Numerical simulation of combustion frozen nanosized aluminum suspension with water

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Abstract. The paper presents a mathematical model for combustion of a frozen nanosized aluminum suspension (ALICE), taking into account the combustion of aluminum in water vapor, the motion of combustion products, and the velocity lag of particles compared to gas. The model was formulated based on Belyaev’s approach to modeling the combustion of volatile fuels. The burning rate calculated is in agreement with the experimental data on the ALICE burning rate and its variation with pressure.

Keywords: aluminum, frozen suspension, combustion, nanosized particles, ALICE, mathematical modeling.

The linear burning rate of the frozen nanosized aluminum suspension is determined by the rate of water evaporation from the aluminum surface. The aluminum particles are considered to be beads, with their size and distribution being uniform. There is supposed to be a chemical reaction between water vapor and aluminum particles, its product being aluminum oxide remaining on the particle surface and hydrogen \(2Al + 3H_2O = Al_2O_3 + 3H_2\). The ignition of aluminum particles occurs when they reach a certain temperature \[1\]. The burning rate of aluminum particles is described based on the experimental data \[2, 3\]. The heat exchange between aluminum particles and gas is defined by Newton’s law. The aluminum particles are in motion due to the friction caused by the gas. Because of the low volume concentration of aluminum particles in the gas their motion has no effect on the gas flow. The agglomeration of aluminum particles on the condensed phase surface and their interaction with each other in the gas phase are not taken into consideration. The combustion regime is supposed to be isobaric and the pressure does not depend on the distance from the burning surface.

\[
c_2\rho_2\left(\frac{\partial T_2}{\partial t} + u \frac{\partial T_2}{\partial x}\right) = \lambda_2 \frac{\partial^2 T_2}{\partial x^2} + 4\pi\alpha r_2^2 n (T_3 - T_2) \tag{1}
\]

\[
\frac{\partial \rho_2}{\partial t} + \frac{\partial (\rho_2 u)}{\partial x} = -G \tag{2}
\]

\[
\frac{\partial \rho_{H_2}}{\partial t} + \frac{\partial (\rho_{H_2} u)}{\partial x} = G \frac{\mu_{H_2}}{\mu_o} \tag{3}
\]
In accord with [4], heat capacitance of aluminum particle in process of warming, melting and combustion of aluminum particles follow the formula:

\[ c_3 \rho_3 \left( \frac{\partial T_3}{\partial t} + w \frac{\partial T_3}{\partial x} \right) = -4\pi a \rho^2 n(T_1 - T_2) + GQ_{al} \frac{2\mu_{al}}{3\mu_o} \]  \hspace{2cm} (4)

\[ \frac{\partial \rho_3 + \partial (\rho_3 w)}{\partial t} = G \]  \hspace{2cm} (5)

\[ \frac{\partial w}{\partial t} + w \frac{\partial w}{\partial x} = -\tau_{w} \]  \hspace{2cm} (6)

\[ \frac{\partial n}{\partial t} + \frac{\partial (nw)}{\partial x} = 0 \]  \hspace{2cm} (7)

\[ P = \rho_2 \left( \frac{m_{H_2O}}{\mu_{H_2O}} + \frac{m_{H_2}}{\mu_{H_2}} \right) RT_2 = \text{const} \]  \hspace{2cm} (8)

\[ m_{H_2O} = \frac{\rho_2 - \rho_{H_2O}}{\rho_2} \quad m_{H_2} = \frac{\rho_{H_2}}{\rho_2} \]

In accord with [4], heat capacitance of aluminum particle in process of warming, melting and combustion of aluminum particles follow the formula:

Here, Equation (1) and Equation (4) are the energy equations for the gas phase and for the particles, respectively. Equation (2) is the gas phase mass conservation equation, Equation (3) is the mass conservation equation for the gaseous reaction products, and Equation (5) is the mass conservation equation for the particles. Equation (6) and Equation (7) describe the motion of the particles and their number, respectively. Equation (8) is the ideal gas equation written for a two-component gas mixture.

