Combustion of aluminum and boron powders suspended in the air

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Abstract. This paper presents results on the numerical solution of the flame propagation problem in the air with suspended aluminum and boron particles. The aim of the study is to determine the combustion rate of the Al-B-air mixture depending on the particle mass concentration and its size. The physical and mathematical model of the process is based on the approaches of the mechanics of two-phase reactive media. The numerical method for solving the problem is based on the decay algorithm of an arbitrary discontinuity. It is shown that the apparent burning rate of the aerosol suspension of the mixture of aluminum and boron powders slightly decreases with an increase in the mass fraction of the powder in the mixture.

1. Introduction
The study is devoted to the combustion of boron (B) and aluminum (Al) powders in the air. The burning of boron powders was actively studied in the 1960s. In particular, some theoretical and numerical studies on the combustion of boron particles were carried out. The main conclusion of the studies is that the burning mechanism of boron particles is different from that of aluminum and strongly depends on the ambient temperature [1 - 2]. Currently, the topic of the fuel combustion, containing boron, is again gaining relevance.

The strong influence of ambient conditions on the oxidation, ignition and combustion regularities of boron particles implies impossibility of predicting the fuel combustion behavior, which contains boron powder. At the same time, boron-based fuels are attractive for their energy characteristics. Therefore it is engaging to investigate the combustion behavior of boron powder and also the features of the combustion processes, including with other high-energy materials, for example, aluminum powder.

The monograph [3] presents an oxidation and combustion model of a boron particle, and provides some experiment results on the flame propagation in a reacting gas suspension. According to the experimental results [4], boron powder does not combust in the air in an open pipe. The combustion rate of boron powder in oxygen is about $8 \, cm/s$ for boron mass concentrations of $0.2 - 0.4 \, kg/m^3$. The addition of the aluminum particles to boron powder-air mixture leads to the combustion potential of the mixture [5].

The combustion rate of the Al-B-air suspension with a boron particle radius of $3.1 \, \mu m$ and aluminum particles of $3 \, \mu m$ strongly depends on the mass content of aluminum powder in the mixture and the total mass concentration of the mixed powders [5].

For example, the flame normal velocity varies from $0.1$ to $0.12 \, m/s$ for the Al-B-air mixture with a content of boron and aluminum particles in the proportion of $m_{Al} = m_{B} = 0.5 \, m_{dust}$, whereas the total powder mass ranges from $0.3$ to $0.4 \, kg/m^3$. 
This paper presents a physico-mathematical model of the Al-B-air suspension combustion, which is based on the combustion model of the aluminum particles [6] and taking into account the oxidation and combustion mechanisms of boron particles [1 - 3]. The problem of the flame propagation speed along the suspension has been solved.

2. Mathematical model
The mathematical model adopts the oxidation and combustion mechanisms of boron powder described in [1-3].

At the first stage, when the particle temperature is under boiling point, boron oxide on the particle surface is in a condensed state, forming an oxide film. The oxidation reaction on the particles surface and the evaporation of the oxide layer are taken into account. There are no reactions in the gas phase. At the second stage, when the temperature of the boron oxide on the particle surface reaches the boiling point or higher temperature, boron oxide evaporates and a heterogeneous reaction occurs. Oxide film does not appear. The boron particle burns similar to a coal particle. It is supposed that the reaction products are formed in gaseous form. The kinetics of boron combustion on the particle surface has been set according to the studies [1 - 3]. The assumptions made for the aluminum particle combustion are consistent with [6]. Other assumptions of the mathematical combustion model correspond to [7] and the model has the following form:

the gas continuity equation:
\[
\frac{\partial \rho_g}{\partial t} + \frac{\partial \rho_g u_g}{\partial x} = G_1 + G_2 - \frac{24}{11} G_3 + G_4 - G_5, \tag{1}
\]

the momentum conservation equation for the gas
\[
\frac{\partial \left( \rho_g u_g \right)}{\partial t} + \frac{\partial \left( \rho_g u_g u_g + p \right)}{\partial x} = -\tau_v + \left( G_1 + G_2 - \frac{24}{11} G_3 + G_4 \right) u_{k,1} - G_6 u_g, \tag{2}
\]

the gas energy equation:
\[
\frac{\partial \rho_g \left( e_g + 0.5 u_g^2 \right)}{\partial t} + \frac{\partial \left[ \rho_g u_g \left( e_g + 0.5 u_g^2 \right) + pu_g \right]}{\partial x} = \left( G_1 + G_2 - \frac{24}{11} G_3 + G_4 \right) \left( c_{k,1} T_{g,1} + \frac{u_{k,1}^2}{2} \right) + \\
\frac{\partial}{\partial x} \left[ \lambda_g \left( T_g \right) \frac{\partial T_g}{\partial x} \right] + \sum_{i=1,2} \left[ \alpha_{k,i} \nu_{k,i} \left( T_{g,1} - T_g \right) - u_{k,i} \tau_{v,i} \right] + \\
\left( Q - Q_1 \right) G_1 + \left( Q - Q_2 \right) G_2 - G_6 \left( c_{i,1} T_g + \frac{u_g^2}{2} \right), \tag{3}
\]

