Features of mathematical model for ignition process of a metallized condensed substance by a local energy source

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Abstract. Comparison of analysis results for regularities of a metallized condensed substance ignition by a single small-sized particle heated to high temperatures and a hot massive plate was carried out. Ignition delay time was defined for metallized condensed substance. Influence of local energy source heat content on integrated characteristics of process was established. It was shown that use of heat transfer mathematical model with perfect thermal contact conditions on surface of a condensed substance is impossible in case of its ignition by a local energy source with limited heat content.

Keywords: metallized condensed substance, particle, plate, heat transfer, ignition, mathematical modeling.

1. Introduction
Numerical and experimental research results of homogeneous solid [1–3] and liquid [4–6] condensed substances ignition at it interaction with single small-sized hot particle and besides massive energy source allowed to establish essential differences of the main integrated characteristic of studied process – ignition delay time for gunpowder, wood, polymethyl methacrylate, gasoline, kerosene, diesel fuel, etc. It is published [7,8] not so much theoretical research results of metallized condensed substance ignition conditions within the models considering structural heterogeneity of substance caused by aluminum particles. Mathematical models [7,8] rather difficult. It is expedient the assessment of it simplification possibility within approaches [9,10] for decrease calculation volume at the numerical researches of ignition processes.

The purpose of the present work is the numerical analysis of macroscopic regularities for metallized condensed substance ignition by local and massive energy sources.

2. Problem Statement
Heat transfer process at solid-phase ignition in a system “local energy source – metallized condensed substance – air” was considered (Figure 1). It was supposed that small-sized energy source (particle warmed to high temperature) in parallelepiped shape is besieged inertial on a surface of the metallized condensed substance [11] with known thermophysical and thermochemical characteristics. Warming of condensed substance near-surface layer happened due to heat accumulated in a hot particle. During the induction period the part of energy of a hot particle was taken away continuously from lateral sides in air. Such heat transfer considered at two-dimensional statement can have essential impact on integrated characteristics of condensed substance ignition by a small-sized hot particle in comparison...
with opportunity of a massive energy source when temperature on a condensed substance heated surface is maintained by a constant during the induction period.

Near the bottom side of an energy source \((y=y_2)\) the rate of exothermic reaction increases and ignition happens as a result of metallized condensed substance near-surface layer warming.

Figure 1. A scheme of the solution domain:

1 – air, 2 – hot particle, 3 – condensed substance, 4 – aluminum particle

At the condensed substance heterogeneous structure modeling (Figure 1) the sites corresponding to composite propellant (butyl rubber and ammonium perchlorate) and the sites corresponding to metal particles (aluminum) were allocated.

A single small-sized \((l_p=x_k=2.5\cdot10^{-3}\text{ m}, h_p=y_3-y_2=2.5\cdot10^{-3}\text{ m})\) heated to high temperatures particle in the parallelepiped shape was considered as an ignition source. In condensed substance and air the areas \((l=10\cdot10^{-3}\text{ m}, h=10\cdot10^{-3}\text{ m})\) were allocated that significantly exceeds a size of a local energy source. Sizes of aluminum particles was \(l_g=x_2-x_1=0.1\cdot10^{-3}\text{ m}, h_g=y_2-y_1=0.1\cdot10^{-3}\text{ m}\).

Ignition conditions were accepted [9]:

1. The energy emitted as a result of exothermic reaction in a near-surface layer of a condensed substance is more than the heat quantity released from energy source to ignition zone.
2. Substance temperature in exothermic reaction zone above the initial temperature of a hot particle.

3. Mathematical Model and Solution Methods

Heat transfer processes in a system “local energy source – metallized condensed substance – air” were described by the system of nonlinear non-stationary differential equations in private derivatives.

Thermal conduction equation for air:

\[
x_k < x < l, \quad y_2 < y < y_3; \quad 0 < x < l, \quad y_3 < y < h, \quad \rho C \frac{\partial T_1}{\partial t} = \lambda \left( \frac{\partial^2 T_1}{\partial x^2} + \frac{\partial^2 T_1}{\partial y^2} \right).
\] (1)

Thermal conduction equation for hot steel particle:
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\[ 0 < x < x_k, \ y_2 < y < y_3, \ \rho_2 C_2 \frac{\partial T_2}{\partial t} = \lambda_2 \left( \frac{\partial^2 T_2}{\partial x^2} + \frac{\partial^2 T_2}{\partial y^2} \right). \]  

(2)

Thermal conduction equation for composite propellant:

\[ 0 < x < l, \ 0 < y < y_1; \ 0 < x < x_1, \ x_2 < x < x_3, \ldots, \ x_n < x < l, \ y_1 < y < y_2, \]

\[ \rho_3 C_3 \frac{\partial T_3}{\partial t} = \lambda_3 \left( \frac{\partial^2 T_3}{\partial x^2} + \frac{\partial^2 T_3}{\partial y^2} \right) + Q^2 W_3, \]

(3)

where \( W_3 = \rho_3 k_3^0 \exp \left( -\frac{E_3}{RT_3} \right) \) is mass rate of exothermic reaction \([10]\).

