Numerical Simulation of TNT-Al Explosives in Explosion Chamber

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Abstract: The Numerical modeling of burning particles burning, initiated from a heavily aluminized HE is being investigated. Reactive multiphase flows must be modeled to properly account for variable-size aluminum particles burning behind the blast wave. The governing equations also include models for solid evaporation and chemical reactions. The final paper will present comparison of experimental data and computational results of mixed TNT-Al detonation and burning in a closed chamber.

Keywords: Computational Fluid Dynamics, Blast Wave, Afterburning, Multi-phase Flow

1 Introduction

Aluminum particles are often mixed into solid propellants or explosives to enhance energy release. However the aluminum particle burning mechanism is very complicated because of its evaporation and slower reaction time, especially for cased weapons. A numerical analysis of heavily aluminized explosive is very important for its safety usage. Reactive multiphase flow models have been incorporated into the usual Euler equations to model this phenomenon. The purpose of this research is to develop numerical models to treat the burning of multiple-sized aluminum particles burning behind the initial blast wave.

2 Governing Equations and Chemical Reaction Modeling

The governing equations are as follows:

\[ \frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} = S_1 + S_2 + S_3 \]  

\[ Q = \begin{bmatrix} \rho_{\phi} \\ \rho_{\phi, e} \\ \rho_{\phi, u} \\ \phi_{\rho, u} \\ \phi_{\rho, E} \\ N_{p} \end{bmatrix}, \quad E = \begin{bmatrix} \rho_{\phi}u \\ \rho_{\phi, e}u \\ \rho_{\phi, u}^2 + P \\ \phi_{\rho, u}u \\ \phi_{\rho, E}u \\ N_{p}u \end{bmatrix}, \quad S_1 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad S_2 = \begin{bmatrix} \frac{1}{1 - \phi_e} \Delta c (1 - \frac{\rho_e}{\rho}) + \phi_e \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad S_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \]
The interphase mass exchange factor $\Delta c$ (the evaporation rate) can be written as follows:

$$\Delta c = (3\phi, \rho, / \tau)(1 + 0.276\sqrt{Re}) \text{ for } T > T_{\text{ignition}} \quad (2)$$

We considered 7 reactions and 10 species in this study as follows:

$$\begin{align*}
\text{Al} + \frac{3}{4} \text{O}_2 & \rightarrow \frac{1}{2} \text{Al}_2\text{O}_3 \quad (\text{if } T < 3500 \text{ K}) \quad (3) \\
\text{Al} + \frac{1}{2} \text{O}_2 & \rightarrow \text{AlO} \quad (\text{if } T > 3500 \text{ K}) \quad (4) \\
\text{Al} + \frac{1}{2} \text{H}_2\text{O} & \rightarrow \frac{1}{2} \text{Al}_2\text{O}_3 + \frac{1}{2} \text{H}_2 \quad (5) \\
\text{Al} + \frac{1}{2} \text{CO}_2 & \rightarrow \frac{1}{2} \text{Al}_2\text{O}_3 + \frac{1}{2} \text{C} \quad (6) \\
\text{H}_2\text{O} + \frac{1}{2} \text{O}_2 & \rightarrow \frac{1}{2} \text{H}_2 \quad (7) \\
\text{C} + \frac{1}{2} \text{O}_2 & \rightarrow \text{CO} \quad (8) \\
\text{CO} + \frac{1}{2} \text{O}_2 & \rightarrow \text{CO}_2 \quad (9)
\end{align*}$$

### 3 Computed example

Figure 1 shows the computed solution at a given time for the detonation and burning of a heavily aluminized HE in confined room. The computed results using the new methodology agreed well with experimental data.

![Computed solution](image)

**Figure 1**: Computed velocity Gouraud shading of Abs. Velocity and Pressure & Impulse history inside the room (Blue: Experiment, Magenta: Computation with Al burning model, Green: Computation without Al burn)

### 4 Future Work

In the final paper, significantly more complex scenarios, involving boxed pre-mixed TNT-Al and TNT-surrounded by an Al shell, will be presented. These tests were conducted in a detonation chamber. The computed results will be compared with experimental data.

### References
