Spark ignition of a mixture of aluminum and boron powders

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Abstract. The paper presents the results of the numerical solutions of the problem of spark ignition aero suspension mixture of powders of aluminum and boron. The physical and mathematical model of gas suspension combustion is based on the approaches of the mechanics of two-phase reacting media. The solution to the problem is based on the decay algorithm of an arbitrary discontinuity S. K. Godunov. From the solution of the problem, the dependence of the minimum energy of spark ignition on the radius, mass concentration and the fraction of aluminum and boron particles in the gas suspension were determined.

1. Introduction
An interest in studying the laws of combustion of boron particles in powder metal fuels, aerosuspensions and mixed solid fuels is dictated by the high calorific value of boron powder. The behavior of boron powder in the composition of gas mixtures is ambiguous, the addition of boron, depending on the conditions, can lead to both an increase and a decrease in the specific enthalpy of fuel combustion [1]. In [2], the study of flame propagation modes in a gas-suspension mixture of boron and aluminum powders was performed. It is shown that for the considered parameter range boron additive particles results in a slowing of flame propagation. With regard to critical conditions spark ignition gas suspension mixture of powders of aluminum and boron, the situation may be different. Boron particles begin to oxidize faster. In this case, energy is released that goes to warm the gas suspension.

In [3], the influence of the composition of a gas suspension of aluminum powder on the critical conditions for spark ignition of bi-dispersed suspension of aluminum particles in air was shown. It is shown that when the mass concentration of aluminum powder increases in the direction of stoichiometric composition, the dependence of the minimum spark ignition energy on the mass concentration of the powder decreases. In this case, the dependence of the minimum spark ignition energy on the particle size and particle size distribution is reduced. In the presence of a fine particle fraction, the minimum spark ignition energy of a bi-disperse air suspension of aluminum powder is significantly reduced compared to the minimum spark ignition energy of a monodisperse air suspension with large particles.

In [4], a physical and mathematical model of the combustion of a gas suspension of a mixture of aluminum and boron powders was presented. The presented physical and mathematical model showed a significant dependence of the behavior of the burning rate on the ignition temperature of aluminum particles.

In this work, we used the model of combustion of boron particles [5] and the assumptions of the physical and mathematical model [4]. The aim of this work was to determine the effect of the
composition of a gas suspension of a mixture of aluminum and boron powders on the critical conditions for spark ignition of a gas suspension.

2. Mathematical model
The physical and mathematical formulation of the problem was based on the assumptions of operation [4] and approaches to the mechanics of two-phase reacting media [6]. It is assumed that a suspension of boron powder with a mass concentration of particles $m_B$ and a suspension of aluminum powder with a mass concentration of particles $m_{Al}$ are evenly distributed in air. Total weight of the powder mixture is determined as $m_{dust} = m_B + m_{Al}$. Chemical, thermal, and inertial interactions between particles were neglected. The initial temperature of aluminum and boron particles is equal to the gas temperature under normal conditions, $T_{gb}$. The filamentous instantaneous ignition source is located in the center. The external boundary of the computational domain is assumed to be infinitely remote from the ignition source. Heat loss to the electrodes is neglected. Inertial interaction between the particles and the gas described analogously to [3]. Details of the physical and mathematical model of boron particle oxidation and combustion are presented in [4]. Details of the physical and mathematical model of combustion of aluminum particles are given in [3].

The equations describing the physical and mathematical formulation of the problem based on the [4] and recorded in a cylindrical coordinate system:

the gas continuity equation:

$$\frac{\partial \rho_g}{\partial t} + \frac{\partial \rho_g u_g}{\partial r} = r [G_1 + G_2 - \alpha_1 G_3 + G_4 - G_5], \quad (1)$$

the momentum conservation equation for the gas:

$$\frac{\partial \rho_g u_g}{\partial t} + \frac{\partial \rho_g u_g^2 + p}{\partial r} = p - r \tau_v + ru_{i,j} \left( G_1 + G_2 - \alpha_3 G_3 + G_4 \right) - rG_5 u_g, \quad (2)$$

the gas energy equation:

$$\frac{\partial \rho_g (e_g + 0.5u_g^2)}{\partial t} + \frac{\partial \rho_g u_g (e_g + 0.5u_g^2) + pu_g}{\partial r} = r \left( G_1 + G_2 - \alpha_3 G_3 + G_4 \right) \left( c_{s1} T_{s1} + \frac{u_{s1}^2}{2} \right) +$$

