Effect of Aerodynamic Breakup on Combustion of Aluminum Particles from Heterogeneous Explosives

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1 Introduction

Heterogeneous blast explosives contain a mixture of condensed-phase explosive, binders, and metal particles. Most often aluminum particles are used for their high heat of combustion when reacted with atmospheric air. Micrometric-sized particles are large enough that they do not react significantly within the detonation zone of the explosive itself, rather they are accelerated and heated by shock compression and are dispersed into the surrounding environment where their reaction may augment the air blast. Most aluminum particles feature a thin passive oxide coating, which is presumed to be cracked or removed by the detonation shock. The remaining pure aluminum particles have a relatively low melting point (933 K at 1 bar) that is easily reached by shock compression heating during detonation of the explosive and convective heating in the detonation products and shocked air. Molten and liquid particles may become unstable under conditions of high relative flow and may possibly fragment through aerodynamic breakup. The melting behavior of the particles under high pressures and the feasibility of subsequent breakup in the initial expansion flow could be critical for the efficient reaction of aluminum particles in the very near-field of detonation of such heterogeneous explosives.

Numerical modeling of aluminized explosives near structures [1, 2] has shown that aerodynamic breakup of molten particles and liquid metal droplets is one of the most significant factors affecting the resulting heterogeneous blast pressure. For the catastrophic droplet breakup mechanism in high relative flow conditions, the resulting fragment droplets are typically 10 times smaller in normalized diameter with a corresponding factor of 1000 increase in number density. The post-breakup size substantially increases the reaction rate in addition to the momentum and heat transfer rates. The burn time becomes significantly different according to $t_b \sim d_{p0}^n$, where $n \leq 2$, since d_{p0} becomes the fragment size, or the rate may become limited by kinetics for small d_{p0} . The increased convective heating rate leads to prompt ignition and reaction of the metal particles. The consequence of higher drag controls whether or not the particles escape the detonation products to reach the air, and therefore

further influences the reaction, since the aluminum reaction rate in the detonation products (CO, CO_2 , and H_2O) and the heat release contribution to the blast are less than those with atmospheric O_2 .

While recent modeling studies have demonstrated the importance of the aerodynamic breakup of metal particles on the resulting heterogeneous blast loading, a number of thermophysical parameters have traditionally been considered as constant, including the heat capacity, liquid surface tension, and melting temperature. The conditions within the condensed heterogeneous matter detonation zone feature pressure levels typically above 100 kbar. At the edge of the charge, the detonation shock transmits into a very strong air shock which decays from 100 kbar to 1 kbar within one charge radius, where the shocked air temperature exceeds 3000 K and gas dissociation effects are significant. The blast pressure further decays to just 10 bar within ten charge radii and the shocked air temperature falls below 1000 K in the absence of particle reaction. Within this transient region of rapid expansion and transition from detonation pressure to air blast, the assumption of constant melting and evaporation temperatures for metal particles becomes inappropriate and may affect the aerodynamic breakup and subsequent combustion. This paper presents a model for high pressure melting of aluminum particles and the subsequent aerodynamic breakup of liquid droplets in the abovementioned transition region from detonation region sexplosives.

2 High-Pressure Melting of Aluminum Particles

The melting point of a metal particle in a surrounding gas at elevated pressure, p_g , may be represented using the Clausius-Clapeyron equation: $T_m = L_m/R \ln(p^*/p_g)$ where L_m is the latent heat of fusion, R is the gas constant, and p^* is a reference pressure. Jayaraman et al. [3] and Lees and Williamson [4] both measured the increase in the melting temperature of aluminum to be nearly linear with pressure in a range up to 45 kbar and 60 kbar, respectively. Experimental data from Lees and Williamson [4] indicates that the melting temperature of aluminum increases to 1320 K at 60 kbar. Shocked particle morphology tests of micrometric aluminum particles saturated in a liquid [5] showed that aluminum particles did not melt during shock compression to pressure levels of 290 kbar within a 1 µs load duration, consistent with elevated melting temperature at high pressure.

Moriarty et al. [6] investigated the aluminum melting curve up to 2000 kbar with first principles calculations using a generalized pseudo-potential theory (GPT). Their theoretical prediction is in good agreement with the experimental data from Lees and Williamson as shown in Figure 1. Using a linear fitting to the data of Lees and Williamson and the prediction from Moriarty et al., a correlation for the high pressure melting curve is therefore suggested:

$$T_m = T_{m0} + p/p$$

where $T_{m0} = 933$ K and $p^* = 150$ bar, and the correlation is assumed to be valid for $p \le 100$ kbar. The model shows the melting temperature of aluminum is 1000 K at 10 kbar and 1600 K at 100 kbar. In the higher pressure regime (p > 100 kbar) polynomial fitting to theory of Moriarty et al. [6] can be used for $p \le 1.5$ Mbar. The upper limit of aluminum melting is dictated through a high-pressure evaporation curve by Gonor [7].



