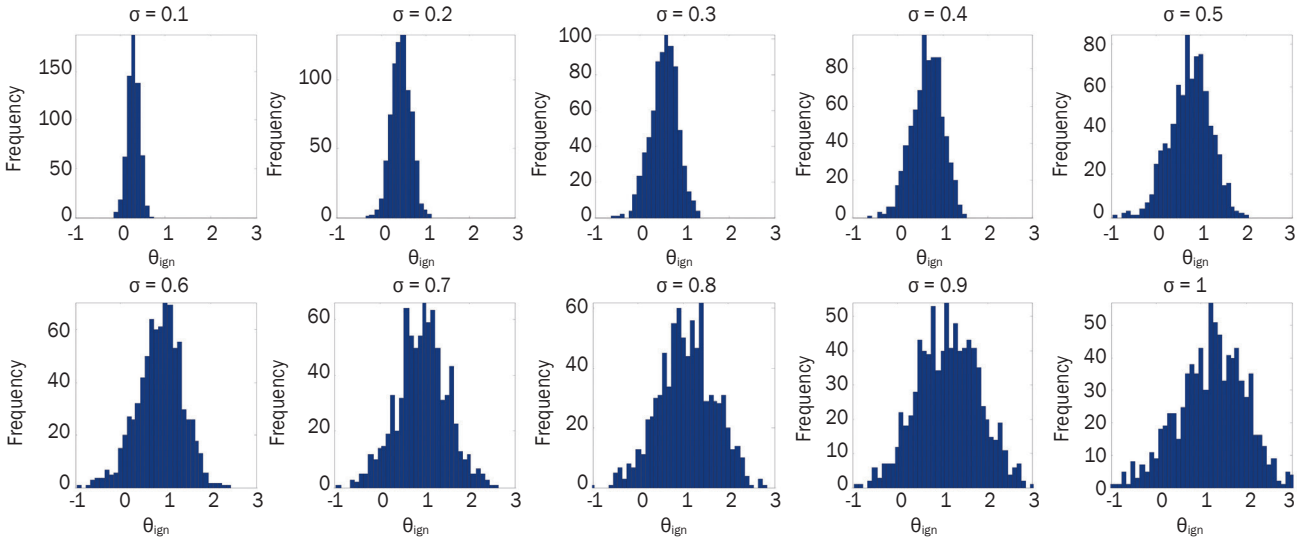

Fig. 4. *Distribution of the environment temperature at the ignition moment for Fk = 0.8 and different σ values*
Рис. 4. *Распределение температуры окружающей среды в момент воспламенения при Fk = 0,8 и различных значениях σ*

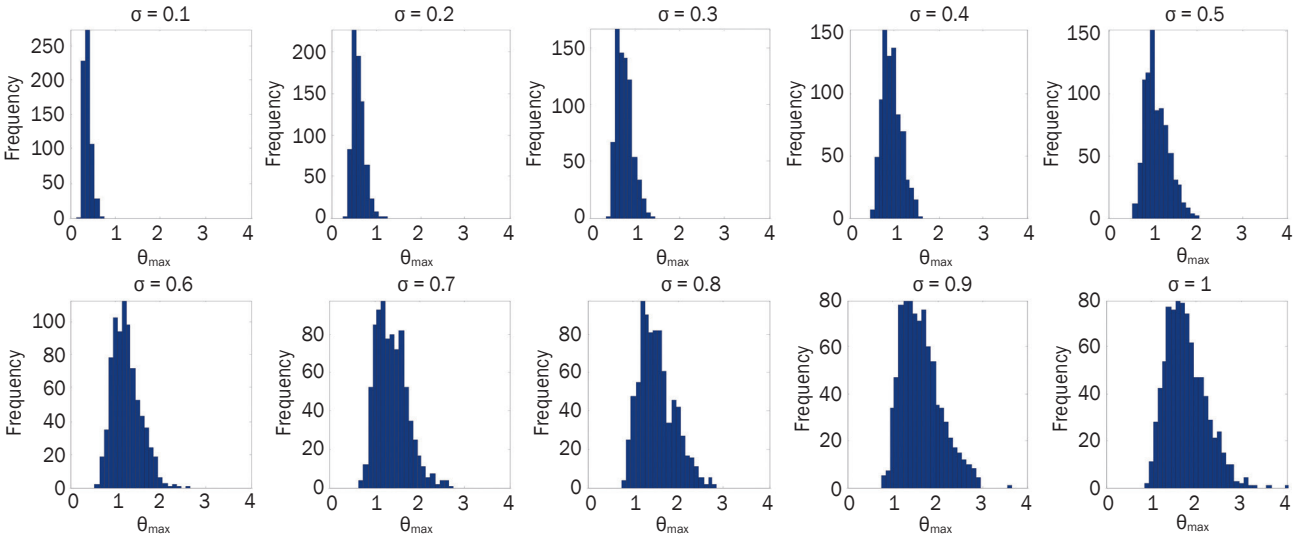

Fig. 5. *Distribution of the maximum environment temperature achieved during random walks for Fk = 0.8 and different σ values*
Рис. 5. *Распределение максимальной температуры окружающей среды, достигнутой при случайных блужданиях при Fk = 0,8 и различных значениях σ*

highest achieved environment temperature (for successful ignition solutions). The higher the average environmental temperature, the lower the ignition time, as shown in Fig. 6. The fraction of solutions with early ignition increases with noise intensity.

