Numerical Modeling of Falling Aluminum Particle Oxidation in Air

Dr. A. Davidy[1]
[1]Israel Military Industry (IMI)
*Corresponding author contact: POB. 1044/66 Ramat-Hasharon, ISRAEL, 47100, alon.davidy@gmail.com

Abstract: Aluminum because of its high enthalpy of combustion has been added to energetic materials. Several research efforts have been directed to understand the mechanism and model the oxidation of aluminum particles. In this work, a two dimensions and time dependent thermal model is developed and assessed to describe the interrelated processes of Aluminum particle oxidation. The thermal model consists of thermal radiation, forced convection and thermal conduction and oxygen diffusion and surface reactions. It is assumed the aluminum particle is coated with Aluminum oxide layer.

Keywords: Aluminum particle**,** Combustion, Oxygen diffusion, diffusion equation, Navier Stokes equation.

1. Introduction

Extensive research on the burning of aluminum particles has been conducted since the early 1960s. Aluminum powder additives have found use in applications ranging from enhancing the specific motor thrust for propellants in rocket motors to the formulation of advanced energetic materials[1] for the design of decoy flares[2].

The ignition of Aluminum particles begins with short heterogeneous combustion and quickly transitions to a quasi steady state diffusion flame[1]. In this work, the two-dimensional combustion of a single aluminum particle free falling in air is studied numerically, including the physical processes of finite oxygen diffusion, surface reactions coupled with forced convection.

2. Model Formulation

In this study, the following has been assumed[3]:
1) The particle is spherical
2) The change in particle diameter is small during combustion (due to oxide deposition)
3) Flow around the particle is laminar
4) The flame has spherical symmetry
5) The aluminum particle is coated with oxide layer
6) The inner diameter of the particle is 10 μm and the outer diameter of the aluminum is 20 μm.

The equation of motion of the falling aluminum particle is:

$$m_p g = \frac{1}{8}\rho_g C_D D_{p,out}^2 u_p^2 \qquad (1)$$

Where m_p is the particle mass, g is the gravity acceleration, ρ_g is the air density, $D_{p,out}$ is the external diameter of the particle and u_p is the particle velocity. C_D is the drag coefficient. This term is calculated from the following empirical equation[1]:

$$C_D = \begin{cases} 24\left(1+\mathrm{Re}_p^{2/3}/6\right)/\mathrm{Re}_p & \text{for } \mathrm{Re}_p \le 1000 \\ 0.424 & \text{for } \mathrm{Re}_p > 1000 \end{cases} \qquad (2)$$

Re_p is Reynolds number of the particle. This term is calculated from:

$$\mathrm{Re}_p = \frac{D_{p,out}\rho_g u_p}{\mu_g}$$

Figure 1 shows the value of the Drag coefficient as a function of particle velocity.

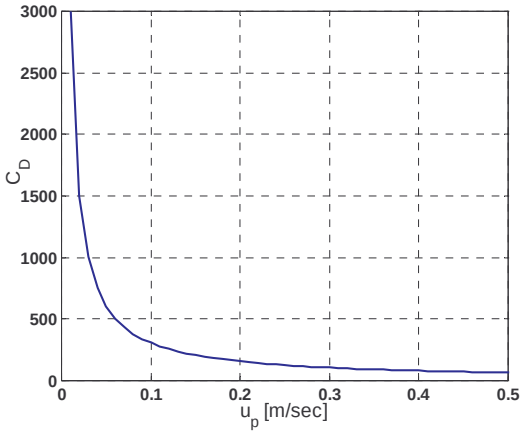

Figure 1: Particle drag coefficient as a function of velocity.