Fig. 1. Aluminum melting curves [6]

3 Aerodynamic Breakup of Aluminum Particles

Aerodynamic breakup has traditionally been correlated to the non-dimensional Weber number, $We = \rho_g |u_g - u_p|^2 d_{p0}/\gamma$, where ρ_g is the gas density, $|u_g - u_p|$ is the slip velocity, and γ is the liquid surface tension.

Ripley, R. C.

For conventional liquid droplets, the limit of stability is $We^* = 12 - 20$ which indicates that the surface tension is insufficient to maintain a coherent droplet shape and breakup occurs [8]. For conditions of aluminum/alumina agglomerates in the combustion products of a propellant, the critical Weber number has been suggested to be $We^* = 20 - 30$ [9].

According to the fact that the mass median droplet fragment size is on the order of half of the stable droplet diameter [8], a model used in the numerical implementation is:

$$d_{frag} = \frac{1}{2} \max\left(We^* \frac{\gamma}{\rho_g |u_g - u_p|^2}, \frac{d_{p0}}{10^2} \right) \quad \text{if } \Delta t_{We > We^*} > \tau_b \frac{d_{p0}}{|u_g - u_p|} \sqrt{\frac{\rho_p}{\rho_g}}$$

where ρ_p is the particle solid density and τ_b is a non-dimensional breakup time ($\tau_b = 4$ to 5 based on aerodynamic breakup in a shock wave). For micrometric aluminum particles, the absolute breakup time is typically less than 10 µs. A lower bound of $d_{frag}/d_{p0} \sim 10^{-2}$ represents the limiting fragment size from the data of Piltch and Erdman [10], which occurs for We > 1000. The above fragment size is applied as an average size for a subgroup of the large number of Lagrange particle group sets and the fragments resulting from aerodynamic breakup therefore feature a transient size distribution of the total particles. The model has been validated for breakup of water and hydrocarbon droplets in air shocks.

To highlight the importance of aerodynamic breakup of melted particles, preliminary numerical results [1] are shown for an essentially uncased cylindrical charge containing a thermobaric explosive mixture with a high mass fraction of aluminum particles (Figure 2). The charge contains a high explosive booster through the centre that is initiated from the top. The numerical model employs a breakup criterion based on Weber number (We > 15), assuming that the particle has already overcome its latent heat of fusion and remained melted. Constant properties for surface tension ($\gamma = 0.86$ N/m) and a fixed melting temperature of 933 K were used.



Figure 2. Two-dimensional axi-symmetric model of multiphase detonation and near-field dispersal from a metalized explosive [1]. The particle state is identified by coloured points. Left: Results during detonation ($t = 15 \mu s$). Right: Results during early expansion to approximately three charge diameters ($t = 100 \mu s$).

Ripley, R. C.

Figure 2 illustrates the extent of particle fragmentation at very early times. During the detonation stage (Figure 2, left) there is widespread detonation damage to the particles during the detonation shock compression that shifts the mean particle size distribution towards smaller diameters as the detonation wave passes. Further behind the detonation shock, aerodynamic break-up of the particles begins, most prominently along the interface with the high-explosive booster and at the free-edges of the charge as the detonation products break out. During the very early expansion (Figure 1, right) there is extensive aerodynamic breakup of the dispersed particles resulting in significantly smaller mean droplet sizes.

Figure 3 provides a comparison of reaction histories with and without aerodynamic breakup of melted particles. Figure 3 (left) gives the results during the timescale of detonation and early dispersal, which shows significantly increased consumption of aluminum due to extensive breakup and corresponding increased reaction rates. On the timescale of 100 μ s, the aluminum reaction is almost exclusively with the detonation products gases. Figure 3 (right) shows the effect of the breakup that occurred during the first 100 μ s on the subsequent later time reaction progress. The early-time aerodynamic breakup and increased reaction in the detonation products resulted in much less particles escaping the fireball and reacting with oxygen in the air.



Figure 3. The effect of aerodynamic breakup of melted particles on the global reaction history. Left: Detonation and early expansion timeframe ($t < 100 \ \mu s$). Right: Late-time reaction during unconfined dispersal ($t < 1.1 \ ms$).

6 Conclusions

The melting of aluminum particles and subsequent aerodynamic breakup of molten aluminum play a significant role in the aluminum reaction and energy release in the near field of detonation of an aluminized condensed explosive. The preliminary numerical results using a constant melting temperature for standard atmospheric pressure exhibit extensive aerodynamic breakup of aluminum particles. Beyond uncertainties in the liquid surface tension and breakup criteria which may alter the stability of liquid droplets, melting of particles is a prerequisite for aerodynamic breakup to occur. Considering the very high pressure regimes during detonation and in the very near field of a heterogeneous explosive, a high pressure melting curve based on published experimental and theoretical data has been adopted. The increased melting temperature of aluminum during the very early particle dispersal is expected to delay the aerodynamic breakup. This will increase the dispersal distance of the particles and facilitate reaction with atmospheric oxygen. Final numerical calculations will be presented to confirm the resulting effect of aerodynamic breakup on the combustion of aluminum particles and results will be compared with experimental data.

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