the oxygen mass balance equation:
\[
\frac{\partial \rho_{O_2}}{\partial t} + \frac{\partial \rho_{O_2} u_g}{\partial x} = \frac{\partial}{\partial x} \left( D_{g} \left( T_g \right) \rho_g \frac{\partial \rho_{O_2}}{\partial x} \right) - \frac{24}{11} \left[ \left( G_1 + G_2 + G_3 \right) - G_5 \right], \tag{4}
\]

the mass balance equation for the gaseous reaction products B2O3(g):
\[
\frac{\partial \rho_{B_2O_3}}{\partial t} + \frac{\partial \rho_{B_2O_3} u_g}{\partial x} = \frac{\partial}{\partial x} \left( D_{g} \left( T_g \right) \rho_g \frac{\partial \rho_{B_2O_3}}{\partial x} \right) + \frac{35}{11} \left( G_1 + G_2 \right) + G_4, \tag{5}
\]

the particle mass balance equation:
\[
\frac{\partial \rho_{k,1}}{\partial t} + \frac{\partial \rho_{k,1} u_{k,1}}{\partial x} = -G_1 - G_2 + \frac{24}{11} G_3 - G_4, \quad \frac{\partial \rho_{k,2}}{\partial t} + \frac{\partial \rho_{k,2} u_{k,2}}{\partial x} = G_5, \tag{6}
\]
the mass balance equation for solid boron oxide:
\[ \frac{\partial \rho_{BO}}{\partial t} + \frac{\partial \rho_{BO} u_{BO}}{\partial x} = \tau_{BO} - \left( G_{1} + G_{2} - \frac{24}{11} G_{3} + G_{4} \right) u_{k,1}, \]
\[ \frac{\partial \rho_{BO}}{\partial t} + \frac{\partial \rho_{BO} u_{BO}}{\partial x} = \tau_{BO} + G_{i} u_{g}, \]  

(7)

the particle momentum conservation equations:
\[ \frac{\partial \rho_{k,1} (u_{k,1} + 0.5 u_{k,1}^2)}{\partial t} + \frac{\partial \rho_{k,1} u_{k,1}}{\partial x} = \left( Q_{i} G_{1} + Q_{g} G_{2} + Q_{s} G_{3} - Q_{s} G_{4} \right) - G_{1} \left( c_{k,1} T_{k,1} + 0.5 u_{k,1}^2 \right) + \tau_{k,1} n_{k,1} \left( T_{k,1} - T_{g} \right), \]
\[ \frac{\partial \rho_{k,2} (u_{k,2} + 0.5 u_{k,2}^2)}{\partial t} + \frac{\partial \rho_{k,2} u_{k,2}}{\partial x} = - \alpha_{k,2} S_{k,2} n_{k,2} \left( T_{k,2} - T_{g} \right) + \]
\[ \left( G_{5} c_{k,2} T_{g} + 0.5 u_{g}^2 + \frac{Q_{g}}{\alpha_{s}} \right) + \tau_{k,2} u_{k,2}, \]  

(8)

the particle energy equations:
\[ \frac{\partial n_{k,1}}{\partial t} + \frac{\partial n_{k,1} u_{k,1}}{\partial x} = 0, \quad i = 1, 2, \]

(10)

the gas equation:
\[ p = \rho_{g} R_{g} T_{g}, \]

(11)

the initial conditions:
\[ T_{g} (x, t) = \begin{cases} T_{g} = T_{b}, & \rho_{k,1} (x, t) = m_{k,b}, \quad \rho_{k,2} (x, t) = m_{k,d}, \\
(T_{b} - T_{g}), & T_{b} < x < \infty, \quad \rho_{k,1} (x, t) = m_{k,b}, \quad \rho_{k,2} (x, t) = m_{k,d}. \end{cases} \]

(12)

the boundary conditions:
\[ \frac{\partial \rho_{k,1} (0, t)}{\partial x} = \frac{\partial \rho_{g} (0, t)}{\partial x} = \frac{\partial \rho_{k,2} (0, t)}{\partial x} = \frac{\partial T_{g} (0, t)}{\partial x} = 0, \]
\[ \frac{\partial n_{k,1} (0, t)}{\partial x} = \frac{\partial n_{g} (0, t)}{\partial x} = \frac{\partial T_{k,1} (0, t)}{\partial x} = 0, \quad u_{k,1} (0, t) = u_{g} (0, t) = 0, \]

(13)

The notations in (1) - (13) are usual and correspond to the studies [6 - 7]. The parameters of boron particles are marked by index 1, and those of 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:
The mass change rate of the boron particles due to the oxidation reaction with the condensed oxide $B_2O_3$ formation:

$$G_3 = \beta_{k,\text{eff}} n_{k,1} \rho_{B_2O_3} S_{k,1},$$

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 $B_2O_3$:

$$G_4 = n_{k,1} \beta_{k,1} (\rho_{B_2O_3}^e - \rho_{B_2O_3}^g),$$

where $\rho_{B_2O_3}^e$ is the density of saturated vapors around a particle.