Thermal conduction equation for aluminum particle:

\[ x_1 < x < x_2, \ldots, \ x_{n-1} < x < x_n, \ y_1 < y < y_2, \ \rho_4 C_4 \frac{\partial T_4}{\partial t} = \lambda_4 \left( \frac{\partial^2 T_4}{\partial x^2} + \frac{\partial^2 T_4}{\partial y^2} \right). \]

(4)

The nomenclature was accepted: \( \rho_i \) is density, \( \text{kg/m}^3 \); \( \lambda_i \) is thermal conductivity, \( \text{W/(m·K)} \); \( C_i \) is specific heat, \( \text{J/(kg·K)} \); \( T \) is temperature, \( \text{K} \); \( k_3^0 \) is preexponential factor, \( \text{s}^{-1} \); \( E_3 \) is activation energy of exothermic reaction, \( \text{J/mole} \); \( Q_i \) is thermal effect of exothermic reaction, \( \text{J/kg} \); \( R \) is absolute gas constant, \( \text{J/(mole·K)} \); subscripts 1, 2, 3, 4 correspond to air, hot steel particle, composite propellant, aluminum particles.

The initial conditions at \( t=0 \):

\( T_1=T_2=T_3=T_0, \ 0<x<l, \ 0<y<y_2; \ x_i<x<l, \ y_2<y<y_3; \ 0<x<l, \ y_3<y<h. \)

\( T_2=T_4, \ 0<x<x_i, \ y_2<y<y_3. \)

The boundary conditions at \( 0<y<t_f: \)

1. Conditions of equal to zero gradients of corresponding functions were accepted for all equations on symmetry axis and external borders:

\[ \frac{\partial T_i}{\partial x} = 0, \ \text{at} \ i=1, 2, 3, \ x=h, 0<y<h; \]

\[ \frac{\partial T_i}{\partial y} = 0, \ \text{at} \ i=1, 3, \ y=0, 0<x<l; \ y=h, 0<x<l. \]

2. Perfect thermal contact conditions were accepted for all equations on borders between system components (Figure 1):

\( x=x_i, x=x_3, \ldots, x=x_{n-1}, y_1<y<y_2; \ T_3=T_4, \ -\lambda_3 \frac{\partial T_3}{\partial x} = -\lambda_4 \frac{\partial T_4}{\partial x}; \)

\( x=x_2, x=x_4, \ldots, x=x_n, y_1<y<y_2; \ T_4=T_3, \ -\lambda_4 \frac{\partial T_4}{\partial x} = -\lambda_3 \frac{\partial T_3}{\partial x}; \)

\( x=x_k, y_2<y<y_3, T_2=T_1; \ -\lambda_2 \frac{\partial T_2}{\partial x} = -\lambda_1 \frac{\partial T_1}{\partial x} - q_i; \)

\( y=y_1, x_1<x<x_2, x_3<x<x_4, \ldots, x_{n-1}<x<x_n; \ T_3=T_4, \ -\lambda_3 \frac{\partial T_3}{\partial y} = -\lambda_4 \frac{\partial T_4}{\partial y}; \)

\( y=y_2, 0<x<x_1, x_2<x<x_3, \ldots, x_{k-1}<x<x_k; \ T_3=T_2, \ -\lambda_3 \frac{\partial T_3}{\partial y} = -\lambda_2 \frac{\partial T_2}{\partial y}; \)

\( y=y_3, x_1<x<x_2, x_3<x<x_4, \ldots, x_{k-2}<x<x_k; \ T_4=T_2, \ -\lambda_4 \frac{\partial T_4}{\partial y} = -\lambda_2 \frac{\partial T_2}{\partial y}; \)

\( y=y_2, x_{k-1}<x<x_k, \ldots, x_n<x<l; \ T_3=T_1, \ -\lambda_3 \frac{\partial T_3}{\partial y} = -\lambda_1 \frac{\partial T_1}{\partial y}; \)

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\[ y = y_2, x_k < x < x_{k+1}, \ldots, x_{n-1} < x < x_n; T_d = T_1, -\lambda_4 \frac{\partial T_4}{\partial y} = -\lambda_1 \frac{\partial T_1}{\partial y}; \]

\[ y = y_3, 0 < x < x_k, T_e = T_1; -\lambda_2 \frac{\partial T_2}{\partial y} = -\lambda_1 \frac{\partial T_1}{\partial y} - q_r. \]

Thermal flow from a local energy source according to radiant heat exchange was calculated on a formula: \( q_r = \sigma \varepsilon T^4 \),

where \( \sigma \) is Stefan–Boltzmann constant, \( W/(m^2 \cdot K^4) \); \( \varepsilon \) is blackness degree of a particle.

Mathematical problem statement is similar given above at the heating of metallized condensed substance by hot steel plate. However perfect thermal contact conditions were accepted for thermal conduction equations on border “hot steel plate – metallized condensed substance” in case of a massive energy source.

