Combustion model of boron-air suspension

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Abstract. This paper presents a physico-mathematical combustion model of the boron-air suspension. The oxidation mechanism and combustion of boron particles are based on the study by King M. K. The physico-mathematical formulation of the problem implies the approaches by R.I. Nigmatulin for the mechanics of two-phase reactive media. The paper provides numerical investigation on the effect of mass concentration and boron particle size on the apparent and normal combustion front velocity of the boron-air suspension.

1. Introduction
Recently, the interest of the researchers to the problems of the boron powder combustion has been manifested again. Boron powder during combustion can provide high temperatures and therefore boron-containing fuels are perspective. One of the main problems of the experimental and theoretical studies on the boron particles combustion is the complex process of their burning. The kinetics of the boron powder combustion is described in [1 - 3] and resolves to the following mechanism of oxidation and combustion:

1. If the particle temperature is under the boiling point, boron oxide on the particle surface is in a condensed state, forming an oxide film. The combustion rate is limited by the diffusion of oxygen through the oxide layer. The film thickness grows in time, thus the diffusion rate of the oxidizer decreases, and the boron particles slow down final combustion.

2. When the temperature of a boron particle exceeds the boiling point of boron oxide, the particle oxide layer starts evaporate to the surrounding gas. The boron particle reacts heterogeneously with oxygen forming the gaseous intermediate products, which are oxidized to the final product ($B_2O_3$) in the gas phase. An intensive high-temperature burning of boron proceeds and the combustion rate is limited by the oxygen diffusion to the particle surface.

The aim of the study is to develop the physico-mathematical combustion model of the boron-air suspension, solve the problem of the flame propagation velocity using the oxidation and combustion regularities of boron from [1 - 3] and conduct a numerical study of the flame propagation velocity dependence on the mass concentration and radius of boron particles.

2. Mathematical model
The formulation of the problem and solution procedure are based on the studies [4, 5]. The right summands of the differential equations responsible for the oxidation and combustion of boron particles are determined according to the following assumptions: the model takes into account boron oxide formation and its evaporation reaction and two heterogeneous reactions between oxygen and boron with the formation of two gaseous reaction products. Heating of the particles leads to their oxidation with formation of an oxide film. Further heating causes evaporation of the film. The
evaporation rate depends on the pressure of the boron oxide saturated vapors around the particles. The boron oxidation through the oxide film is defined by the effective mass transfer coefficient, taking into account the oxide layer on the particle. Heating the particles to a temperature above the boiling point of boron oxide induces rapid evaporation of the oxide film and the beginning of heterogeneous chemical reactions on the surface of the particles. Heterogeneous chemical reactions on the surface of particles are described using the kinetic constants from [1] taking into account mass transfer [5].

Under the assumptions made, the mathematical formulation of the problem in the Cartesian coordinate system is:

the gas continuity equation:

$$\frac{\partial \rho_g}{\partial t} + \frac{\partial \rho_g u_g}{\partial x} = G_1 + G_2 - \frac{24}{11} G_3 + G_4,$$  

(1)

the momentum conservation equation for the gas:

$$\frac{\partial \left( \rho_g u_g \right)}{\partial t} + \frac{\partial \left( \rho_g u_g^2 + p \right)}{\partial x} = -\tau_u + \left( G_1 + G_2 - \frac{24}{11} G_3 + G_4 \right) u_i,$$  

(2)

the gas energy equation:

$$\frac{\partial \rho_g \left( e_g + 0.5 u_g^2 \right)}{\partial t} + \frac{\partial \left( \rho_g u_g \left( e_g + 0.5 u_g^2 \right) + p u_g \right)}{\partial x} = \frac{\partial}{\partial x} \left( \lambda_g \left( T_g \right) \frac{\partial T_g}{\partial x} \right) + \alpha_e n_k S_k \left( T_k - T_g \right) +$$

$$+ \left( G_1 + G_2 - \frac{24}{11} G_3 + G_4 \right) \left( c_k T_k + \frac{u_k^2}{2} \right) - u_k \tau_u + \left( Q - Q_i \right) G_1 + \left( Q - Q_2 \right) G_2,$$  

(3)

the oxygen mass balance equation:

$$\frac{\partial \rho_{O_2}}{\partial t} + \frac{\partial \rho_{O_2} u_g}{\partial x} = \frac{\partial}{\partial x} \left( \rho_g D_g \left( T_g \right) \frac{\partial a_{O_2}}{\partial x} \right) - \frac{24}{11} \left[ G_1 + G_2 + G_3 \right],$$  

(4)

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

$$\frac{\partial \rho_{B_2O_3}}{\partial t} + \frac{\partial \rho_{B_2O_3} u_g}{\partial x} = \frac{\partial}{\partial x} \left( \rho_g D_g \left( T_g \right) \frac{\partial a_{B_2O_3}}{\partial x} \right) + \frac{35}{11} \left[ G_1 + G_2 \right] + G_4,$$  

