Investigation on focal ignition and combustion of aluminum-air suspension

K M Moiseeva and A Yu Krainov
Tomsk State University, Tomsk, 634050 Russia
E-mail: Moiseeva_KM@t-sk.ru

Abstract. The paper provides a numerical investigation on focal ignition and flame propagation in an aluminum-air suspension. The aim of the research was to determine the apparent flame propagation velocity in the aluminum-air suspension depending on the size and mass concentration of the aluminum particles. Numerical simulation showed that the smaller the particle radius the stronger the apparent burning velocity of the suspension depends on the initial mass concentration of the aluminum powder. The obtained results qualitatively correspond to the experimental data described in the scientific papers.

1. Introduction
The dependence of the flame propagation rate in the aluminum-air suspension on the characteristics of aluminum powder has been determined in [1-6]. The work [1] provides a review of theoretical and experimental works on ignition and combustion of aluminum-air suspension in an oxidizing environment. An experimental study of the flame propagation rate in the case of oxidant-rich environment was performed in [2]. According to the results the normal flame velocity in the aluminum-air suspension varies from 0.192 to 0.25 m/s. For aluminum particles with a diameter of 4-6 μm the normal flame velocity ranges from 0.1 to 0.3 m/s at mass concentration of the particles in the air from ranged from 0.1 to 0.4 kg/m³ [3]. An increase in mass concentration of aluminum in the suspension in the predetermined range resulted in an increase in the normal propagation velocity of the combustion front. The propagation velocity of the combustion front in a tube with one open end was investigated in [4] for an aluminum-air suspension with a particle diameter of 5.4 μm. The research [4] shows that for a fuel-rich suspension the apparent flame propagation velocity comes close to the same value which is approximately equal to 0.8 m/s. A decrease in oxidant excess coefficient leads to an increase in the apparent flame propagation velocity in the air for the suspension with aluminum ASD-1 and ASD-4 [5, 6].

In the present paper we numerically investigate the problem of the combustion front propagation in aluminum-air suspension. In order to obtain a sufficiently correct result of the numerical simulation which describes the propagation velocity of the combustion front, it is necessary to involve methods of two-phase flow dynamics. The solution of the equations system describing dynamics of the two-phase flow which include the equations of mass, momentum, and energy conservation for gas and particles allows us to correctly reproduce the initial ignition period when a considerable temperature and gas pressure drop occurs in the mixture. The aim of this work was to determine the dependence of the combustion front propagation velocity in aluminum-air suspension on the size and mass concentration of aluminum particles.
2. Mathematical model

The mathematical formulation of the problem is based on [7, 8]. A monodisperse aluminum suspension with a particle mass concentration \( \rho_{kb} \) and particle size \( r_{Al0} \) is uniformly distributed in the air. There is an ignition spot with radius \( r_0 \) in the center of the particle cloud. The right boundary of the area is assumed to be infinitely remote from the ignition source. The diffusion and thermal conductivity coefficients of the gas depend on the temperature [7]. Radiation transport is neglected. Heat exchange coefficient is defined from the posture of continuum mechanics. The combustion of aluminum particles is described on the basis of experimental data [9], the ignition of an aluminum particle occurs when it reaches the ignition temperature \( T_{kz} \). The rate of a heterogeneous chemical reaction on particle surfaces is described taking into account the mass transfer [10]. The approach includes thermal and dynamic interaction between particles and the gas. As the aluminum particle burns out, the radius of aluminum in the particle \( r_{Al} \) decreases, the radius of the whole particle \( r_k \) grows due to the buildup of the oxide layer. Before the chemical reactions in the particle \( r_1 = r_{Al0} \). The mathematical formulation of the problem under the made assumptions is determined by an equation system written in a cylindrical coordinate system:

\[
\frac{\partial \rho_{g} u_{g}}{\partial t} + \frac{\partial \rho_{g} u_{g}^{2} + p}{\partial r} = -rG, \tag{1}
\]

\[
\frac{\partial \rho_{g} u_{g}}{\partial t} + \frac{\partial \rho_{g} u_{g}^{2} + p}{\partial r} = \frac{\partial}{\partial r} \left( r \lambda_{g} \left( T_{g} \right) \frac{\partial T_{g}}{\partial r} \right) - rG \left( c_{e} T_{g} + u_{g}^{2}/2 \right) - ru_{k} \tau_{w} + r \alpha_{k} n_{k} S_{k} \left( T_{k} - T_{g} \right), \tag{2}
\]