The system of differential equations (1) – (4) with corresponding initial and boundary conditions was solved by the method of finite differences. The local one-dimensional method was applied to solve different analogues of differential equations. The sweep method using the implicit four-dot difference scheme was applied to solve one-dimensional equations in difference form.

4. Results and Discussion

Numerical investigations were carried out at the following values of process parameters [11]: initial temperature of air and metallized condensed substance \( T_0 = 300 \) K; initial temperature of energy source \( T_p = 800 \text{–} 1700 \) K. Blackness degree of a particle \( \varepsilon = 0.6 \); Stefan–Boltzmann constant \( \sigma = 5.67 \cdot 10^{-8} \) \( W/(m^2 \cdot K^4) \); universal gas constant \( R = 8.31 \) J/(mole·K). Kinetic parameters of ignition process \( E_3 = 50 \cdot 10^3 \) J/mole, \( Q_{hk3} = 1.9 \cdot 10^9 \) J/(kg·s).

Thermophysical characteristics of components (Figure 1):

- \( \lambda_1 = 0.026 \) W/(m·K); \( \rho_1 = 1.161 \) kg/m³; \( C_1 = 1190 \) J/(kg·K);
- \( \lambda_2 = 36 \) W/(m·K); \( \rho_2 = 8100 \) kg/m³; \( C_2 = 545 \) J/(kg·K);
- \( \lambda_3 = 0.472 \) W/(m·K); \( \rho_3 = 1776 \) kg/m³; \( C_3 = 1500 \) J/(kg·K);
- \( \lambda_4 = 343 \) W/(m·K); \( \rho_4 = 2700 \) kg/m³; \( C_4 = 930 \) J/(kg·K).

At the numerical research the dependence of metallized condensed substance ignition delay time on initial temperature of local energy source \( - t_{d1} \) and massive hot plate \( - t_{d2} \) was established (Table 1). The results obtained at use of mathematical model for a condensed substance ignition by an energy source with limited heat content (Figure 1) exceed more than for 100% the results calculated at use of mathematical model with perfect thermal contact conditions on a heated surface in all range of initial source temperature changing. At comparing \( t_{d1} \) with experimental values of ignition delay time \( t_{d3} \) [11] was established good correlation of research results. Obtained regularities are caused by specifics of studied process. Change of hot particle temperature happens during the induction period at local heating of metallized condensed substance. This result can be explained follows. At the heat transfer on horizontal coordinate quantity of energy of hot particle expenditure for air warming increases. Another part of energy is spent for warming near-surface layer of a metallized condensed substance. In case of a massive energy source such heat transfer on horizontal coordinate is absent and all accumulated energy is spent for warming of condensed substance.

| Table 1. The dependence of metallized condensed substance ignition delay time on initial temperature of energy source at \( l_p = h_p = 2 \) mm |
|---|---|---|---|---|---|---|---|---|---|---|
| \( T_p, \) K | 1700 | 1600 | 1500 | 1400 | 1300 | 1200 | 1100 | 1000 | 900 | 800 |
| \( t_{d1}, \) s | 0.057 | 0.069 | 0.088 | 0.118 | 0.171 | 0.266 | 0.446 | 0.789 | 1.609 | no ignition |
| \( t_{d2}, \) s | 0.019 | 0.021 | 0.023 | 0.025 | 0.028 | 0.034 | 0.047 | 0.082 | 0.179 | 0.486 |
| \( t_{d3}, \) s | 0.064 | 0.091 | 0.132 | 0.198 | 0.305 | 0.487 | 0.809 | 1.413 | 2.614 | no ignition |

\( t_{d1} \) is metallized condensed substance ignition delay time at it interaction with hot particle (numerical research);
\(t_{d2}\) is metallized condensed substance ignition delay time at it interaction with hot plate (numerical research);

\(t_{d3}\) is metallized condensed substance ignition delay time at it interaction with hot particle (experimental research [11]).

The established specifics of studied process are illustrated a temperature field (Figure 2) in solution area at the ignition moment. Figure 2 shows that temperature change of a local energy source during the induction period makes more than 150 K (at \(T_p=1300\) K). Also considerable change of air temperature near the hot particle was observed. It testifies to the additional heat sink in environment.

![Figure 2. Temperature field in a system “local energy source – metallized condensed substance – air” at ignition moment \((t_d=0.171\) s) at \(T_p=1300\) K](image)

At the engineering calculations, as a rule, the great interest is represented to the limit conditions of ignition process in system (Figure 1). It was established that \(T=900\) K is minimum initial temperature of a local energy source with sizes \(l_p=h_p=2\) mm when ignition is realized.

5. Conclusion
As a result of numerical researches restrictions on application of mathematical model with perfect thermal contact conditions on a heated surface for analysis of ignition characteristics of a metallized condensed substance by energy source with limited heat content were set. Also minimum value of initial hot particle temperature \(T_p=900\) K was defined at which in system “local energy source – metallized condensed substance – air” ignition happens.

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