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A reaction progress variable modeling approach for non-ideal multiphase explosives

K.P. Ruggirello [a], P.E. DesJardin [a,*], M.R. Baer [b], M.J. Kaneshige [b], E.S. Hertel [b]

[a] Department of Mechanical and Aerospace Engineering, University at Buffalo, Buffalo, NY 14228, USA
[b] Sandia National Laboratories, Albuquerque, NM 87123, USA

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ABSTRACT

This study concerns the development of a mixture fraction based reaction progress variable formulation for aluminized explosives. Highlights of the formulation include a fully compressible treatment of both the gas and solid phases (both aluminum and alumina), heterogenous and homogenous reactions, and effects of group combustion. Isolated particle simulations are validated against experimental data and DNS and show good agreement of burn times over a range of pressure and oxygen environments. The new models are implemented in the CTH shock physics code using a fractional step approach to allow for efficient computation of particle dynamics. Comparisons are made to experimental pressure data for a thermobaric explosive in the Sandia Explosive Components Facility (ECF). Parametric studies are conducted to determine pressure response and impulse to charge equivalence ratio and particle size. Overall good agreement is observed between simulation predictions of pressure time history and impulse.

1. Introduction

While the behavior of ideal explosives is well understood and mature scaling theories are established (Cooper, 1996), much less is known about non-ideal multiphase explosives. In an ideal explosive, the effects of reactions can be explained by well established Chapman–Jouget (CJ) theory for detonations and the resulting expansion process can be explained by non-reacting gas dynamics. Non-ideal explosives, however, do not follow the same well defined detonation jump relations and therefore significant deviations are expected for the CJ pressure, velocity, or expansion isentrope predicted from equilibrium, steady-state calculations such as those typically used in BKW (Mader, 1998), TIGER (Cowperthwaite, 1973), and CHEETAH (Fried and Souers, 1994). The observed detonation pressures can be hundreds of kilobars below the predicted steady-state calculations (Orth and Krier, 1998). Non-ideal explosives also show increased sensitivity to confinement, diameter, and oxidizing environment which are all controlled by local turbulent mixing processes. Additionally they can have reaction zones which are on the order of centimeters rather than microns found in ideal explosives (Jackson et al., 2011), and have delayed reactions that take place in the expansion wave which support the air shock. The reactions in the expansion wave of a non-ideal explosive occur as both anaerobic from reactions with the detonation products, and aerobic reactions from mixing with surrounding oxidants such as oxygen in the air. Even though the detonation pressures are lower, the detonation wave from non-ideal explosives have wider pressure profiles which leads to an increased impulse ($I = \int p\,dt$), as illustrated in Fig. 1.

Non-ideal multiphase explosives do not have the fuel and oxidizer mixed on a molecular level, and usually a fine reactive metal powder such as aluminum is added to a mixture of high explosive(s), and binder. The metallic powders nominal diameter has a significant effect on the detonation behavior and is typically of the order of 10s of microns to nanometers in size in more recent compositions, where the smaller particle size is desirable due to lower thermal inertia and increased reaction surface area. The shape of the particles also has an effect on the explosive properties, where metallic flakes are typically used to further increase the surface area for reactions. This metalized high explosive mixture is then placed around a booster charge which serves to initiate the explosive and also to disperse the metallic fuel to the surrounding atmosphere where it may use the excess oxygen if the mixture is fuel rich.

In an effort to improve the predictions made by the equilibrium thermodynamics codes Keshavarz et al. (2006) recently developed a simple empirical relationship to predict the detonation pressure for a general $C_aH_bN_cO_dAl_e$ non-ideal explosive, but more advanced physics based models for the prediction of the detonation properties of non-ideal explosives are still lacking. The focus of this study is to explore the ignition and burning of aluminum particles in a multiphase high pressure and temperature shock environment following the detonation of a non-ideal aluminized high explosive (TBX) where both anaerobic and aerobic reactions occur.

* Corresponding author. Tel.: +1 716 645 1467.
E-mail address: ped3@buffalo.edu (P.E. DesJardin).

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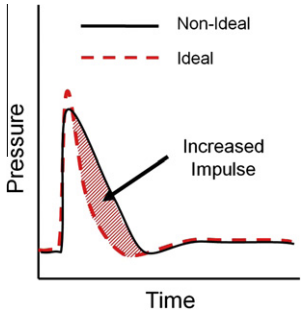

Fig. 1. Representative pressure profile for an ideal vs. non-ideal explosive.