In the first phase, a simple MATLAB is developed in order to calculate the particle motion equation (see equation (1)). By using trial and error technique, It was found that the particle velocity is $u_p = 0.0276\,\mathrm{m/s}$. The convection coefficient was calculated according to following equation[1]:

$$h_{conv} = \frac{2k_g}{D_{p,out}}\left[1 + Re_p^{1/2}\,Pr_g^{1/3}/3\right]$$

$$= 4597.6\,\frac{W}{m^2 \cdot K}$$

Where k_g is the thermal conductivity of the air, Pr_g is the Prandtl number of the particle, and $D_{p,out}$ id the outer diameter of the particle. In the second phase, the COMSOL software solved the Continuity, Navier-Stokes, mass balance and heat conduction equation. The solution provides the structure of the diffusion layer and the temperature field inside the burning Aluminum particle from the simultaneous solution of these equations. Figure 2 shows a schematic representation of the coated particle. The gas is introduced at the bottom of the model and exits at the top. Symmetry is assumed at the vertical boundaries, implying symmetry in the *y*-axis and that the modeled unit cell is typical for the system. Furthermore, it has been assumed that the density of the air does not change due to the chemical reaction between the particle and the oxygen.

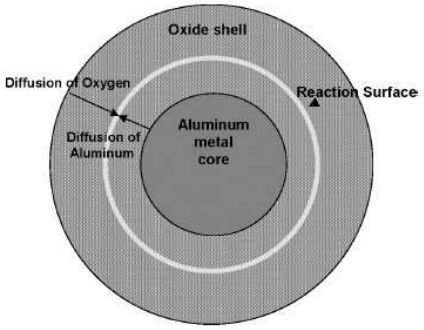

Figure 2: Schematic of an oxide-coated aluminium particle showing the metal core, oxide shell and the dynamic reaction surface[4].

The equations that describe the fluid flow in the free fluid sub-domain, are the momentum transport equation and the mass transport equation

$$\frac{\partial \rho}{\partial t} + \eta \nabla^2 u + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p = 0 \qquad (3)$$

$$\nabla \cdot \mathbf{u} = 0 \qquad (4)$$

Where η denotes the dynamic viscosity, **u** is the velocity vector, ρ is the density of the fluid, and p denotes the pressure. To couple the equations of motion to the mass transport equation, for the reactant in the fluid at transient state, we use the following equation:

$$\frac{\partial c}{\partial t} + \nabla(-D\nabla C) + u\nabla c = 0 \qquad (5)$$

Where D denotes the diffusion coefficient and c is the oxygen concentration. The expression within parentheses on the left side is the flux vector for the reacting species.

The heat conduction equation in the Solid phase is:

$$\rho c_p \frac{\partial T}{\partial t} + \nabla(-k_{solid}\nabla T) = 0 \qquad (6)$$

The mass and heat balance at external boundary of the particle surface are:

$$\nabla \cdot (-D\nabla c) - kc^2 = 0 \quad (7)$$

Where D denotes the diffusion coefficient in the particle and k is the rate constant for the second order reaction.

$$-n(-k_{solid}\nabla T) = h_{conv}(T_f - T) + \varepsilon\sigma\left(T_0^4 - T^4\right) \quad (8)$$

Where k_{solid} denotes the thermal conductivity of the Alumina.

3. Input Parameters for the Model

It is assumed that the following chemical reaction occurred between the Aluminum particle and the Oxygen[3]:

$$AlO + O_2 \rightarrow AlO_2 + \frac{1}{2}O_2 \quad (9)$$

Where the reaction rate constant is calculated from the Arrhenius equation[6]:

$$k = 4.63E+8 \cdot \exp(-10{,}008/T) \left[m^3/mole \cdot s\right] \quad (10)$$

For the equations of motion, the following boundary conditions apply[5]:

$$\begin{aligned} &\mathbf{u}\cdot\mathbf{n} = v_0 && \text{at } \partial\Omega_{inlet} \\ &u \cdot n = 0 && \text{at } \partial\Omega_{ff,1} \text{ and } \partial\Omega_{ff,2} \\ &u = (0,0) && \text{at } \partial\Omega_{pl,1} \\ &p = 0 && \text{at } \partial\Omega_{outlet} \end{aligned} \quad (11)$$

Where $\partial\Omega_{pl}$ is a subdomain boundary, because the Navier-Stokes and Continuity equations are not defined in the particle domain. To find the boundary conditions for the mass transport equation, we assume that the inlet oxygen concentration is known. In addition, we assume that the reactant transport, in the gas at the outlet, is mainly driven by convection, that is, we neglect diffusion in the main direction of the convective flow:

$$\begin{aligned} &c = c_0 && \text{at } \partial\Omega_{inlet} \\ &(-D\nabla c + c\mathbf{u})\cdot\mathbf{n} = 0 && \text{at } \partial\Omega_{ff,1} \text{ and } \partial\Omega_{ff,2} \\ &(-D\nabla c)\cdot\mathbf{n} = 0 && \text{at } \partial\Omega_{pl,1} \\ &(-D\nabla c + c\mathbf{u})\cdot\mathbf{n} = c\mathbf{u}\cdot\mathbf{n} && \text{at } \partial\Omega_{outlet} \end{aligned} \quad (12)$$

The input parameters are shown in Table 1.