(5)

the particle mass balance equation:

$$\frac{\partial \rho_k}{\partial t} + \frac{\partial \rho_k u_k}{\partial x} = -\left( G_1 + G_2 - \frac{24}{11} G_3 + G_4 \right),$$  

(6)

the mass balance equation for solid boron oxide:

$$\frac{\partial \rho_{B_2O_3}^s}{\partial t} + \frac{\partial \rho_{B_2O_3}^s u_k}{\partial x} = \frac{35}{11} \left[ G_3 - G_4 \right],$$  

(7)

the particle momentum conservation equations

$$\frac{\partial \left( \rho_k u_k \right)}{\partial t} + \frac{\partial \rho_k u_k^2}{\partial x} = \tau_u - \left( G_1 + G_2 - \frac{24}{11} G_3 + G_4 \right) u_k,$$  

(8)
the particle energy equations:

\[ \frac{\partial \rho_k \left( \epsilon_k + 0.5 u_k^2 \right)}{\partial t} + \frac{\partial \rho_k u_k \left( \epsilon_k + 0.5 u_k^2 \right)}{\partial x} = (Q_1 G_1 + Q_2 G_2 + Q_3 G_3 - Q_4 G_4) - \left( G_1 + G_2 - \frac{24}{11} G_3 + G_4 \right) \left( c_k T_k + \frac{u_k^2}{2} \right) + \tau_g u_k - \alpha_k \rho_k n_k \left( T_g - T_k \right), \]

the particle concentration equation:

\[ \frac{\partial n_k}{\partial t} + \frac{\partial n_k u_k}{\partial x} = 0, \]

the gas equation:

\[ p = \rho_g R T_g. \]

the initial conditions:

\[ T_g(x,t_z) = \begin{cases} T_z, & 0 \leq x \leq x_0 \\ T_z, & x_0 < x \leq \infty \end{cases}, \quad T_k(x,t_z) = T_z, \quad \rho_{o_2}(x,t_z) = \rho_{o_2,b}, \quad \rho_{g,023} = \rho_{g,023}^0 = 0, \]

\[ \rho_k(x,t_z) = \rho_{b,b}, \quad u_g(x,t_z) = u_k(x,t_z) = 0, \quad \rho_g(x,t_z) = \rho_{b,b}, \quad n_k(x,t_z) = n_{b,b}, \]

the boundary conditions:

\[ \left. \frac{\partial T_g(0,t)}{\partial x} \right|_{x=0} = \left. \frac{\partial T_k(0,t)}{\partial x} \right|_{x=0} = \left. \frac{\partial T_g(\infty,t)}{\partial x} \right|_{x=\infty} = \left. \frac{\partial T_k(\infty,t)}{\partial x} \right|_{x=\infty} = 0. \]

The notations in (1) - (13) are usual and correspond to the studies [4, 6]. The rates of the boron particle mass change during the heterogeneous reactions on the particle surface are defined as:

\[ G_i = \frac{k_{o_1} \exp\left(-\frac{E_i}{RT_{k,i}}\right) \beta_{k,i}}{k_{o_0} \exp\left(-\frac{E_1}{RT_{k,i}}\right) + \beta_{k,i}} n_{i,b} \rho_{o_2} S_{k,i}, \quad G_2 = \frac{k_{o_2} \exp\left(-\frac{E_2}{RT_{k,i}}\right) \beta_{k,i}}{k_{o_0} \exp\left(-\frac{E_2}{RT_{k,i}}\right) + \beta_{k,i}} n_{i,b} \rho_{o_2} S_{k,i}. \]

The mass change rate of the boron particles due to the oxidation reaction with the condensed oxide \( B_2O_3 \) formation:

\[ G_3 = \beta_{k,off} n_{i,b} \rho_{o_2} S_{k,i}, \]

where \( \beta_{k,off} \) is the effective mass transfer coefficient taking into account the diffusion through the spherical oxide, the diffusion resistance of the oxide layer and gas surrounding the particle:

\[ \beta_{k,off} = \left[ \frac{r_o^2}{D_g} + \frac{1}{D_d} \left( \frac{1}{r_o} - \frac{1}{r_i} \right) \right]^{-1}. \]
where $D_d$ is the preexponential coefficient as function of the diffusion coefficient depending on temperature, $E_d$ is the diffusion activation energy.

The mass change rate of the boron particles due to the evaporation of a melted oxide $B_2O_3$:

$$G_4 = n_{k,1} β_{k,1} \left( \rho_{B_2O_3}^* - \rho_{B_2O_3}^{\infty} \right) S_{k,1},$$

where $\rho_{B_2O_3}^* = \left( \rho_{\text{m, } \mu g} \right) / \left( R_u T_g \right)$ is the density of saturated vapors around a particle.

