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Effect of temperature fluctuations of fluid on thermal stability of particles with exothermic chemical reaction

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ABSTRACT

Effect of temperature fluctuations in liquid phase on heat explosion of individual particles with internal heat release is investigated. Heat emission due to chemical reaction inside particles describes as Arrhenius low. Fluctuations of temperature of carrier phase are modeled as random statistically stationary Gaussian process uniformly distributed in space. Method of functional derivations is used for obtaining closed equation for probability density function of temperature fluctuations of particles. Closed system of moments of particles temperature fluctuations is derived. Reasons leading to loss of thermal stability of particles are studied by numerical and analytical methods. Comparison between various scenarios of heat explosion of particles with temperature fluctuations is carried out. On the base of reverse Kolmogorov equation for probability density function of transition new effect of stochastic drift of particle temperature to the critical value of heat explosion was discovered. Results of numerical integration of the closed equation for probability density function of temperature fluctuations of particles are also presented.

1. Introduction

We study process of heat explosion of individual particle with internal heat emission due to chemical exothermic reaction inside a particle. Temperature of liquid carrier phase surrounding particles fluctuates around averaged stationary value.

Results of this paper have practical value for modeling ignition of dispersed fuels (droplets or particles) in power stations, aviations motors in chemical engineering. Results of this investigation may be used for estimation safety related heat explosion of dispersed materials in coal mines, warehouse for evaluation heat stability of catalytic bed reactors of synthesis.

In classical theory of heat explosion thermal stability of particles is studied as deterministic relation between temperature of surrounding fluid and power of heat generation inside particles due to exothermic chemical reactions [1–3]. Balance between heat transfer from particle surface in liquid phase and power of heat release determines boundaries of thermal stability. Semenov's diagram is familiar instrument for investigation various scenarios of heat explosion. Temperature fluctuations are not entering in classical theory of heat explosion. Stochastic temperature variations significantly alter heat release due to chemical reactions [4]. Main origin of temperature fluctuations in fluid phase is turbulence [5,6] or random variations of parameters in chemical reactions of synthesis [7,8]. Temperatures fluctuations qualitatively change dynamic of heat explosion and disturb boundaries of regions of thermal stability.

Present work is executed in the frame of some restrictions. Fluctuations of concentrations of oxidizers are not including into consideration. Distribution of temperature is uniform in a particle volume. The influence of particles on temperature of carrying fluid is not including into analysis. Temperature fluctuations of fluid phase are modeled as Gaussian statistically stationary process. We investigate model case, where fluctuation of temperature of carrying phase uniformly distributed in space. This approximation allows finishing investigation without modeling assumptions, which are common in the theory of turbulence.

In present paper, closed equation for probability density function (PDF) of temperature fluctuations of particles is derived. Closed system for averaged temperature and dispersion of temperature fluctuations of particles are obtained. Approximation of temperature fluctuation of particles as Gaussian random process is suggested. Numerical and analytical investigations of various scenarios of heat explosion are carried out. Equation for averaged time of first passage of a particle temperature from given temperature interval is derived.

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Nomenclature

A	rate of a chemical reaction (s^{-1})
B	coefficient of 'diffusion' in phase space of temperature (K^2/s)
a_f	coefficient of thermal diffusion in a fluid (m^2/s)
c	thermal capacity (J/(kg K))
d_p	diameter of particles (m)
E	activation energy (J/mol)
f_θ	response function
G	probability density function of transition
J	drift coefficient in phase space of temperature (K/s)
m_p	mass of a particle (kg)
Nu_p	Nusselt number of a particle
Q	thermal effect of a chemical reaction (J/kg)
q_θ	response function
R^0	universal gas constant (J/(mol K))
S_p	area of a particle surface (m^2)
T_θ	integral temporary macroscale (s)
W_Q	growth rate of temperature due to a chemical reaction (K/s)

Greek symbols

α_p	heat transfer coefficient ($W/(m^2 K)$)
β	nondimensional coefficient in the Kolmogorov' reveres equation
Γ_p	nondimensional temperature of particles
γ	nondimensional temperature fluctuations
$\delta(x)$	Dirac delta-function
$\delta\Theta$	temperature variations (K)
Θ	temperature (K)
θ	fluctuations of temperature (K)
χ	nondimensional coefficient in the Kolmogorov' reveres equation
λ	increment of temperature growth (s^{-1})
Ξ	passage time of particles temperature (s)
ξ	nondimensional time
ρ	density (kg/m^3)
σ_θ^2	intensity of temperature fluctuations (K^2)
σ_γ^2	nondimensional intensity of temperature fluctuations
τ_θ	thermal relaxation time of a particle (s)
Φ	probability density function
φ	indicator function
Ω_θ	parameter of thermal inertia of particles

Subscripts/superscripts

cr	critical value
f	fluid phase
p	particles
$\circ$	initial value
$*$	nondimensional variables
$\langle\,\rangle$	averaging over of an ensemble of random realizations

New effect of stochastic drift of particles random temperature to the critical value of heat explosion is illustrates.