Further, calculations were carried out for a constant σ with varying *Fk*. The ignition characteristics were the same: the environmental temperature at which ignition occurred, the highest environment temperature reached before ignition, and the ignition time delay. In contrast to varying the noise intensity, varying the value of *Fk* has little effect on the shape of the ignition temperature distribution. As shown in Fig. 7, an increase in reactivity leads to a shift in the distribution toward lower temperatures (following eq. (6)). That is, after reaching the ignition limits, the environment temperature changes similarly for all values of *Fk*, which results from the randomness of the walk.

Fig. 8 shows similar shifts in the distribution for the maximum temperature. The left shoulder of the distribution decays more sharply (since ignition is less likely at low temperatures). The right shoulder of the distribution follows the same pattern as in the previous figure.

The higher the *Fk* value, the lower the ignition temperature and, therefore, the less the average time needed to reach a critical temperature. The distribution of ignition times is then concentrated in the region of small values.

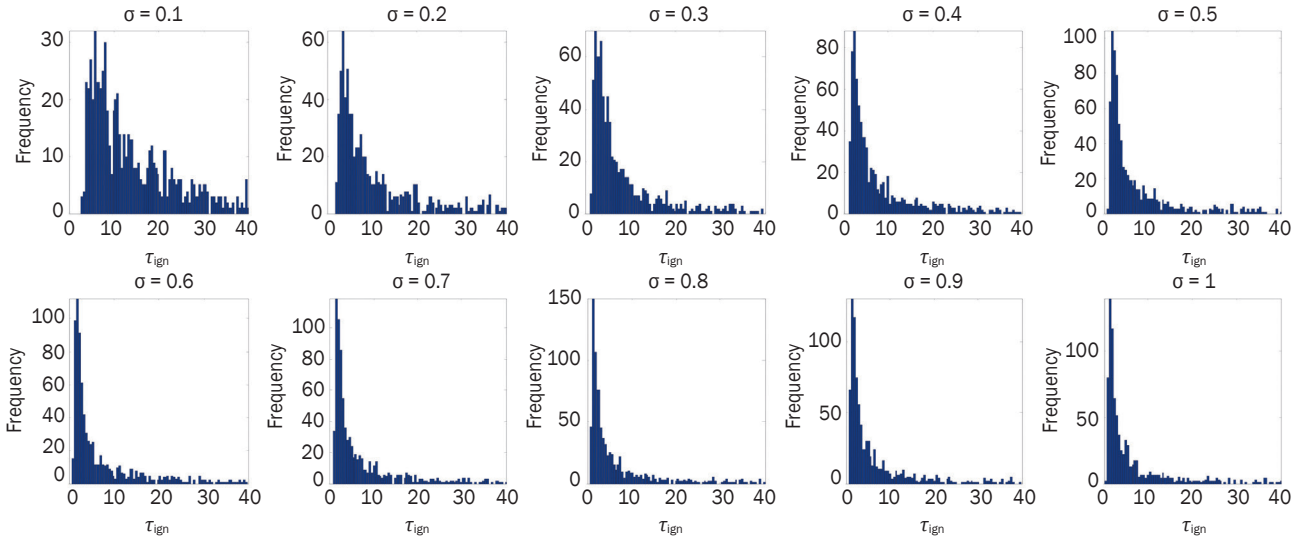

Fig. 6. *Distribution of ignition time for Fk = 0.8 and different σ values*
Рис. 6. *Распределение времени зажигания для Fk = 0,8 и различных значений σ*

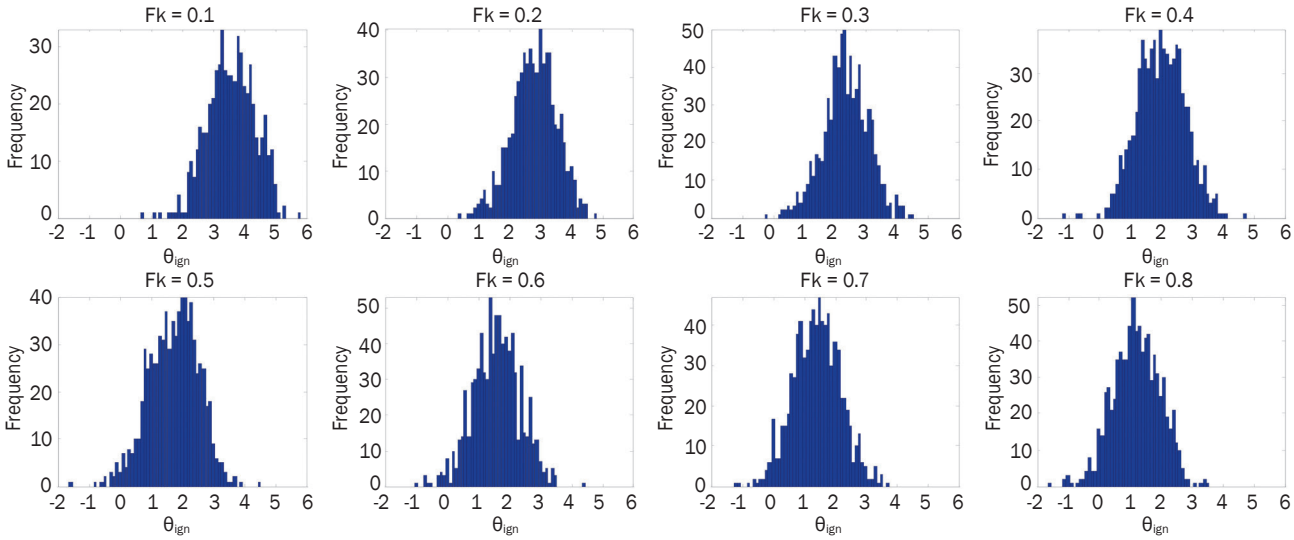

Fig. 7. *Distribution at the environment temperature at the ignition moment for σ = 1 and different Fk values*
Рис. 7. *Распределение температуры окружающей среды в момент воспламенения при σ = 1 и различных значениях Fk*