The coordinate \( x = 0 \) corresponds to the burning surface. The following relations are valid on the evaporation surface, namely mass conservation of the water flow (Equation (9)) and conservation of the mass flow for the aluminum particles (Equation (10)):

\[ (1 - M_{al}) \rho V = \rho_2 u|_{x=0} \]  \hspace{2cm} (9)

\[ M_{al} \rho V = (\rho_3 w)|_{t=0} \]  \hspace{2cm} (10)

The equality of the water, vapor and particles temperatures is defined by:

\[ T_1|_{x=0} = T_2|_{x=0} = T_v \]  \hspace{2cm} (11)

The temperature of the saturated vapor \( T_v \) above the evaporation surface is defined based on the Clausius-Clapeyron equation:

\[ P = A \exp \left( -\frac{L}{RT} \right) \quad T_v = \frac{L}{R \ln \left( \frac{P}{P_a} \right) + L/T_{v,a}} \]  \hspace{2cm} (12)

The initial conditions are as follows:
The heat flow from the gas to the evaporation surface is consumed to warm up the condensed phase to the ice melting temperature, to melt the ice, to heat the water to its evaporation temperature and to evaporate it:

\[
T_2(x, 0) = T_{gw}; \quad T_3(x, 0) = T_{gw}; \quad \rho_2(x, 0) = \frac{\mu_{H_2O} P}{RT_2(x, 0)}; \quad \rho_{H_2}(x, 0) = 0; \\
\rho_3(x, 0) = 0; \quad u(x, 0) = 0; \quad w(x, 0) = 0; \quad n(x, 0) = 0
\] (13)

The water vapor density above the evaporation surface of the condensed phase is defined by the ideal gas equation:

\[
\lambda_2 \frac{\partial T}{\partial x}_{x=0} = \rho_2 V (c_i T_{2,1,0} - c_i T_{1,0}) + \rho_3 (1 - M_{Al}) V (L + \Lambda)
\] (14)

The water vapor density above the evaporation surface of the condensed phase is defined by the ideal gas equation:

\[
\rho_2 |_{x=0} = \frac{\mu_{H_2O} P}{R T_2 |_{x=0}}\; ; \; P = \text{const}
\]

The number of particles per unit volume is determined by the following relation:

\[
n |_{x=0} = \frac{\rho_3 |_{x=0}}{(4/3) \pi r_{Al,0}^3 \rho_k},
\]

where \( r_{Al,0} \) is the initial radius of the aluminum particle; \( \rho_k \) is the particle density.

There is assumed to be no gaseous reaction products near the evaporation surface,

\[
\rho_{H_2} |_{x=0} = 0
\]

At \( x = \infty \) the boundary condition is the following:

\[
\frac{\partial T}{\partial x} |_{x=\infty} = 0
\] (15)

The force of interaction between the aluminum particles and the gas is calculated applying the formula:

\[
\tau_r = \frac{F_r}{4/3 \pi r_k^3 \rho_k}; \quad F_r = \frac{C_R}{S_m} \rho_2 \left( \frac{w-u}{2} \right) |u-w|
\]

Here, the resistance coefficient is defined according to the empirical formula given in [5]:

\[
C_R = \frac{24}{Re} \left( 1 + 0.15 Re^{0.682} \right) ; \quad \text{Re} = \frac{2r_k \rho_k |u-w|}{\eta}
\]

The coefficient of heat transfer is determined as follows:

\[
\alpha = \frac{Nu \lambda}{2r_k}; \quad Nu = 2 + \sqrt{Nu_i^2 + Nu_l^2}, \; \text{where} \; Nu_l = 0.664 Re^{0.5}; \; Nu_i = 0.037 Re^{0.8} \; [5]
\] (16)

\[
G = \frac{3 \mu_{Al}}{2 \mu_{Al}} n \rho_k 4 \pi r_{Al} k_{Al}, \; \text{where} \; k_{Al} \; \text{is assumed to be constant}
\] (17)
When deriving Equation (18), we assumed for simplification that the alumina remained on the particle surface as a spherical layer. This assumption is introduced to determine the actual radius of the aluminum bead and has no effect on its burning rate since the latter is taken based on the experimental data. The burning rate of the aluminum particle was calculated according to the experimental data on the time of aluminum particle combustion in water vapor [3]. In calculations, the ignition temperature for the aluminum particles of the size given was considered to be 1400 K [6].