2. Equation for PDF

Equation for nonstationary temperature $\Theta_p(t)$ of spherical particle with regards of heat exchange through fluid phase, which temperature is $\Theta_f(t)$, and heat release due to chemical reaction modeling by Arrhenius low has the following form

$$m_p c_p \frac{d\Theta_p(t)}{dt} = \alpha_p S_p[\Theta_f(t) - \Theta_p(t)] + Qm_pA\exp\left(-\frac{E}{R^0\Theta_p(t)}\right), \quad (1)$$

where m_p is mass of a particle, c_p is thermal capacity of material of a particle, Q is thermal effect of chemical reaction, A is rate constant of the chemical reaction, E is activation energy, R^0 is universal gas constant, S_p is area of a particle surface, α_p is heat transfer coefficient.

Particles thermal relaxation time τ_θ, which represent effect of particles thermal inertia is follows from Eq. (1)

$$\tau_\theta = \frac{1}{6}\frac{\rho_p c_p}{\rho_f c_f}\frac{d_p^2}{Nu_p a_f}, \quad (2)$$

where d_p is a particle diameter, ρ_p is density of material of a particle, ρ_f, c_f are density and heat capacity of fluid phase, a_f is coefficient of thermal diffusion in fluid phase, Nu_p is Nusselt number of a particle.

With regards of Eqs. (1) and (2) equation for actual particle temperature is written as

$$\frac{d\Theta_p(t)}{dt} = \frac{1}{\tau_\theta}[\Theta_f(t) - \Theta_p(t)] + \frac{QA}{c_p}\exp\left(-\frac{E}{R^0\Theta_p(t)}\right). \quad (3)$$

As a result of averaging over an ensemble of realizations of random temperature of fluid phase averaged and fluctuating part of temperature are separated

$$\Theta_f(t) = \langle\Theta_f(t)\rangle + \theta_f(t), \quad \langle\theta_f(t)\rangle = 0. \quad (4)$$

Here angle brackets denote results of ensemble avenging. Using Dirac delta-function $\delta(x)$ we define an indicator function [9], which cuts out in phase space of temperature a random particle 'trajectory'

$$\varphi(\Theta_p, t) = \delta(\Theta_p - \Theta_p(t)). \quad (5)$$

Here Θ_p is temperature consider as coordinate in phase space of temperature, $\Theta_p(t)$ is actual temperature of a particle.

From formulas (3)–(5) one can see that indicator function (5) is functional from random process of temperature fluctuation of carried phase. Averaging of indicator function (5) over an ensemble of random realization of fluid temperature leads to PDF of particles temperature

$$\Phi(\Theta_p, t) = \langle\delta(\Theta_p - \Theta_p(t))\rangle = \langle\varphi(\Theta_p, t)\rangle. \quad (6)$$

PDF (6) has normalization on one particle

$$\int_0^\infty \Phi(\Theta_p, t)d\Theta_p = \int_0^\infty \langle\delta(\Theta_p - \Theta_p(t))\rangle d\Theta_p = 1.$$

With the help of PDF averaged temperature of particles is calculated as

$$\langle\Theta_p(t)\rangle = \int_0^\infty \Theta_p\Phi(\Theta_p, t)d\Theta_p = \int_0^\infty \Theta_p\langle\delta(\Theta_p - \Theta_p(t))\rangle d\Theta_p. \quad (7)$$

We define fluctuation of particles temperature with the help of averaging temperature (7)

$$\theta_p = \Theta_p - \langle\Theta_p(t)\rangle. \quad (8)$$

Proving zero value of averaged fluctuations of temperature (8) is carried out as

$$\langle\theta_p\rangle = \int_0^\infty \theta_p\Phi(\Theta_p)d\Theta_p = \int_0^\infty [\Theta_p - \langle\Theta_p(t)\rangle]\Phi(\Theta_p)d\Theta_p = 0.$$