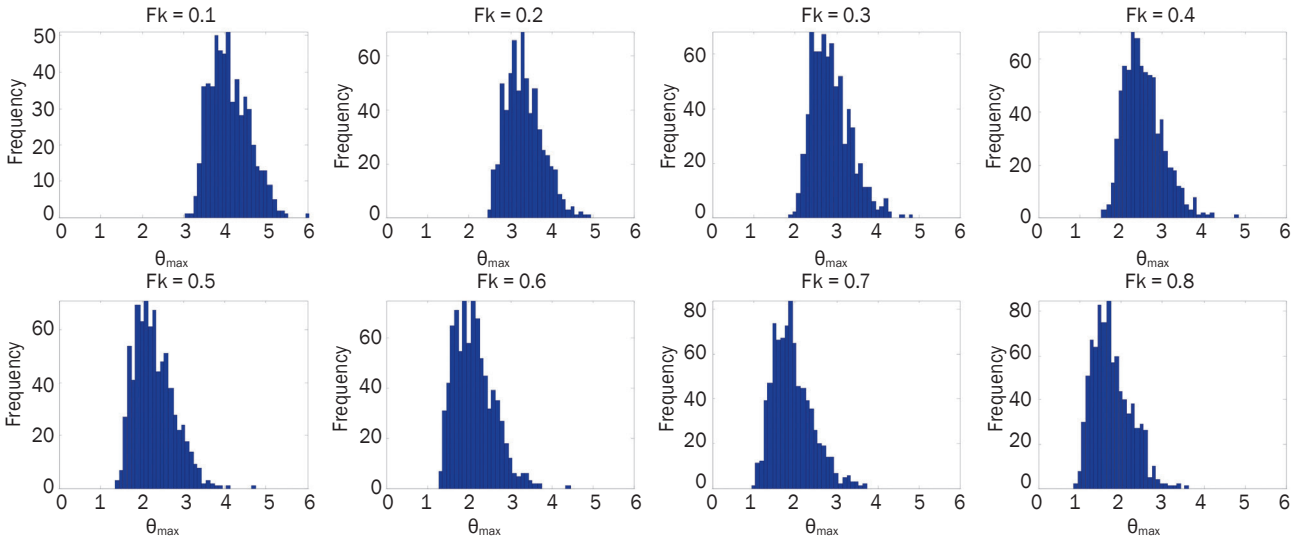

Fig. 8. *Distribution of the maximum environment temperature achieved during random walks for σ = 1 and different Fk values*
Рис. 8. *Распределение максимальной температуры окружающей среды, достигнутой при случайных блужданиях, для σ = 1 и для различных значений Fk*

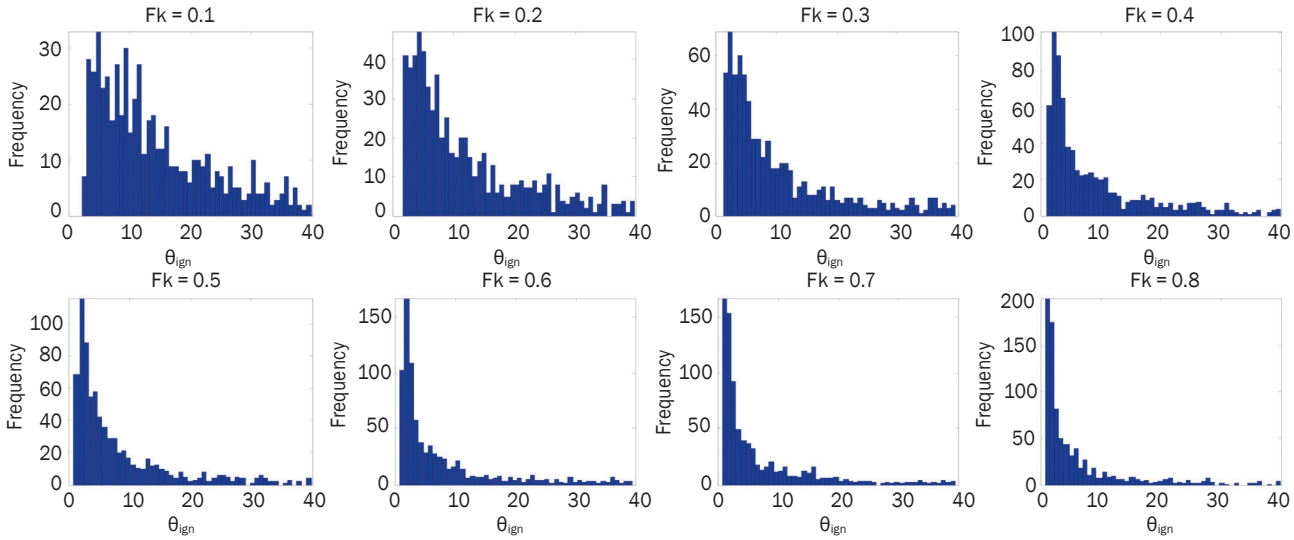

Fig. 9. *Distribution of ignition times for σ = 1 and different Fk values*
Рис. 9. *Распределение времени зажигания для σ = 1 и для различных значений Fk*

Figs. 10 and 11 show the changes in moments. As indicated earlier, with increasing noise intensity, the variance of the characteristic temperature increases, and this growth is approximately linear. With a constant noise intensity, the distribution temperature width changes slightly, while the dependences of critical temperatures on variance follow qualitatively eq. (6) but with a shift relative to the y-axis (1–2 temperature units). The variance of the ignition temperature distribution for all the cases is greater than the variance of the maximum temperature distribution. This difference may be explained by the difference in the time scales of heating and ignition. The reaction rate is approximately constant along the curves in the graphs; therefore, for ignition to occur before the environmental temperature drops and the sample cools, a higher temperature is needed. The average reaction rate increases by 5–10 times compared to the reaction rate for quasi-stationary conditions, which ensures that the sample ignites within the thermal relaxation time.

