Numerical Modeling of Falling Aluminum Particle Oxidation in Air

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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 for the design of decoy flares.

Composition of Decoy Flare

<table>
<thead>
<tr>
<th>Composition No. 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>● Magnesium</td>
</tr>
<tr>
<td>● Aluminium</td>
</tr>
<tr>
<td>● Boron</td>
</tr>
<tr>
<td>● Urotropine</td>
</tr>
<tr>
<td>● Ammonium perchlorate</td>
</tr>
<tr>
<td>● Potassium nitrate</td>
</tr>
<tr>
<td>● PTFE</td>
</tr>
<tr>
<td>● Viton®</td>
</tr>
</tbody>
</table>
Model’s Assumptions

In this study, the following assumptions have been assumed:

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.
Calculation of the Particle Velocity

The equation of motion of the falling particle is:

\[ m_p g = \frac{1}{8} \rho g C_D D_p^{2, \text{out}} u_p^2 \]  \hspace{1cm} (1)

The Drag coefficient of the particle is:

\[ C_D = \begin{cases} 
24 \left( 1 + \frac{Re_p^{2/3}}{6} \right) / Re_p & \text{for } Re_p \leq 1000 \\
0.424 & \text{otherwise}
\end{cases} \]  \hspace{1cm} (2)
The Flow Equations and Boundary Conditions

The Navier Stokes equations equations is:

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

The continuity equation:

\[ \nabla \cdot \mathbf{u} = 0 \]  \( )4( \)

The boundary equation for these equations are:

\[ \mathbf{u} \cdot \mathbf{n} = v_0 \]  at \( \partial \Omega_{\text{inlet}} \)
\[ \mathbf{u} \cdot \mathbf{n} = 0 \]  at \( \partial \Omega_{\text{ff,1}} \) and \( \partial \Omega_{\text{ff,2}} \)
\[ \mathbf{u} = (0,0) \]  at \( \partial \Omega_{\text{pl,1}} \)
\[ p = 0 \]  at \( \partial \Omega_{\text{outlet}} \)
The Diffusion Equation and Boundary Conditions

The Oxygen diffusion equation is:

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D \nabla c + cu) = 0$$  \hspace{1cm} (6)$$

The boundary conditions are:

$$c = c_0 \quad \text{at } \partial \Omega_{\text{inlet}}$$  \hspace{1cm} (7)$$

$$(-D \nabla c + cu) \cdot n = 0 \quad \text{at } \partial \Omega_{\text{ff,1}} \text{ and } \partial \Omega_{\text{ff,2}}$$

$$(-D_{\text{eff}} \nabla c) \cdot n = 0 \quad \text{at } \partial \Omega_{\text{pl,1}}$$

$$(-D \nabla c + cu) \cdot n = cu \cdot n \quad \text{at } \partial \Omega_{\text{outlet}}$$
The Heat Conduction and Boundary Conditions

The heat conduction equation is:

\[ \rho c_p \frac{\partial T}{\partial t} + \nabla (-k_{\text{solid}} \nabla T) = 0 \]  

(8)

The boundary conditions is:

\[ -n(-k_{\text{solid}} \nabla T) = h_{\text{conv}} (T_f - T) + \varepsilon \sigma (T_0^4 - T^4) \]

(9)

Where:

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

\[ = 4597.6 \frac{W}{m^2 \cdot K} \]
Model’s Assumptions

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

\[ \text{AlO} + \text{O}_2 \rightarrow \text{AlO}_2 + \frac{1}{2}\text{O}_2 \]

Where the reaction rate constant is calculated from the Arrhenius equation:

\[ k = 4.63 \times 10^8 \exp\left(-\frac{10,008}{T}\right) \left[ m^3/mole \cdot sec \right] \]

### Input Parameters Values

<table>
<thead>
<tr>
<th>Name</th>
<th>Expression</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>rho</td>
<td>0.66</td>
<td>0.66</td>
<td>Density [kg/m^3]</td>
</tr>
<tr>
<td>eta</td>
<td>2.6e-5</td>
<td>2.6e-5</td>
<td>Dynamic viscosity [kg/(m*sec)]</td>
</tr>
<tr>
<td>D</td>
<td>7.4E-9</td>
<td>7.4e-9</td>
<td>Diffusion coefficient [m^2/s]</td>
</tr>
<tr>
<td>Deff</td>
<td>7.4e-9</td>
<td>7.4e-9</td>
<td>Effective diffusion coefficient [m^2/sec]</td>
</tr>
<tr>
<td>k</td>
<td>1106.3</td>
<td>1106.3</td>
<td>Rate constant [m^3/(s*mol)]</td>
</tr>
<tr>
<td>v0</td>
<td>0.001</td>
<td>0.001</td>
<td>Inlet velocity [m/s]</td>
</tr>
<tr>
<td>c0</td>
<td>0.2</td>
<td>0.2</td>
<td>Inlet concentration [mol/m^3]</td>
</tr>
</tbody>
</table>
Oxygen velocity field around the aluminum particle at $t=0.05$ sec
Oxygen concentration field around the aluminum particle at t=0.05 sec
Temperature field inside the aluminum particle at t=0.05 sec
Concluding Remarks

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.
Thank You for Your Attention

Questions?