$$+ \frac{\partial}{\partial r} \left( \rho_g \left( \frac{T_g}{\rho} \frac{\partial T_g}{\partial r} \right) + r \sum_{i=1}^{i=2} \left[ a_{i,j} n_{k,i} S_{k,i} (T_{k,i} - T_g) - u_{k,i} \tau_{v,i,j} \right] +$$

$$+ r (Q - Q_1) G_1 + (Q - Q_2) G_2 - G_1 (c_{s1} T_{s1} + 0.5u_{s1}^2), \quad (3)$$

the oxygen mass balance equation:

$$\frac{\partial \rho_g O_2}{\partial t} + \frac{\partial \rho_{g2O3} u_g}{\partial r} = \frac{\partial}{\partial r} \left( r D_g (T_g) \rho_g \frac{\partial a_{g2O3}}{\partial r} \right) - r \left[ \alpha_3 G_1 + \alpha_3 G_2 + \alpha_3 G_3 \right] - rG_5, \quad (4)$$

the mass balance equation for the gaseous reaction products $B_2O_3(g)$:

$$\frac{\partial \rho_{g2O3}}{\partial t} + \frac{\partial \rho_{g2O3} u_g}{\partial r} = \frac{\partial}{\partial r} \left( r D_g (T_g) \rho_g \frac{\partial a_{g2O3}}{\partial r} \right) + (1 + \alpha_1) r \left( G_1 + G_2 \right) + rG_4, \quad (5)$$

the particle mass balance equation:

$$\frac{\partial \rho_{k,i}}{\partial t} + \frac{\partial \rho_{k,i} u_{k,i}}{\partial r} = -r \left( G_1 + G_2 - \alpha_3 G_3 + G_4 \right), \quad \frac{\partial \rho_{k,i}}{\partial t} + \frac{\partial \rho_{k,i} u_{k,i}}{\partial r} = rG_5, \quad (6)$$

the mass balance equation for solid boron oxide:
\[
\frac{\partial r \rho_{203}^k}{\partial t} + \frac{\partial r \rho_{203}^k u_{k,1}}{\partial r} = r\left((1 + \alpha_1)G_1 - G_4\right),
\]

(7)

the particle momentum conservation equations:

\[
\frac{\partial r (\rho_{k,1}u_{k,1})}{\partial t} + \frac{\partial r \rho_{k,1}u_{k,1}^2}{\partial r} = r \tau_p - r\left(G_1 + G_2 - \alpha_2G_5 + G_4\right)u_{k,1}, \quad \frac{\partial r (\rho_{k,2}u_{k,2})}{\partial t} + \frac{\partial r \rho_{k,2}u_{k,2}^2}{\partial r} = r \tau_p + rG_3u_{k,2},
\]

(8)

the particle energy equations:

\[
\frac{\partial r \rho_{k,1}\left(e_{k,1} + 0.5u_{k,1}^2\right)}{\partial t} + \frac{\partial r \rho_{k,1}u_{k,1}\left(e_{k,1} + 0.5u_{k,1}^2\right)}{\partial r} = r\left(QG_1 + QG_2 + QG_3 - Q_4G_4\right) - r\left(G_1 + G_2 - \alpha_2G_5 + G_4\right)\left(c_{k,1}T_{k,1} + 0.5u_{k,1}^2\right) + r\left[\tau_p u_{k,1} - \alpha_2S_{k,1}n_{k,1}\left(T_{k,1} - T_g\right)\right] -
\]

\[
\frac{\partial r \rho_{k,2}\left(e_{k,2} + 0.5u_{k,2}^2\right)}{\partial t} + \frac{\partial r \rho_{k,2}u_{k,2}\left(e_{k,2} + 0.5u_{k,2}^2\right)}{\partial r} = -r\alpha_{k,2}S_{k,2}n_{k,2}\left(T_{k,2} - T_g\right) + r\tau_p u_{k,2},
\]

(9)

the particle concentration equation:

\[
\frac{\partial r n_{k,i}}{\partial t} + \frac{\partial r n_{k,i}u_{k,i}}{\partial r} = 0, \quad i = 1, 2,
\]

(10)

the gas equation:

\[
p = \rho_g^r R T_g^r,
\]