Average ignition time decreases almost monotonically with an increase of reactivity and noise intensity (Fig. 11). Its variance does not significantly change. It should be noted that the values were calculated based on successful ignition cases only.

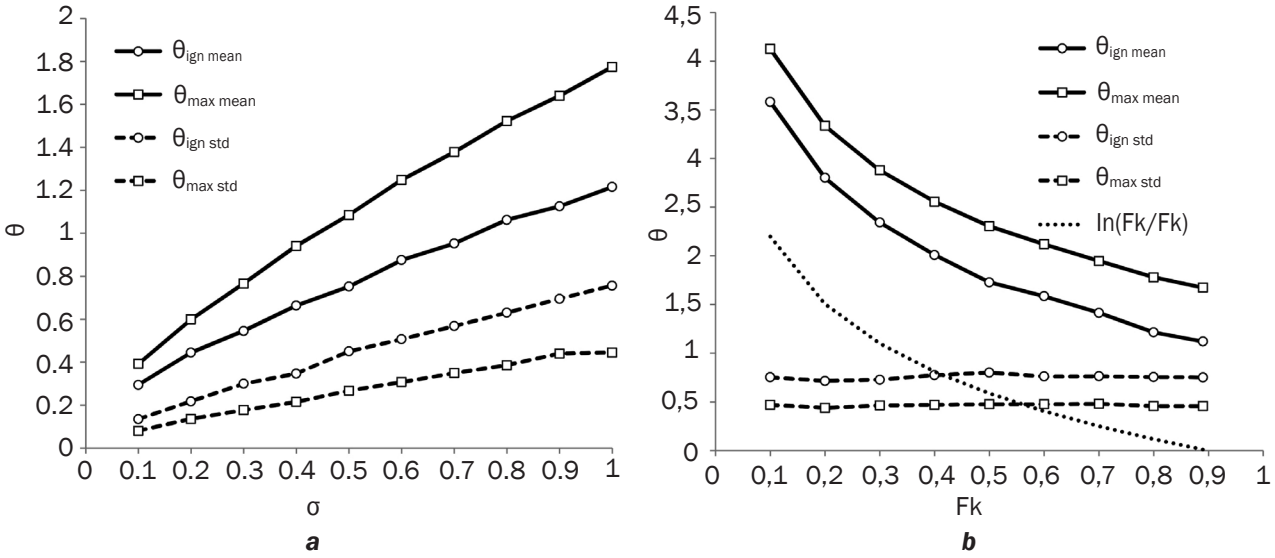

Fig. 10. *Average values and variances of ignition temperature from the maximum temperature*
Рис. 10. *Средние значения и отклонения температуры воспламенения от максимальной температуры*

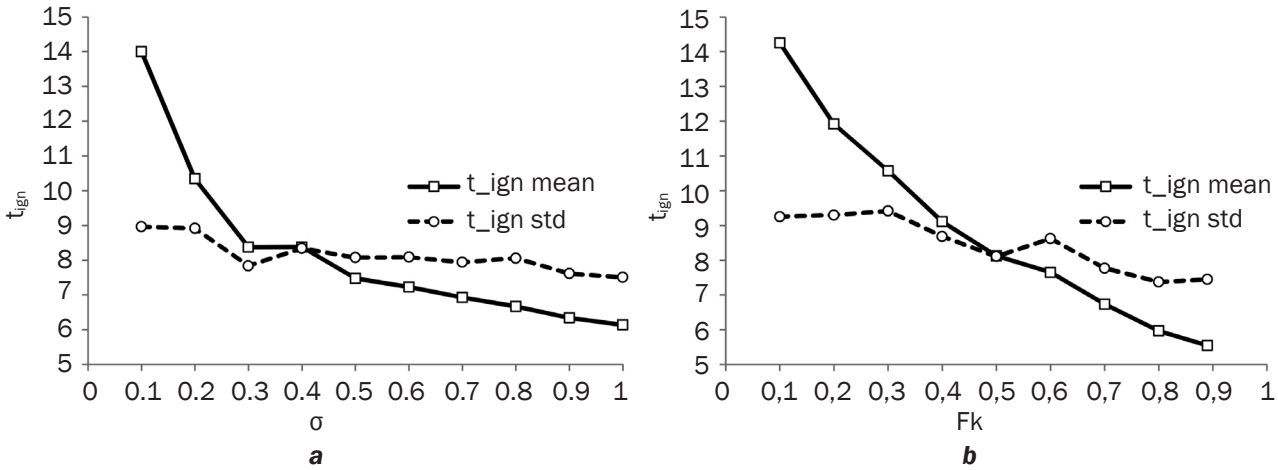

Fig. 11. *Average values and variances of ignition time values when changing parameters σ and Fk*
Рис. 11. *Средние значения и отклонения значений времени зажигания при изменении параметров σ и Fk*

Thus, the influence of non-stationarity can be reduced, with some degree of approximation, to a change in the critical temperature. Indeed, the curve in Fig. 3 *a*, reduced to the critical temperature from eq. (6) with a constant additive term of 1.2 temperature units (the average difference for Fig. 10 *b*), agrees quite well with the results of the quasi-stationary analysis (4)–(8): this comparison is presented in Fig. 1 with circles.