The radius of a whole particle and its unreacted boron part are calculated by the formulas:

$$r_e = \left( \frac{3\rho_k}{4\pi \rho_{\infty} n_k} \right)^{\frac{1}{3}}, \quad r_\beta = \left( \frac{3\left( \rho_k - \rho_{B_2O_3}^* \right)}{4\pi \rho_k^2} \right)^{\frac{1}{3}}.$$

3. Results and discussion

The solution method of the posed problem is similar to the methods described in [4, 6]. Study [4] provides a detailed description of the calculation algorithms. The space grid step is set to constant and equals $\Delta h = 2 \cdot 10^{-5}$ m. The time step is chosen from a comparison of two Courant stability conditions:

$$\Delta t = 0.4 \min \left[ \frac{\Delta h}{\max \left[ \mu_g + c_g \right]}, \frac{\Delta h^2}{2\chi_g} \right],$$

where $c_g$ is the gas acoustic velocity, $\chi_g = \lambda_g / \left( c_g \rho_g \right)$ is the gas heat diffusivity.

We have carried out a parametric analysis for the mass concentration of boron powder in the range from 0.2 to 0.4 kg/m$^3$ (these values correspond to the lack of oxidizer). The particle radius has been ranged from 0.5 to 4 $\mu$m. The kinetic constants of the heterogeneous combustion reaction for boron particles ($G_1, G_2$) have been taken from [1, 2]. The diffusion rate through the oxide layer is determined by the values $D_d = 1.89 \cdot 10^{-8}$ m$^2$/s and $E_d = 10$ kJ/mol [7]. Other parameters have been set according to the table indicated values from the reference literature. The calculation results are presented in Figures 1 – 4.

![Figure 1](attachment:image1.png)  
Figure 1. The apparent combustion rate of Boron-Air suspension.

![Figure 2](attachment:image2.png)  
Figure 2. The normal combustion rate of Boron-Air suspension.
Figures 1, 2 show the dependence of the apparent and normal combustion rate of a boron-air suspension on the mass concentration of the boron powder. Whilst the mass concentration of the powder changes from 0.2 kg/m$^3$ to 0.4 kg/m$^3$, the normal combustion rate of the suspension changes slightly: the change is about 1–2 cm/s (Figure 2), whereas the apparent combustion rate shifts significantly (Figure 1).

The obtained regularities differ from those obtained for the aluminum-air suspension [6]. The study established that an increase in the mass concentration of aluminum particles does not affect the apparent combustion rate. In case of the boron-air suspension combustion, the obtained regularities (Figures 1, 2) are explained by the diffusion of the oxidizing agent through the oxide film.

The obtained result contradicts with results of [1, 8]. The studies [1, 8] indicate that the boron powder in the air does not combust. The results of the numerical investigation on the boron-air combustion problem (1) - (13) for the boron mass concentration of 0.3 kg/m$^3$ and different particle radii are presented in Figures 3, 4.

The normal combustion rate is 0.1–0.12 m/s for particles with a radius of 2–3 μm (Figure 4). According to data from [1, 8], the normal burning rate of boron powder in oxygen with the average particle diameter of 4 – 6 μm and the particle mass concentration of 0.2 – 0.4 kg/m$^3$ is about 0.08 m/s. The contradiction of the calculation results by the model (1) - (13) with experimental one can be associated with the selected parameters of the diffusion rate through the oxide layer or with the experimental conditions [8]. This problem requires further investigation.

**Conclusions**

We have developed the physico-mathematical model of boron-air suspension combustion and conducted a numerical analysis of the suspension combustion problem using the model. The numerical study has provided the data on the apparent and normal combustion rate of the suspension depending on the particle size and the mass concentration of boron powder in the suspension. The obtained
results have shown that an increase in boron particle size for a suspension with the powder mass concentration of 0.3 kg/m³ leads to a decrease of the apparent and normal combustion rate.

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References:
[1] Yagodnikov D A 2009 Ignition and combustion of powdered metals (Moscow: MGTU im. N. E. Baumana)
[2] King M K 1972 Combust Sci Technol 5 (4) 155
[3] Vovchuk Ya I, Zolotko A N, Klyachko L A and Polishchuk D I 1975 Combust Explos Shock Waves 11 (4) 556
[4] Moiseeva K M and Krainov A Yu 2018 Combust Explos Shock Waves 54 (2) 179
[5] Frank-Kamenetskiy D A 1987 Diffusion and Heat Transfer in Chemical Kinetics (Moscow: Nauka)
[6] Moiseeva K M and Krainov A Yu 2018 J Phys Conf Ser 1105 012034
[7] Poryazov V A and Krainov A Yu 2018 MATEC Web Conf 243 00023
[8] Boichuk L V 1993 Investigation of flame propagation processes in two-component gas mixtures (Odessa: OSU)