(11)

the initial conditions:

\[
T_g(r,t) = T_0 + \frac{Q}{4\lambda_d T_0}\exp\left(-\frac{r^2}{4\lambda_d T_0}\right), \quad T_{k,i}(r,t_z) = T_0, \quad \rho_{k,1}(r,t_z) = m_g, \quad \rho_{k,2}(r,t_z) = m_{d_1},
\]

(12)

\[
u_g(r,t_z) = u_{k,i}(r,t_z) = 0, \quad \rho_{0,2}^r, \quad \rho_g^r(r,t_z) = \rho_g^r, \quad n_{k,i}(r,t_z) = n_{k,i}, \quad \rho_{203}^{k,1} = \rho_{203}^k = 0;
\]

the boundary conditions:

\[
\frac{\partial r \rho_{203}^k(0,t)}{\partial r} = \frac{\partial r \rho_{203}^k(\pi,t)}{\partial r} = \frac{\partial r \rho_{0,2}^r(0,t)}{\partial r} = \frac{\partial r \rho_{0,2}^r(\pi,t)}{\partial r} = 0,
\]

(13)

\[
\frac{\partial r \rho_{k,1}(0,t)}{\partial r} = \frac{\partial r \rho_{k,1}(\pi,t)}{\partial r} = \frac{\partial r T_{k,1}(0,t)}{\partial r} = \frac{\partial r T_{k,1}(\pi,t)}{\partial r} = 0, \quad u_{k,i}(0,t) = u_g(0,t) = 0,
\]

The notations in (1)–(13) are usual and correspond to the studies [3,4]. The parameters of boron particles are marked by index 1, aluminum by index 2.

The rates of the boron particle mass change during the heterogeneous reactions on the particle surface (during the second stage) are defined as:

\[
G_1 = \frac{k_{0,1} \exp\left(-E_1/RT_{k,1}\right)\beta_{k,1}}{k_{0,1} \exp\left(-E_1/RT_{k,1}\right) + \beta_{k,1} n_{k,1}\rho_{0,2}S_{k,1}}, \quad G_2 = \frac{k_{0,2} \exp\left(-E_2/RT_{k,1}\right)\beta_{k,1}}{k_{0,2} \exp\left(-E_2/RT_{k,1}\right) + \beta_{k,1} n_{k,1}\rho_{0,2}S_{k,1}}.
\]
The mass change rate of the boron particles due to the oxidation reaction with the condensed oxide $\text{B}_2\text{O}_3$ formation:

$$G_3 = \beta_{k,\text{eff}} n_{k,i} \rho_{\text{O}_2} S_{k,i},$$

where $\beta_{k,\text{eff}}$ is the effective mass transfer coefficient taking into account the diffusion through the spherical oxide layer.

The mass change rate of the boron particles due to the evaporation of a melted oxide $\text{B}_2\text{O}_3$:

$$G_4 = n_{k,i} \beta_{k,1} \left( \rho_{\text{B}_2\text{O}_3}^u - \rho_{\text{B}_2\text{O}_3}^g \right),$$

where $\rho_{\text{B}_2\text{O}_3}^u$ is the density of saturated vapors around a particle.

The mass change rate of the aluminum particles according to [3] is:

$$G_5 = \alpha_{a,\text{eff}} n_{k,2} \rho_{a,2} S_{a,l} \frac{k(a_{o2,2} r_{al}) \beta_{k,2}}{k(a_{o2,2} r_{al}) + \beta_{k,2}}.$$

The radii of the boron and aluminum particles (including oxide layer) and the radii of the unreacted boron and aluminum in the particles were calculated by the formulas:

$$r_{k,i} = \left( \frac{3\rho_{k,i}}{4\pi n_{k,i} n_{k,i}} \right)^{1/3}, \quad i = 1, 2, \quad r_{al} = \left[ \left( \frac{\mu_{al} + 1.5\mu_{al}}{\mu_{al}} \right) r_{al,0}^3 - \frac{3\rho_{k,2}}{4\pi n_{k,2} \rho_{k,2}} \right]^{1/3}, \quad r_{B} = \left( \frac{3(\rho_{k,1} - \rho_{\text{B}_2\text{O}_3})}{4\pi n_{k,1} \rho_{k,1}} \right)^{1/3}.$$

3. Results and discussion

We have solved the problem (1)–(13) using the method based on the studies [7,8]. The detailed description of the used calculation algorithms is given in [3].