The main result is the dependence of expected ignition time on reaction conditions: this dependence can be used for the control of reactive systems in stochastic environments (for example, to detect runaway or to select a method of extinguishing). This kind of problem is of interest in energy storage systems design, taking into account fire safety issues. Other problems are also to be studied, including optimal control, collective effects in connected heat networks, the “inverse” problem of ensuring stable combustion, etc.

CONCLUSION

The paper shows that the development of a thermal explosion in a stochastic environment differs significantly from the predictions of classical theory. A thermal explosion can occur for arbitrarily low levels of reactivity because there is a nonzero probability of reaching an arbitrarily high ambient temperature; on the other hand, even if a reactivity is higher than

the critical value, the onset of a thermal explosion is not guaranteed since there is a symmetric probability of achieving an arbitrarily low temperature.

Calculations carried out using the Monte Carlo method make it possible to estimate the ignition probability depending on the parameters of the problem (reactivity, noise intensity, observation time). As the noise intensity increases, the width of the characteristic temperature distribution increases; with increasing reactivity, the variance in the characteristic temperatures practically does not change, while the average values change qualitatively in a way expected from quasi-stationary theory. The average ignition time decreases with increasing noise intensity and reactivity; the variance in the ignition time distribution is slightly reduced.

The results obtained can be applied to the analysis of critical phenomena in stochastic media.

References

1. Mallick S., Gayen D. Thermal behaviour and thermal runaway propagation in lithium-ion battery systems – a critical review. *Journal of Energy Storage*. 2023;62:106894. https://doi.org/10.1016/j.est.2023.106894. EDN: VDIKWS.
2. Fu Hui, Wang Junling, Li Lun, Gong Junhui, Wang Xuan. Numerical study of mini-channel liquid cooling for suppressing thermal runaway propagation in a lithium-ion battery pack. *Applied Thermal Engineering*. 2023;234:121349. https://doi.org/10.1016/j.applthermaleng.2023.121349. EDN: OAMIOZ.
3. Frank-Kamenetsky D.A. *Fundamentals of macrokinetics. Diffusion and heat transfer in chemical kinetics*. Moscow: Nauka; 2008, 407 p. (In Russ.). EDN: QKBWWN.
4. Baras F., Nicolis G., Mansour M.M., Turner J.W. Stochastic theory of adiabatic explosion. *Journal of Statistical Physics*. 1983;32:1-23. https://doi.org/10.1007/BF01009416.
5. De Pasquale F., Mecozzi A. Theory of chemical fluctuations in thermal explosions. *Physical Review A.* 1985;31:2454. https://doi.org/10.1103/PhysRevA.31.2454.
6. Fernandez A. Theory of scaling for fluctuations in thermal explosion conditions. *Berichte der Bunsengesellschaft fur physikalische Chemie*. 1987;91(2):159-163. https://doi.org/10.1002/bbpc.19870910216.
7. Frankowicz M., Nicolis G. Transient evolution towards a unique stable state: stochastic analysis of explosive behavior in a chemical system. *Journal of Statistical Physics*. 1983;33:595-609. https://doi.org/10.1007/BF01018836.
8. Frankowicz M., Mansour M.M., Nicolis G. Stochastic analysis of explosive behaviour: a qualitative approach. *Physica A: Statistical Mechanics and its Applications*. 1984;125(1):237-246. https://doi.org/10.1016/0378-4371(84)90011-6.
9. Van Kampen N.G. Intrinsic fluctuations in explosive reactions. *Journal of Statistical Physics*. 1987;46(5):933-948. https://doi.org/10.1007/BF01011150. EDN: ECYFKX.
10. Vlad M.O., Ross J. A stochastic approach to nonequilibrium chain reactions in disordered systems: breakdown of eikonal approximation. *International Journal of Thermophysics*. 1997;18:957-975. https://doi.org/10.1007/BF02575241.
11. Gorecki J., Popielawski J. On the stochastic theory of adiabatic thermal explosion in small systems — numerical results. *Journal of Statistical Physics.* 1986;44:941-954. https://doi.org/10.1007/BF01011916.
12. Zheng Qiang, Ross J. Comparison of deterministic and stochastic kinetics for nonlinear systems. *Journal of Chemical Physics*. 1991;94(5):3644-3648. https://doi.org/10.1063/1.459735.
13. Chou Dong-Pao, Lackner T., Yip Sidney. Fluctuation effects in models of adiabatic explosion. *Journal of Statistical Physics*. 1992;69:193-215. https://doi.org/10.1007/BF01053790.
14. Nowakowski B., Lemarchand A. Thermal explosion near bifurcation: stochastic features of ignition. *Physica A: Statistical Mechanics and its Applications*. 2002;311(1-2):80-96. https://doi.org/10.1016/S0378-4371(02)00824-5. EDN: AYCRRJ.
15. Lemarchand A., Nowakowski B. Fluctuation-induced and nonequilibrium-induced bifurcations in a thermochemical system. *Molecular Simulation*. 2004;30(11-12):773-780. http://dx.doi.org/10.1080/0892702042000270151.
16. Buyevich Yu.A., Fedotov S.P. Formation of heterogeneous reaction modes under the influence of multiplicative noise. *Journal of Engineering Physics and Thermophysics.* 1987;53(5):802-807. (In Russ.).
17. Wei James. Irreversible thermodynamics in engineering. *Industrial and Engineering Chemistry*. 1966;50(10):55-60. https://doi.org/10.1021/ie50682a010.
18. Van der Broeck C., Parrondo J.M.R., Toral R., Kawai R. Nonequilibrium phase transitions induced by multiplicative noise. *Physical Review E*. 1997;55:4084. https://doi.org/10.1103/PhysRevE.55.4084.
19. Bedeaux D., Pagonabarraga I., De Zarate J.M.O., Sengers J.V., Kjelstrup S. Mesoscopic non-equilibrium thermodynamics of non-isothermal reaction-diffusion. *Physical Chemistry Chemical Physics*. 2010;12(39):12780-12793. https://doi.org/10.1039/C0CP00289E. EDN: OBNEQV.
20. Bochkov G.N., Orlov A.L., Kolpashchikov V.L. Fluctuation-dissipation models of mass transfer in systems with chemical reactions. *International Communications in Heat and Mass Transfer*. 1985;12(1):33-43. https://doi.org/10.1016/0735-1933(85)90005-3.

