Thermal explosion theory of moving heterogeneous media

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Abstract

The mathematical models for description of the flow of a gas and reactive solid particles taking into account the lag in the phase velocities and temperatures are proposed. A catastrophe/ignition manifold for a pointwise model of single magnesium particle ignition that takes into account the chemical oxidation reaction, metal evaporation, and convective heat exchange with the ambient gas has been analyzed qualitatively and quantitatively. It is shown that this model can describe experimental data on ignition delay and stability of a given parameter to a set of kinetic constants. A theory of thermal explosion of moving continua of magnesium particles has been developed. This theory is adequate to experimental data and extends the classical Semenov theory to the case of a moving two-phase medium. Namely, analytical conditions that separate the domain of explosive action of a SW into a cloud of particles and a region of regular (explosionless) heating of the cloud are presented. A steady structure of the flow is constructed as an ignition wave that steadily propagates over the mixture.

1. General model of the motion of a composite mixture taking into account the ignition of metal particles.

A mathematical model of the motion of a mixture of gas and metal particles with a chemical reaction of particles oxidation is proposed. It is closed by equations of state and by determining the source terms of production of each phase via the growth rate of the oxide film on the particles by the functions of the parameters of state. Two approximations of this model (pointwise and distributed) are considered.

2. The study of the thermal explosion of a magnesium particle taking into account metal evaporation.

Within the framework of the pointwise approximation of the proposed mathematical model, the effect of metal evaporation on the process of particle ignition under the action of a high-temperature ambient gas is studied. To analyze qualitatively the solution of the corresponding Cauchy problem, we investigate in the domain of determining parameters the zero isocline of the equation for particle temperature T_2 using methods of elementary catastrophe theory. Similarly to [1, 2], a catastrophe manifold is constructed, i.e., the steady-state temperature T_2 as a function of the bifurcation parameter α which is determined as the ratio of the characteristic time of convective heat transfer to the characteristic time of the oxidation reaction. The catastrophe manifold is constructed in cross-sections c=const where c is the ratio of characteristic times of evaporation and oxidation processes. Ignition delays predicted by the model after its verification according to [3] and similar data of the model [1] which ignores evaporation are compared. For small particles (particle radius 30-60 μm) the differences in induction period are insignificant. For large particles (300-600 μm) they do not exceed 11%.

3. Thermal explosion theory in a moving heterogeneous medium.

The problems of physical and mathematical theory of the thermal explosion of heterogeneous media have been numerically studied by the authors in [4 – 6]. It seems of interest to present analytical conditions of thermal explosion in a moving heterogeneous medium within the framework of the new proposed model and to classify the types of heating of particle clouds due to the action of shock waves on the basis of these conditions.

Formulation of the problem.

We consider an adiabatic one-dimensional channel filled by a mixture of gas and small magnesium particles. In the one-velocity approximation, the equations that describe a steady motion of the mixture behind the shock wave (SW) have the following form:

$$\frac{dT_2}{d\zeta} = B\left\{ (T_m - T_2)\, exp\left(-\frac{E_a}{T_2} \right) - \alpha\,(T_2 - T_1) \right\},.$$

$$\rho\, U = C_1, \quad C_1 U + P = C_2, \quad e + \frac{U^2}{2} + \frac{P}{\rho} = C_3, \tag{1}$$

where $B,...,C_3$ are some dimensionless constants. As the initial data for the mixture, we use the conditions behind the frozen shock wave front and the stationary conditions at $+\infty$

$$\overset{\rho}{\Phi} = (\rho, U, P, T_1, T_2) = (\tilde{\rho}, \tilde{U}, \tilde{P}, \tilde{T}_1, \tilde{T}_2) \quad \text{for } \zeta = 0\,, \quad d\overset{\rho}{\Phi} / d\zeta \to 0 \quad \text{for } \zeta \to \infty\,. \tag{2}$$

Classification of stationary regimes in the mixture flow.

In accordance with [7], the equilibrium states of equations (1) have been studied. Like in the classical theory of thermal explosion proposed by N.N.Semenov, it is shown that the dependence of the particle temperature T_{2k} in the equilibrium state of the mixture on the heat transfer parameter α is a one-valued curve for $\alpha < \alpha_-$ or $\alpha > \alpha_+$ and a three-valued curve for $\alpha_- < \alpha < \alpha_+$ where $\alpha_\pm$ is the known function of the initial parameters of the mixture. For $\tilde{T}_2 = T_0 < T_e$ (where T_0 is the initial temperature of the mixture and T_e is the temperature of phase equilibrium) the following is valid.

- **Statement.** (a) if $0 < \alpha < \alpha_-$, then $T_{2k} \in (T_{2+}, T_m)$; (b) if $\alpha > \alpha_-$, then $T_{2k} \in (T_e, T_{2-})$; here $T_{2\mu} = T_{2k}(\alpha_\mu)$.

In accordance to [7], case (a) corresponds to the flow regime of the mixture behind the SW with particle ignition and case (b) to the flow regime without ignition, with regular heating of particles. The structure of the ignition wave (a) is determined by energy output from the gas phase, heating of particles and their ignition. The temperature T_1 and velocity U monotonically decrease, and the particle temperature T_2 monotonically increases to its final value T_{2k}.