Table 1: Input parameters values.

Parameter	Value	Unit
ρ	0.66	kg/m^3
η	2.6E-5	$\frac{kg}{m\cdot s}$
c_0	0.2	$\frac{mol}{m^3}$
D	7.4E-9	$\frac{m^2}{s}$
D_p	10	μm
$D_{p,out}$	20	μm
k	1106.3	$\frac{m^3}{mol\cdot s}$
k_g	0.044	$\frac{w}{m\cdot K}$
Pr_g	0.668	-
v_0	0.0276	$\frac{m}{s}$

The thermophysical properties of the Alumina and Aluminum material are shown in Table 2.

Table 2: Thermophysical properties of Alumina and Aluminum materials.

Parameter	Value	Unit
$\rho_{Al_2O_3}$	3,900	kg/m^3
$k_{Al_2O_3}$	27	$\frac{w}{m \cdot K}$
$c_{p\,Al_2O_3}$	900	$\frac{J}{kg \cdot K}$
ρ_{Al}	2,700	kg/m^3
k_{Al}	160	$\frac{w}{m \cdot K}$
$c_{p\,Al}$	900	$\frac{J}{kg \cdot K}$

Dreizin[7] found that the combustion of aluminum particles free falling in air has three stages: stable, strong oscillation and weak combustion stage. The current study investigates the first stage of combustion. In this study, the flame temperature is 2,559 K[2], and the particle falling velocity is 0.0276m/s. Figure 3 shows that the maximum velocity occurs in the contraction between the particle and the symmetry line on the right side.

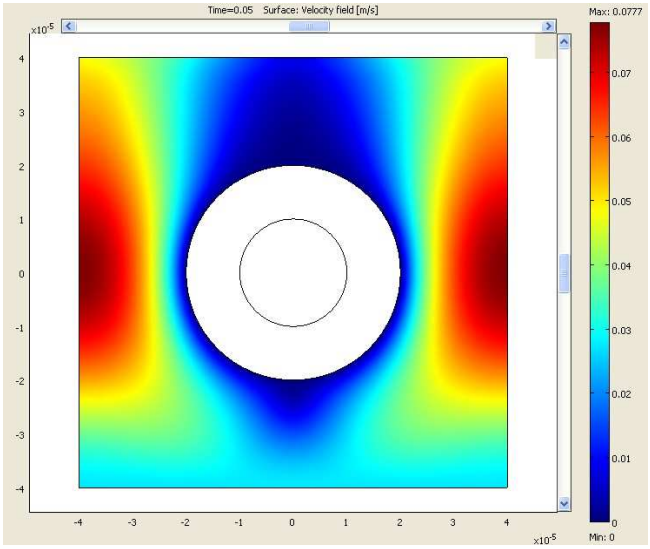

Figure 3: Oxygen velocity field around the aluminum particle at t=0.05 sec.

From Figure 3 it is shown that there are two stagnation zones in front and behind the particle. Figure 4 shows the oxygen concentration field around the burning aluminum particle.

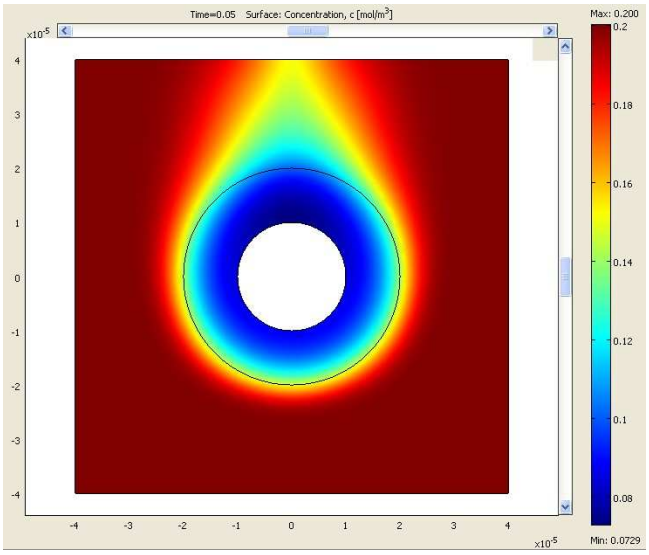

Figure 4: Oxygen concentration field around the aluminum particle at t=0.05 sec.