21. Schmiedl T., Seifert U. Stochastic thermodynamics of chemical reaction networks. *Journal of Chemical Physics*. 2007;126(4):044101. https://doi.org/10.1063/1.2428297.
22. Ge Hao, Qian Hong. Mathematical formalism of nonequilibrium thermodynamics for nonlinear chemical reaction systems with general rate law. *Journal of Statistical Physics*. 2017;166(1):190-209. https://doi.org/10.1007/s10955-016-1678-6. EDN: YAXFNJ.
23. Darvey I.G., Staff P.J. Stochastic approach to first-order chemical reaction kinetics. *Journal of Chemical Physics*. 1966;44(3):990-997. https://doi.org/10.1063/1.1726855.
24. Van Kampen N.G. The equilibrium distribution of a chemical mixture. *Physics Letters A*. 1976;59(5):333-334. https://doi.org/10.1016/0375-9601(76)90398-4.
25. Gillespie D.T. Stochastic simulation of chemical kinetics. *Annual Reviews of Physical Chemistry*. 2007;58:35-55. https://doi.org/10.1146/annurev.physchem.58.032806.104637.
26. Higham D.J. Modeling and simulating chemical reactions. *SIAM review*. 2008;50(2):347-368. https://doi.org/10.1137/060666457.
27. Sandu A. A new look at the chemical master equation. *Numerical Algorithms*. 2014;65:485-498. https://doi.org/10.1007/s11075-013-9758-z.
28. Schlögl F. Stochastic measures in nonequilibrium thermodynamics. *Physics Reports*. 1980;62(4):267-380. https://doi.org/10.1016/0370-1573(80)90019-8. EDN: XSQZOA.
29. Öttinger H.C., Peletier M.A., Montefusco A. A framework of nonequilibrium statistical mechanics. I. Role and types of fluctuations. *Journal of Non-Equilibrium Thermodynamics*. 2020;46(10):1-13. https://doi.org/10.1515/jnet-2020-0068. EDN: UJNFDB.
30. Fernandez A., Rabitz H. *The scaling of nonequilibrium fluctuations in gaseous thermal explosions*. *Berichte der Bunsengesellschaft fur physikalische Chemie.* 1988;92(6):754-760. https://doi.org/10.1002/bbpc.198800184.
31. Baer M.R., Gartling D.K., Desjardin P.E. Probabilistic models for reactive behaviour in heterogeneous condensed phase media. *Combustion Theory and Modelling*. 2012;16(1):75-106. https://doi.org/10.1080/13647830.2011.606916.
32. Fedotov S.P. Stochastic analysis of the thermal ignition of a distributed explosive system. *Physics Letters A*. 1993;176(3-4):220-224. https://doi.org/10.1016/0375-9601(93)91038-7. EDN: ZYVJQJ.
33. Derevich I.V. Effect of temperature fluctuations of fluid on thermal stability of particles with exothermic chemical reaction. *International Journal of Heat and Mass Transfer*. 2010;53(25-26):5920-5932. https://doi.org/10.1016/j.ijheatmasstransfer.2010.07.031. EDN: MXGOGN.
34. Derevich I., Galdina D. Simulation of thermal explosion of catalytic granule in fluctuating temperature field. *Journal of Applied Mathematics and Physics.* 2013;1(5):1-7. http://doi.org/10.4236/jamp.2013.15001.
35. Derevich I.V., Fokina A.Y., Ermolaev V.S., Mordkovich V.Z., Solomonik I.G. Heat and mass transfer in Fischer–Tropsch catalytic granule with localized cobalt microparticles. *International Journal of Heat and Mass Transfer.* 2018;121:1335-1349. https://doi.org/10.1016/j.ijheatmasstransfer.2018.01.077. EDN: XXMULJ.
36. Donskoy I.G., Gross E.I. Numerical analysis of thermal ignition statistics in a stochastic reacting medium. *Information and mathematical technologies in science and management*. 2024;1:66-77. (In Russ.). https://doi.org/10.25729/ESI.2024.33.1.006. EDN: BWDPTW.
37. Derevich I.V., Klochkov A.K. Thermal explosion of single particles in a random temperature field of the medium. *High temperature*. 2023;61(1):108-117. (In Russ.). https://doi.org/10.31857/S0040364423010039. EDN: PYOCSJ.
38. Donskoy I.G. Steady-state equation of thermal explosion in a distributed activation energy medium: numerical solution and approximations. *iPolytech Journal*. 2022;26(4):626-639. https://doi.org/10.21285/1814-3520-2022-4-626-639. EDN: BNSPEZ.
39. Kloeden P.E., Platen E. *Numerical solution of stochastic differential equations*. Berlin: Springer; 1991, vol. 19, Iss. 11, 636 p. https://doi.org/10.1007/978-3-662-12616-5.