Parametric calculations has been performed for a suspension with the mass content of aluminum and boron particles $m_{k,\text{Al}} = m_{k,B} = 0.5 \, m_{\text{dust}}$. The total mass of the powder suspended in the air has been set in the range from 0.2 to 0.4 kg/m². The physical specifications the gas and aluminum particles corresponded to [3]. The kinetic constants for the boron powder corresponded to the values described in the [5].

First, we show the results obtained for the problem of spark ignition of a monodisperse air suspension of boron powder. Figure 1 shows the profiles of the gas temperature (solid curve) and particles (dashed line) at the initial moment of ignition of the gas suspension of boron powder. Figure 2 shows the dependence of the minimum spark ignition energy of particles on the mass concentration.

According to figure 1, at the beginning of the process, the temperature in the spark heat release zone falls, and the gas and particles are slowly warmed up at a distance from this area (curves 1-3). In the heating zone, the oxidation of particles begins with the release of heat, the heating rate of gas and particles increases (curves 4–6). With the heating of particles, the process of oxidation and heat evolution accelerates (curves 7–8). After sufficient heating, the oxide layer evaporates; heterogeneous reactions begin on the surface of the particles and in the gas phase. The temperature of the particles increases, and begins to exceed the temperature of the gas; a combustion zone is formed, which propagates from the ignition zone (curve 9). According to figure 2 the relative change in the minimum energy spark ignition with an increase in the mass concentration of the particles is small. According to the calculation results, the minimum spark ignition energy of an aer suspension of boron powder with a particle radius of $10^{-6}$ m is less than the minimum spark ignition energy of an aer suspension of aluminum powder with the same particle size.

Further, the calculation of the minimum spark ignition energy of an air suspension of a mixture of aluminum and boron powders was performed. The ignition temperature of aluminum particles was set by the ratio from [9], $T_z = \exp \left( 0.087 \cdot \lg (2 \cdot 10^6 \cdot r_{k,2}^b) + 7.28 \right)$. The results are shown in
figures 3 and 4. For the calculation, a gas mixture was taken with the ratio of mass concentrations of aluminum powder and boron powder in the mixture of 50% to 50%.

Figure 1. Distributions of gas temperature (solid curve) and particles (dashed line) over space at time $t = 1 - 1.2 \cdot 10^{-3}$, $2 - 2.4 \cdot 10^{-3}$, $3 - 3.6 \cdot 10^{-3}$, $4 - 4.8 \cdot 10^{-3}$, $5 - 6 \cdot 10^{-3}$, $6 - 7.2 \cdot 10^{-3}$, $7 - 8.4 \cdot 10^{-3}$, $8 - 9.6 \cdot 10^{-3}$, $9 - 1.08 \cdot 10^{-2}$.

Figure 2. Dependence of the minimum spark ignition energy of a monodisperse air suspension of boron powder on the mass concentration of particles. $R_k = 10^{-6} m$.

Figure 3. Dependence of the minimum spark ignition energy of an air suspension mixture of aluminum and boron powders on the mass concentration of particles. $r_{k,1} = 3 \cdot 10^{-6} m$, $r_{k,2} = 0.5 \cdot 10^{-6} m$.

Figure 4. Dependence of the minimum spark ignition energy of an air suspension mixture of aluminum and boron powders on the radius of aluminum particles. $r_{k,1} = 3 \cdot 10^{-6} m$, $m_{dust} = 0.4 kg/m^3$. 
According to the results shown in figures 3 and 4, the minimum spark ignition energy of the gas suspension of the powder mixture increased in comparison with the minimum spark ignition energy of the gas suspension of boron powder and the gas suspension of aluminum powder. There are two reasons for this. The first reason may be the competition of reactions on the surface of the particles. Competition of reactions leads to insufficient oxygen for each of the particle fractions. A second reason may be used as the ignition temperature of the particles expressions [9].

4. Conclusions
A physical and mathematical model of spark ignition of a gas suspension of a mixture of aluminum and boron powders has been developed. The dependence of the minimum spark ignition energy of an air suspension of a mixture of aluminum and boron powders on the composition of the mixture is obtained from calculations. The effect of the mass concentration and radius of particles on the minimum spark ignition energy of a gas suspension is shown.

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