\[
\frac{\partial \rho_{g} \left( e_{g} + 0.5 u_{g}^{2} \right)}{\partial t} + \frac{\partial \left( \rho_{g} u_{g} \left( e_{g} + 0.5 u_{g}^{2} \right) + pu_{g} \right)}{\partial r} = \frac{\partial}{\partial r} \left( r \lambda_{g} \left( T_{g} \right) \frac{\partial T_{g}}{\partial r} \right) - rG \left( c_{e} T_{g} + u_{g}^{2}/2 \right) - ru_{k} \tau_{w} + r \alpha_{k} n_{k} S_{k} \left( T_{k} - T_{g} \right), \tag{3}
\]

\[
\frac{\partial \rho_{o2}}{\partial t} + \frac{\partial \rho_{o2} u_{g}}{\partial r} = \frac{\partial}{\partial r} \left( r D_{o2} \rho_{g} \left( T_{g} \right) \frac{\partial a_{o2}}{\partial r} \right) - rG, \tag{4}
\]

\[
\frac{\partial \rho_{k}}{\partial t} + \frac{\partial \rho_{k} u_{k}}{\partial r} = \frac{\partial}{\partial r} \left( r \lambda_{k} \left( T_{k} \right) \frac{\partial T_{k}}{\partial r} \right) - rG, \tag{5}
\]

\[
\frac{\partial \rho_{g} u_{g}}{\partial t} + \frac{\partial \rho_{g} u_{g}^{2}}{\partial r} = \frac{\partial}{\partial r} \left( r \lambda_{g} \left( T_{g} \right) \frac{\partial T_{g}}{\partial r} \right) - rG \left( c_{e} T_{g} + u_{g}^{2}/2 \right) - ru_{k} \tau_{w} + r \alpha_{k} n_{k} S_{k} \left( T_{k} - T_{g} \right), \tag{6}
\]

\[
\frac{\partial \rho_{g} \left( e_{g} + 0.5 u_{g}^{2} \right)}{\partial t} + \frac{\partial \rho_{g} u_{g} \left( e_{g} + 0.5 u_{g}^{2} \right) + p u_{g}}{\partial r} = \frac{\partial}{\partial r} \left( r \lambda_{g} \left( T_{g} \right) \frac{\partial T_{g}}{\partial r} \right) - rG \left( c_{e} T_{g} + u_{g}^{2}/2 \right) - ru_{k} \tau_{w} + r \alpha_{k} n_{k} S_{k} \left( T_{k} - T_{g} \right) + \frac{rQG}{\alpha_{k}} - r \alpha_{k} n_{k} S_{k} \left( T_{k} - T_{g} \right) + \frac{rG \left( c_{e} T_{g} + u_{g}^{2}/2 \right) + ru_{k} \tau_{w}}{\alpha_{k}}, \tag{7}
\]

\[
\frac{\partial n_{k}}{\partial t} + \frac{\partial n_{k} u_{k}}{\partial r} = 0, \tag{8}
\]

\[
p = \rho_{g} R_{g} T_{g}. \tag{9}
\]

\[
T_{g} \left( r, t \right) = \begin{cases} 
T_{g}, & 0 \leq r \leq r_{0} \\
T_{b}, & r_{0} < r < \infty,
\end{cases} \quad T_{k} \left( r, t \right) = T_{b}, \quad \rho_{o2} \left( r, t \right) = \rho_{o2,b}, \tag{10}
\]

\[
\rho_{k} \left( r, t \right) = \rho_{k,b}, \quad u_{g} \left( r, t \right) = u_{g} \left( r, t \right) = 0, \quad \rho \left( r, t \right) = \rho_{b}, \quad n_{k} \left( r, t \right) = n_{k,b}.
\]
\[
\frac{\partial \rho_{O_2}(0,t)}{\partial r} = \frac{\partial T_g(0,t)}{\partial r} = \frac{\partial \rho(0,t)}{\partial r} = \frac{\partial \rho_k(0,t)}{\partial r} = 0,
\]
\[
\frac{\partial n_k(0,t)}{\partial r} = \frac{\partial T_k(0,t)}{\partial r} = 0, u_k(0,t) = u_g(0,t) = 0,
\]
\[
\frac{\partial \rho_{O_2}(\infty,t)}{\partial r} = \frac{\partial T_g(\infty,t)}{\partial r} = 0. \tag{11}
\]