Список источников

1. Mallick S., Gayen D. Thermal behaviour and thermal runaway propagation in lithium-ion battery systems – a critical review // Journal of Energy Storage. 2023. Vol. 62. P. 106894. https://doi.org/10.1016/j.est.2023.106894. EDN: VDIKWS.
2. Fu Hui, Wang Junling, Li Lun, Gong Junhui, Wang Xuan. Numerical study of mini-channel liquid cooling for suppressing thermal runaway propagation in a lithium-ion battery pack // Applied Thermal Engineering. 2023. Vol. 234. P. 121349. https://doi.org/10.1016/j.applthermaleng.2023.121349. EDN: OAMIOZ.
3. Франк-Каменецкий Д.А. Основы макрокинетики. Диффузия и теплопередача в химической кинетике: монография. 4-е изд. М.: Наука, 2008. 407 с. EDN: QKBWWN.
4. Baras F., Nicolis G., Mansour M.M., Turner J.W. Stochastic theory of adiabatic explosion // Journal of Statistical Physics. 1983. Vol. 32. P. 1–23. https://doi.org/10.1007/BF01009416.
5. De Pasquale F., Mecozzi A. Theory of chemical fluctuations in thermal explosions // Physical Review A. 1985. Vol. 31. P. 2454. https://doi.org/10.1103/PhysRevA.31.2454.
6. Fernandez A. Theory of scaling for fluctuations in thermal explosion conditions // Berichte der Bunsengesellschaft fur physikalische Chemie. 1987. Vol. 91. Iss. 2. P. 159–163. https://doi.org/10.1002/bbpc.19870910216.

7. Frankowicz M., Nicolis G. Transient evolution towards a unique stable state: stochastic analysis of explosive behavior in a chemical system // Journal of Statistical Physics. 1983. Vol. 33. P. 595–609. https://doi.org/10.1007/BF01018836.
8. Frankowicz M., Mansour M.M., Nicolis G. Stochastic analysis of explosive behaviour: a qualitative approach // Physica A: Statistical Mechanics and its Applications. 1984. Vol. 125. Iss. 1. P. 237–246. https://doi.org/10.1016/0378-4371(84)90011-6.
9. Van Kampen N.G. Intrinsic fluctuations in explosive reactions // Journal of Statistical Physics. 1987. Vol. 46. No. 5. P. 933–948. https://doi.org/10.1007/BF01011150. EDN: ECYFKX.
10. Vlad M.O., Ross J. A stochastic approach to nonequilibrium chain reactions in disordered systems: breakdown of eikonal approximation // International Journal of Thermophysics. 1997. Vol. 18. P. 957–975. https://doi.org/10.1007/BF02575241.
11. Gorecki J., Popielawski J. On the stochastic theory of adiabatic thermal explosion in small systems — Numerical results // Journal of Statistical Physics. 1986. Vol. 44. P. 941–954. https://doi.org/10.1007/BF01011916.
12. Zheng Qiang, Ross J. Comparison of deterministic and stochastic kinetics for nonlinear systems // Journal of Chemical Physics. 1991. Vol. 94. Iss. 5. P. 3644–3648. https://doi.org/10.1063/1.459735.
13. Chou Dong-Pao, Lackner T., Yip Sidney. Fluctuation effects in models of adiabatic explosion // Journal of Statisa tical Physics. 1992. Vol. 69. P. 193–215. https://doi.org/10.1007/BF01053790.
14. Nowakowski B., Lemarchand A. Thermal explosion near bifurcation: stochastic features of ignition // Physica A: Statistical Mechanics and its Applications. 2002. Vol. 311. Iss. 1-2. P. 80–96. https://doi.org/10.1016/S0378-4371(02)00824-5. EDN: AYCRRJ.
15. Lemarchand A., Nowakowski B. Fluctuation-induced and nonequilibrium-induced bifurcations in a thermochemical system // Molecular Simulation. 2004. Vol. 30. Iss. 11-12. P. 773–780. http://dx.doi.org/10.1080/0892702042000270151.
16. Буевич Ю.А., Федотов С.П. Формирование режимов гетерогенной реакции под воздействием мультипликативного шума // Инженерно-физический журнал. 1987. Т. 53. № 5. С. 802–807.
17. Wei James. Irreversible thermodynamics in engineering // Industrial and Engineering Chemistry. 1966. Vol. 50. Iss. 10. P. 55–60. https://doi.org/10.1021/ie50682a010.
18. Van der Broeck C., Parrondo J.M.R., Toral R., Kawai R. Nonequilibrium phase transitions induced by multiplicative noise // Physical Review E. 1997. Vol. 55. P. 4084. https://doi.org/10.1103/PhysRevE.55.4084.
19. Bedeaux D., Pagonabarraga I., De Zarate J.M.O., Sengers J.V., Kjelstrup S. Mesoscopic non-equilibrium thermodynamics of non-isothermal reaction-diffusion // Physical Chemistry Chemical Physics. 2010. Vol. 12. Iss. 39. P. 12780–12793. https://doi.org/10.1039/C0CP00289E. EDN: OBNEQV.
20. Bochkov G.N., Orlov A.L., Kolpashchikov V.L. Fluctuation-dissipation models of mass transfer in systems with chemical reactions // International Communications in Heat and Mass Transfer. 1985. Vol. 12. Iss. 1. P. 33–43. https://doi.org/10.1016/0735-1933(85)90005-3.
21. Schmiedl T., Seifert U. Stochastic thermodynamics of chemical reaction networks // Journal of Chemical Physics. 2007. Vol. 126. Iss. 4. P. 044101. https://doi.org/10.1063/1.2428297.
22. Ge Hao, Qian Hong. Mathematical formalism of nonequilibrium thermodynamics for nonlinear chemical reaction systems with general rate law // Journal of Statistical Physics. 2017. Vol. 166. Iss. 1. P. 190–209. https://doi.org/10.1007/s10955-016-1678-6. EDN: YAXFNJ.
23. Darvey I.G., Staff P.J. Stochastic approach to first-order chemical reaction kinetics // Journal of Chemical Physics. 1966. Vol. 44. Iss. 3. P. 990–997. https://doi.org/10.1063/1.1726855.
24. Van Kampen N.G. The equilibrium distribution of a chemical mixture // Physics Letters A. 1976. Vol. 59. Iss. 5. P. 333–334. https://doi.org/10.1016/0375-9601(76)90398-4.
25. Gillespie D.T. Stochastic simulation of chemical kinetics // Annual Reviews of Physical Chemistry. 2007. Vol. 58. P. 35–55. https://doi.org/10.1146/annurev.physchem.58.032806.104637.
26. Higham D.J. Modeling and simulating chemical reactions // SIAM review. 2008. Vol. 50. Iss. 2. P. 347–368. https://doi.org/10.1137/060666457.
27. Sandu A. A new look at the chemical master equation // Numerical Algorithms. 2014. Vol. 65. P. 485–498. https://doi.org/10.1007/s11075-013-9758-z.
28. Schlögl F. Stochastic measures in nonequilibrium thermodynamics // Physics Reports. 1980. Vol. 62. Iss. 4. P. 267–380. https://doi.org/10.1016/0370-1573(80)90019-8. EDN: XSQZOA.
29. Öttinger H.C., Peletier M.A., Montefusco A. A framework of nonequilibrium statistical mechanics. I. Role and types of fluctuations // Journal of Non-Equilibrium Thermodynamics. 2020. Vol. 46. Iss. 1. P. 1–13. https://doi.org/10.1515/jnet-2020-0068. EDN: UJNFDB.
30. Fernandez A., Rabitz H. The scaling of nonequilibrium fluctuations in gaseous thermal explosions // Berichte der Bunsengesellschaft fur physikalische Chemie. 1988. Vol. 92. Iss. 6. P. 754–760. https://doi.org/10.1002/bbpc.198800184.
31. Baer M.R., Gartling D.K., Desjardin P.E. Probabilistic models for reactive behaviour in heterogeneous condensed phase media // Combustion Theory and Modelling. 2012. Vol. 16. Iss. 1. P. 75–106. https://doi.org/10.1080/13647830.2011.606916.
32. Fedotov S.P. Stochastic analysis of the thermal ignition of a distributed explosive system // Physics Letters A. 1993. Vol. 176. Iss. 3-4. P. 220–224. https://doi.org/10.1016/0375-9601(93)91038-7. EDN: ZYVJQJ.