Numerical analysis for combustion of the frozen suspension of nanosized aluminum powder in water was carried out at the mass concentration of aluminum powder corresponding to the stoichiometric mixture of aluminum with water. The following values of the thermophysical parameters were taken in calculations: \( \rho_1 = 1460 \, \text{kg/m}^3, \, M_{\text{Al}} = 0.499, \, c_1 = c_{\text{wat}}(1 - M_{\text{Al}}) + c_{\text{Al}}M_{\text{Al}}, \, c_{\text{wat}} = 4185 \, J/(\text{kg} \cdot \text{K}), \, c_{3,\text{solid}} = 903 \, J/(\text{kg} \cdot \text{K}), \, c_{3,\text{liquid}} = 1090 \, J/(\text{kg} \cdot \text{K}), \, c_{\text{H}_2O} = 2600 \, J/(\text{kg} \cdot \text{K}), \, c_{\text{H}_2} = 14300 \, J/(\text{kg} \cdot \text{K}), \, \rho_k = 2600 \, \text{kg/m}^3, \, R = 8.31 \, J/(\text{mol} \cdot \text{K}), \, \eta = 0.00002 \, \text{Pa} \cdot \text{s}, \, \lambda_2 = 1 \, W/(\text{m} \cdot \text{K}), \, k_{d} = 1.2 \times 10^{-10} \, \text{m}^2/\text{s}, \, T_{i,0} = 270 \, \text{K}, \, Q_{\text{Al}} = 15.0 \, \text{MJ/kg} \, [8], \, \Lambda = 332400 \, J/\text{kg}, \, L = 1712940 \, J/\text{kg}, \, c_2 = m_{\text{H}_2O}c_{\text{H}_2O} + m_{\text{H}_2}c_{\text{H}_2}, \, \mu_{\text{Al}} = 0.027 \, \text{kg/mol}, \, \mu_{\text{OG}} = 0.016 \, \text{kg/mol}, \, \mu_{\text{H}_2} = 0.002 \, \text{kg/mol}, \, r_{d,0} = 0.04 \, \mu\text{m} = 40 \, \text{nm}, \, P = 4 \div 20 \, \text{MPa}.

The set of equations (Equations (1)-(8)) with the initial and boundary conditions (Equations (9)-(15)) and the relations for the right-hand terms was solved numerically using the procedure described in [7].

The aluminum particle radius was considered to be 40 nm, the pressure above the burning surface varying within the range of \( 4.0 \leq P \leq 20.0 \, \text{MPa} \), according to [5]. The ignition temperature for the aluminum particles of the size given was taken equal to 1400 K.

In [2, 3] there is a formula for the burning time of the aluminum particle in water vapor (its diameter is within the range of 150-300 \( \mu\text{m} \)), which defines the coefficient \( k_{d,1} \) used in Equation (19).

Calculations with the coefficient given in [3] showed overestimated values of the burning rate for the frozen suspension of nanosized aluminum powder comparing with the experimental data given in [8], so in the mathematical model (Equations (1-20)) the coefficient \( k_{d,1} \) is considered as the only one for the matching calculations with the experimental data [8]. The experimental data on the effect of pressure on the burning rate for the frozen suspension of nanosized aluminum in water [8] are given in the range of \( 4.0 \leq P \leq 20.0 \, \text{MPa} \). The coefficient \( k_{d,1} \) is selected so that the burning rate calculated matches its experimental value [6] at the pressure of 10 MPa. Note, the authors [8] approximated the experimental data obtained using the following formula: \( V_e = 0.7027 P^{0.57019} \, \text{sm/s} \), where pressure was measured in MPa. The value of \( k_{d,1} = 1.2 \times 10^{-10} \, \text{m}^2/\text{s} \) obtained after the matching described was used in our calculations of the burning rate at other pressure values.

Figure 1 shows how the linear burning rate for combustion of the frozen nanosized aluminum suspension in water depends on pressure. The dotted line presents the experimental data approximated in [8] by the following formula: \( V_e = 0.7027 P^{0.57019} \, \text{sm/s} \) (the pressure is measured in MPa). The difference between the burning rate calculated and the experimental one does not exceed 8%.

\[
r_{d,1} = \left[ \left( \frac{\mu_{d,1} + 3/2 \mu_{d,0} r_{d,0}^3}{\mu_{d,1}} \right)^{0.5} \right]^2;
\]

\[
r_3 = \left[ r_{d,1}^3 + \frac{\mu_{d,1} + 3/2 \mu_{d,0} \left( r_{d,1,0}^3 - r_{d,1}^3 \right)}{\mu_{d,1}} \right]^{0.5}.
\]
A mathematical model for combustion of a frozen nanosized aluminum suspension in water has been developed. The numerical results obtained for the burning rate are in good agreement with the experimental data for the dependence of burning rate on pressure for the combustion of frozen nanosized aluminum suspension in water.

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References