The mass change rate of the aluminum particles according to [6] is:

$$G_5 = \alpha_{k,1} n_{k,1} \rho_{k,2}^0 S_{k,1} \left( \frac{k(a_{k,2} r_{k,1})}{\rho_{k,2}^0 + \beta_{k,2}} \right).$$

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:

$$r_{k,i} = \left( \frac{3 \rho_{k,i}^0}{4 \pi n_{k,i} \rho_{k,i}^0} \right)^{1/3}, \quad i=1,2, \quad r_{d,1} = \left[ \frac{(\mu_d + 1.5 \mu_O) r_{d,0}}{\mu_d} - \frac{3 \rho_{k,2}^0}{4 \pi n_{k,2} \rho_{k,2}^0} \right]^{1/3},$$

$$r_{d,2} = \left( \frac{3 (\rho_{k,1} - \rho_{B_2O_3}^g)}{4 \pi n_{k,1} \rho_{k,1}^0} \right)^{1/3}.$$

3. Results and discussion

We have solved the problem (1)-(13) using the method based on the studies [6 - 7]. The detailed description of the used calculation algorithms is given in [7].

Parametric calculations have been performed for a suspension with the mass content of aluminum and boron particles $m_{k,Al} = m_{k,B} = 0.5 m_{dust}$. The total mass of the powder suspended in the air has been set in the range from 0.2 to 0.4 kg/m$^3$. The physical specifications of the gas and aluminum particles corresponded to [6]. The kinetic constants for the boron powder corresponded to the values described in the monograph [3]. Other parameters were set according to table indicating values from the reference literature. The calculations were conducted for two suspension compositions with particle radii $r_{k,1}$, $r_{k,2}=10^{-6}$ m and $r_{k,1}=10^{-6}$ m, $r_{k,2}=0.5\cdot10^{-6}$ m (Figure 1-2). Figure 1 shows the dependence of the apparent propagation velocity of the combustion front in the Al-B-air suspension on the total mass concentration of the particles.

The apparent velocity has been defined as the motion speed of the combustion front. The coordinate of the combustion front has been determined as the coordinate $x$ at which the mass fraction of the oxidizer in the gas is reduced many times in comparison with its initial value. The dependence of the normal combustion velocity on the total mass concentration of the particles is shown in Figure 2. The normal velocity was determined as the difference between the apparent propagation velocity and the velocity of the gas suspension.

As it can be seen from the Figure 1, the apparent combustion velocity of the suspension drops slightly with an increase in the mass fraction of the powder in it. The apparent combustion velocity of the suspension with aluminum particle radii $r_{k,2}=0.5\cdot10^{-6}$ m is higher than for the suspension with aluminum particles radii $r_{k,2}=10^{-6}$ m. With an increase in the total mass concentration of the particles $m_{dust}$, the apparent combustion velocity of the suspension with aluminum particle radii $r_{k,2}=0.5\cdot10^{-6}$ m changes almost linearly. Depending on the dispersity of aluminum particles and the total mass concentration of...
the powder in the suspension, the normal combustion velocity varies from 0.23 m/s to 0.16 m/s. In this case, the highest value of the normal velocity is achieved for the suspension with the mass concentration $m_{dust} = 0.2 \text{ kg/m}^3$ and the aluminum particle radii $r_{k,2} = 0.5 \cdot 10^{-6} \text{ m}$.

![Figure 1. Apparent combustion velocity of the Al-B-air suspension with the particle radii $r_{k,1} = 1 \mu m$, $m_{k,Al} = m_{k,B} = 0.5 m_{dust}$](image1)

![Figure 2. Normal combustion velocity of the Al-B-air suspension with the particle radii $r_{k,1} = 1 \mu m$, $m_{k,Al} = m_{k,B} = 0.5 m_{dust}$](image2)

The obtained values of the normal flame propagation velocity are higher than the values from [5]. This is explained by the fact that in the present study powders with a smaller particle radii have been examined. Decreasing the particle radii raises the normal and apparent velocity of the flame propagation.

Conclusions
We have developed a physical and mathematical model of the Al-B-air suspension combustion. The study provides data on the apparent and normal combustion velocity of the suspension, depending on the size of aluminum particles and the mass concentration of the metal powder in the suspension. It is shown that for the selected initial data the apparent burning rate of the mixture of aluminum and boron powders varies slightly with a change in the total mass concentration.

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