We determine the kinetic constants in the oxide film growth law $(T_m, E_a, ...)$ by means of processing the experimental data of [8] on ignition of a mixture of gas and magnesium particles. A series of calculations allowed us to verify the mathematical model (Fig. 1).

Nonstationary approach of the ignition problem.

Based on numerical simulation of the Cauchy problem for an unsteady model with an stationary ignition wave as initial data, a stable propagation of this steady structure over the mixture was established (Fig. 2). The case of ignition wave initiation also was studied. The computing results are presented in the Fig.3.

Conclusion

Based on a new mathematical model of heterogeneous reactive medium, a theory of thermal explosion of moving continua of magnesium particles has been developed. This theory is adequate to some known experimental data concerning ignition delay time and extends the classical Semenov theory to the case of a moving two-phase medium. Namely, analytical conditions that separate the domain of explosive action of a SW into a cloud of particles and a region of regular (explosionless) heating of the cloud are presented. A steady structure of the flow is constructed as an ignition wave that steadily propagates over the mixture.

A catastrophe/ignition manifold for a pointwise model of single magnesium particle ignition that takes into account the chemical oxidation reaction, metal evaporation, and convective heat exchange with the ambient gas has been analyzed qualitatively and quantitatively. It is shown that this model can describe experimental data on ignition delay and stability of a given parameter to a set of kinetic constants.

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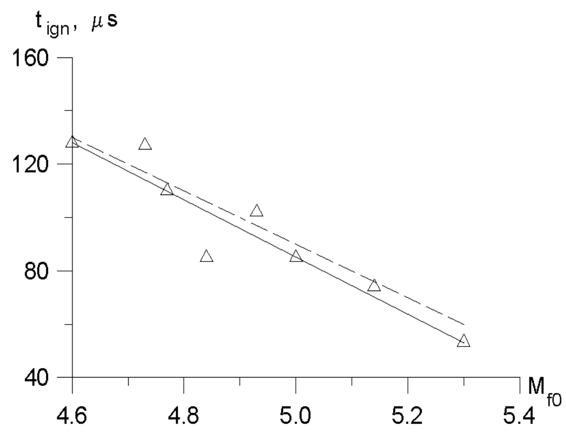

Fig.1 Ignition delay time in a mixture of magnesium particles in oxygen versus the shock wave Mach number: solid lines – our calculation, dashed line – calculation [9], ó – experiment [8].

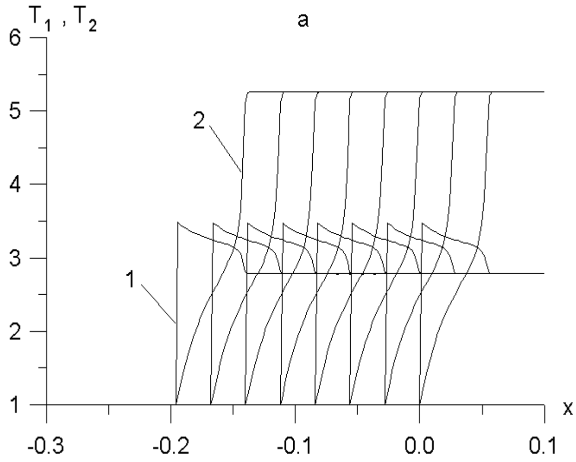

Fig. 2 Propagation of an ignition wave over the mixture. Phase temperatures: 1 – gas, 2 – particles.

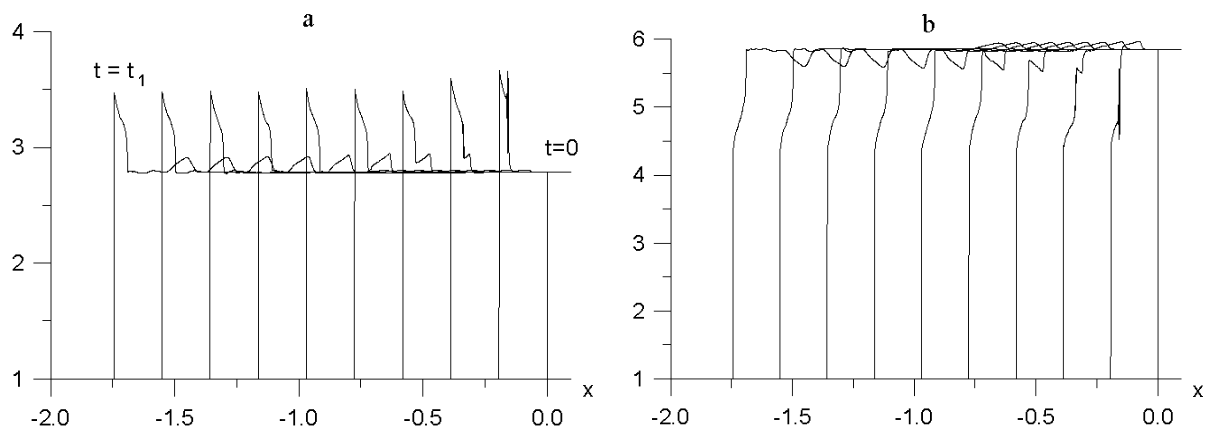

Fig. 3 Initiation of ignition wave: a – temperature of gas phase, b – density of mixture.

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