Figure 5 shows the temperature field around the burning aluminum particle.

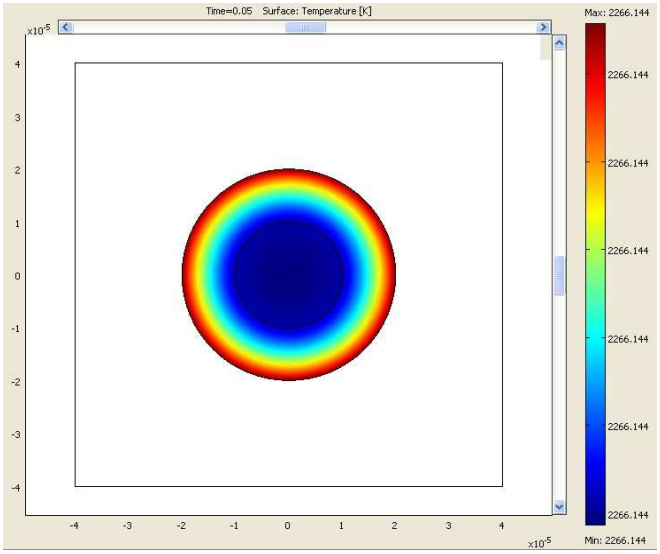

Figure 5: Temperature field inside the aluminum particle at t=0.05 sec.

4. Summary and Conclusions

Several research efforts have been directed to understand the mechanism and model the oxidation of aluminum particles. In this work, a two dimensions and time dependent thermal model was developed and assessed to describe the interrelated processes of Aluminum particle oxidation. The thermal model consists of thermal radiation, forced convection and thermal conduction and oxygen diffusion and surface reactions. It is assumed the aluminum particle is coated with Aluminum oxide layer.

The current study investigates the first stage of combustion. In this study, the flame temperature is 2559 K, and the particle falling velocity is 0.02761m/s. In this study, the following has been assumed[3]:

1) The particle is spherical
2) The change in particle diameter is small during combustion (due to oxide deposition)
3) Flow around the particle is laminar
4) The flame has spherical symmetry
5) The aluminum particle is coated with oxide layer
6) The inner diameter of the particle is 10 μm and the outer diameter of the aluminum is 20 μm.

It has been found out that there are stagnation zones in front and behind the particle

5. References

1. DesJardin Paul .E., Felske James D., & Carrara Mark D. Mechanistic Model for Aluminum Particle Ignition and Combustion in Air, JOURNAL OF PROPULSION AND POWER, **21**, 478-485 (2005).
2. Koch E. C., Pyrotechnic Countermeasures II, Advanced Aerial Infrared Countermeasures, Propellants, Explosives, Pyrotechnics, **31**, 3-19 (2006).
3. Liang, Y. & Beckstead, M.W., Numerical Simulation of Quasi-Steady, Single Aluminum Particle Combustion in Air, AIAA-1998-0254.
4. Rai, A., Park, K. Zhou, L. & Zachariha, M.R., Understanding the mechanism of aluminum nanoparticle oxidation, Combustion Theory and Modeling, **10**, No. 5, 843–859 (2006).
5. Anonymous, COMSOL Multiphysics – Chemical Engineering Module. Version 3.2, September 2005.
6. Bucher, P., Yetter, R.A., Dryer, F.L., Parr, T.P., Hanson, Parr, D.M. & Vicenzy, E.P., Flame Structure Measurement of Single Isolated Aluminum Particles Burning in Air, 26th Symposium International Conference (1996).
7. Dreizin, E.L., Experimental study of stages in aluminum particle combustion in air, Combstion & Flame **105**, 541-556 (1996).