The following notations are used in (1) – (11): \(t\) – time, \(r\) – radius coordinate, \(\rho_g\), \(\rho_{O_2}\) – gas and oxygen partial density, \(\rho_k\) – aluminum particle mass per unit volume, \(u\) – velocity, \(r_k\) – particle radius, \(n_k\) – particle count, \(p\) – pressure, \(\lambda\) – thermal conductivity coefficient, \(\lambda = \lambda_o (T/T_o)^{2/3}\), \(D\) – diffusion coefficient, \(D_g(T_g) = \lambda_s(T_g)/(c_p \rho_g)\), \(Q\) – the heat of the reaction on the surface, \(T\) – temperature, \(\eta\) – the absolute viscosity coefficient of the gas. \(\alpha_g = N_u \lambda_g/(2 r_k)\) – the gas-particles heat exchange coefficient, \(\varepsilon_g = p/(\rho_g (\gamma - 1))\) – the gas internal energy, \(\gamma = c_p/c_v\) – the adiabatic exponent, \(\varepsilon_k = c_k T_k\) – the particle internal energy, \(G\) – the rate of particle mass changing during the combustion, \(S_k = 4 \pi r_k^2\) – particle surface area, \(S_m = \pi r_k^2\) – particle cross-sectional area, \(\tau_v = n_k F_v\) – friction force, \(F_v = C_s S_m \rho_g (u_g - u_k) \left| u_g - u_k \right|/2\) – the interaction force of a single particle with the gas, \(C_r = 24 \left(1 + 0.15 \text{Re}^{0.682}\right)/\text{Re}\) – friction coefficient, \(\text{Re}\) – Reynolds number, \(\text{Nu}_k = 2 + \left(\text{Nu}_l^2 + \text{Nu}_r^2\right)^{1/2}\) – Nusselt number, where \(\text{Nu}_l = 0.664 \text{Re}^{0.5}\), \(\text{Nu}_r = 0.037 \text{Re}^{0.8}\) [8], \(\alpha_o\) – the oxygen stoichiometric coefficient in reaction with aluminum particles. Indexes: \(b\) – the initial values of the parameters, \(k\) – the particle parameters, \(g\) – the gas parameters, \(Al\) – the aluminum parameters inside the oxide layer.

The summands on the right side of equations (1) - (8) which is responsible for the chemical interaction of the gas and particles depend on the radius of aluminum inside the oxide layer of the particle. The summands responsible for the inertial and thermal interaction are defined by the radius of the whole particle consisting of aluminum and oxide layer. To determine the rate of mass change of the particles during their combustion we assume that the combustion product of aluminum is the oxide \(\text{Al}_2\text{O}_3\), which envelops the particle; the particle density does not change during the combustion. The radius of the unreacted part of aluminum in the particle is determined by:

\[
r_{al} = \left[\left(\frac{\mu_o + 3/2 \mu_o}{\mu_{al}}\right) r_{al,0}^3 - \frac{\rho_k}{(4/3) \pi n \rho_k^0}\right]^{1/2}, \tag{12}
\]

where \(\mu_o\), \(\mu_{al}\) are oxygen and aluminum molar masses.

The equation of the particle radius \(r_k\) taking into account that it consist of unreacted aluminum and oxide layer \(\text{Al}_2\text{O}_3\) is:

\[
r_k = \sqrt[3]{\frac{3 \rho_k}{4 \pi \rho_k^0 n_k}}. \tag{13}
\]

The detailed derivation of the equations (12) – (13) is presented in [8].

Accounting the diffusional resistance of the reaction the rate of the particle mass change has the following form:
\[ G = \alpha, p_0, \rho_0 S_{al} \frac{k(a_{O_2} r_{al})}{k(a_{O_2} r_u) + \beta_k} \]

where \( k(a_{O_2} r_{al}) = k_0 a_{O_2}^{\alpha} / \sqrt{r_{al}} \) — the combustion law of a single particle in the oxidant-rich environment, \( S_{al} = 4\pi r_{al}^{2} \) — area of the unburnt aluminum in the particle, \( k_0 \) — the constant of the chemical reaction rate, \( \beta_k = \lambda_k(T) N_{D}/\left(c_g \rho_k r_k^{\beta} \right) \) — particle mass-transfer coefficient, \( \rho_k^{\beta} \) - aluminum density.

The problem (1) – (14) was solved numerically by S.K. Goduvov’s method [11]. The solution of the equations for particles was carried out using the decay of discontinuity algorithm in an environment without its ‘own’ pressure [12]. A detailed technique of the numerical solution is described in [7].