33. Derevich I.V. Effect of temperature fluctuations of fluid on thermal stability of particles with exothermic chemical reaction // International Journal of Heat and Mass Transfer. 2010. Vol. 53. Iss. 25-26. P. 5920–5932. https://doi.org/10.1016/j.ijheatmasstransfer.2010.07.031. EDN: MXGOGN.
34. Derevich I., Galdina D. Simulation of thermal explosion of catalytic granule in fluctuating temperature field // Journal of Applied Mathematics and Physics. 2013. Vol. 1. No. 5. P. 1–7. http://doi.org/10.4236/jamp.2013.15001.
35. Derevich I.V., Fokina A.Y., Ermolaev V.S., Mordkovich V.Z., Solomonik I.G. Heat and mass transfer in Fischer–Tropsch catalytic granule with localized cobalt microparticles // International Journal of Heat and Mass Transfer. 2018. Vol. 121. P. 1335–1349. https://doi.org/10.1016/j.ijheatmasstransfer.2018.01.077. EDN: XXMULJ.
36. Донской И.Г., Гросс Е.И. Численный анализ стохастических закономерностей теплового зажигания в стохастической среде // Информационные и математические технологии в науке и управлении. 2024. № 1. С. 66–77. https://doi.org/10.25729/ESI.2024.33.1.006. EDN: BWDPTW.
37. Деревич И.В., Клочков А.К. Тепловой взрыв одиночных частиц в случайном поле температуры среды // Теплофизика высоких температур. 2023. Т. 61. № 1. С. 108–117. https://doi.org/10.31857/S0040364423010039. EDN: PYOCSJ.
38. Донской И.Г. Стационарное уравнение теплового взрыва в среде с распределенной энергией активации: численное решение и приближения // iPolytech Journal. 2022. Т. 26. № 4. С. 626–639. https://doi.org/10.21285/1814-3520-2022-4-626-639. EDN: BNSPEZ.
39. Kloeden P.E., Platen E. Numerical solution of stochastic differential equations. Berlin: Springer, 1991. Vol. 19. Iss. 11. 636 p. https://doi.org/10.1007/978-3-662-12616-5.

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Author contribution

The author performed a comprehensive analysis, made a generalization on the basis of the results obtained and prepared the manuscript for publication.

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Conflict of interests

The author declares no conflict of interests.

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