3. Results and discussion

The value \( k_0 \) in combustion law (14) is set to provide the equality of calculated and experimental [1] normal combustion rate for the suspension with particle radius of 2 \( \mu m \). The calculated results are in a good agreement with experimental data [1] for aluminum particle mass concentration \( \rho_{ab} = 0.1 \pm 0.3 \) kg / \( m^3 \) and fitted value \( k_0 = 1.11 \times 10^{-6} \) \( m^{1.5} / \) s. Other physical parameters used in the calculation were: \( Q = 36.6 \) \( MJ/kg \), \( \alpha = 0.889 \), \( \lambda_{al} = 0.025 \) \( W/(m \cdot K) \), \( \mu_{al} = 27 \times 10^{-3} \) \( kg/mol \), \( \mu_0 = 16 \times 10^{-3} \) \( kg/mol \), \( \gamma = 1.39 \), \( c_{pg} = 1065 \) \( J/(kg \cdot K) \), \( c_{vg} = 768.2 \) \( J/(kg \cdot K) \), \( c_k = 904 \) \( J/(kg \cdot K) \), \( T_b = 300 \) \( K \), \( \rho_k^{\beta} = 2380 \) \( kg/m^3 \), \( \eta = 2 \times 10^{-5} \) \( Pa \cdot s \), \( \rho_{O_2,b} = 0.264 \) \( kg/m^3 \), \( \rho_b = \rho_p / R_g T_b \), \( p_b = 0.1 \) \( MPa \).

The size of the ignition spot was set to \( r_i = 2 \times 10^{-3} \) \( m \). The initial particle radius varied within the range of \( r_i = r_{d,0} = 2 \times 10^{-7} \pm 4 \times 10^{-6} \) \( m \), particle mass concentration was \( \rho_{ab} = 0.07 \pm 0.3 \) \( kg/m^3 \). The results of the calculations are presented in figures 1–4.

**Figure 1.** Temperatures of the gas and particles (a), radius of unburnt aluminum (solid line) and whole particle (dotted line) (b), time interval \( \Delta t = 10^{-3} \) \( s \), \( r_{d,0} = 6 \times 10^{-7} \) \( m \).
Figures 1 – 2 show the gas and particles temperature distributions (1a, 2a) and the radius of unburnt aluminum and particles (1b, 2b) changing in time with the interval $\Delta t = 10^{-3} \text{s}$. Figure 1 is plotted for the case of focal ignition of an Al-air suspension with particle radius $r_{d,0} = 6 \cdot 10^{-7} \text{m}$, figure 2 – $r_{d,0} = 2 \cdot 10^{-7} \text{m}$. The initial mass concentration of the particles in cases 1, 2 was equal to $\rho_{kb} = 0.09 \text{kg/m}^3$. Gas and particles temperatures in the end of the calculation are close to each other, there is no visible difference between gas and particles temperature curves in figures 1a and 2a.

The smaller is the particle radius, the higher is the apparent propagation velocity of the flame front in the suspension. The calculated apparent propagation velocity of the combustion front in the suspension with particles radius $r_{d,0} = 6 \cdot 10^{-7} \text{m}$ (figure 1) is $u_f = 1.2 \text{m/s}$, the normal propagation velocity of the combustion front is $u_n = 0.05 \text{m/s}$. For particle radius $r_{d,0} = 2 \cdot 10^{-7} \text{m}$ (figure 2) the apparent propagation velocity is $u_f = 2.8 \text{m/s}$, the normal propagation velocity is $u_n = 0.07 \text{m/s}$.

![Figure 2. Temperatures of the gas and particles (a), radius of unburnt aluminum (solid line) and the whole particle (dotted line) (b), time interval $\Delta t = 10^{-3} \text{s}$, $r_{d,0} = 2 \cdot 10^{-7} \text{m}$.](image)

![Figure 3. Apparent flame propagation velocity-initial particle mass concentration curve $r_{d,0} = 0.5 \cdot 10^{-6} \text{m}$ (1), $r_{d,0} = 3.25 \cdot 10^{-6} \text{m}$ (2).](image)

![Figure 4. Apparent flame propagation velocity-initial particle radius curve $\rho_{kb} = 0.15 \text{kg/m}^3$.](image)
The dependence of the apparent flame propagation velocity in the monodisperse Al-air suspension on the size and mass concentration of the particles was determined by a series of parametric studies. The results are presented in figures 3, 4.

According to the obtained results the smaller is the particle radius the stronger the apparent flame propagation velocity depends on the initial mass concentration of aluminum in the suspension. As the initial particle size increases the apparent flame propagation velocity in the Al-air suspension tends to the same value regardless of the particle radius.

The obtained results qualitatively correspond to the experimental data presented in [1 – 6]. The effect of particle size on the apparent flame propagation velocity in an aluminum-air suspension coincides with the data from the scientific papers. The results described in this paper show the combustion regularities of the particles in case of oxidant-rich combustion.

4. Conclusions
We have numerically investigated the flame propagation in an aluminum-air suspension. It has been shown that the mass concentration and size of the aluminum particles in a suspension influences the apparent flame propagation velocity of the combustion front. The increase in size of the particles leads to the decrease of the apparent flame propagation velocity meanwhile its value converge to the same constant magnitude which does not depend on the particle size.

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