Early semi-analytical theoretical models of aluminum combustion have focused on the quasi-steady burning stages (Brzustowski and Glassman, 1964; Law, 1973; Turns et al., 1987). These models employ flame sheet approximations and decompose the transport of heat and mass into two zones: a region between the particle surface and the flame, and a region beyond the flame. Results using these models have been shown to provide reasonable predictions for burning rates in a variety of oxidizing environments (Turns et al., 1987; Brooks and Beckstead, 1995). Beckstead et al. investigated a more detailed description of the flame and flow around the particle but found that many of the aspects of the flame structure and overall burning rates are close to those obtained using flame sheet assumptions (Liang and Beckstead, 1998; Widener et al., 1998). Babuk and Vasilyev have devised a five zone model that includes a more complete description of oxide cap formation, growth and movement (Babuk and Vasilyev, 2002). They demonstrate that their model is capable of capturing many of the observed dynamics of agglomerate motion. Most recently, Washburn et al. (2008, 2010) have combined the Liang/Beckstead (Liang and Beckstead, 1998; Widener et al., 1998) model with a detailed chemical-kinetics mechanism and direct numerical simulation (DNS) of the gas phase around the particle to examine the combustion characteristics for a range of oxidizing and pressure environments. In the current study a previously developed aluminum particle combustion model (DesJardin et al., 2005; Ruggirello et al., 2010) is used which relies on Shvab–Zel'dovich coupling functions (Kuo, 1986) to efficiently solve the coupled heat and mass transfer for the particle.

In order to extend the single particle model to a reactive particulate cloud consisting of potentially millions of particles, a multiphase model is used in the current study to solve the solid and gas phases along with their interactions. Multiphase flow theory has an extensive background and range of applications including fluidized beds (Mathiesen et al., 2000; Samuelsberg and Hjertager, 1996), powder compaction (Saurel et al., 2010), and deflagration to detonation transition in granular materials (Baer and Nunziato, 1986; Bdzil et al., 1999; Kapila et al., 2001). The majority of the multiphase models are based off the two-phase mixture model developed by Baer and Nunziato (1986). It allows for disequilibrium of pressures, velocities, and temperatures between the phases and uses the second law of thermodynamics to construct admissible phase interaction terms. There are several challenges in multiphase flow modeling, which are outlined by Bdzil et al. (1999). The phase interaction terms lead to non-conservative governing equations for each phase and the very short time scales ($\approx 10^{-8}$ s) associated with the equilibrium processes make the equations very stiff. In an effort to alleviate the stiffness several authors have developed reduced equation models which assume a single pressure (Paillre et al., 2003; Liou et al., 2008; Chang and Liou, 2007), a single velocity, or a single velocity and pressure (Kapila et al., 2001). When a single pressure is assumed between the phases the hyperbolic nature of the equations is lost, and a pressure correction term is usually added to the interface pressure to restore hyperbolicity (Stuhmiller, 1977; Chang and Liou, 2007; Liou et al., 2008). Another method to reduce the stiffness of the equations is by using a pressure relaxation method. The pressure relaxation methods subcyle the pressure work term between the phases separately from the hydrodynamics by adjusting the volume fractions until mechanical equilibrium is reached. There are several different pressure relaxation algorithms presented in the literature (Saurel and Abgrall, 1999; Chinnayya et al., 2004; Petitpas et al., 2009; Saurel et al., 2009; Benson, 1992; Lallemand et al., 2005). In this study the multiphase model of Baer and Nunziato (1986) is used to model the solid and gas phases and a pressure relaxation method based on the algorithm presented by Saurel et al. (2009) is used to alleviate the stiffness of the equations.

To recast the previously developed Lagrangian aluminum particle combustion model (DesJardin et al., 2005; Ruggirello et al., 2010) into an Eulerian framework, a reaction progress variable description is used. An Eulerian framework for the aluminum particles is chosen because of the desire to account for the group combustion burning mode for aluminum rich charges. Reaction progress variable approaches have been used in non-premixed turbulent combustion (Pitsch et al., 2003; Bray et al., 2005; Pitsch and Ihme, 2005) to reduce the degrees of freedom and account for subgrid scale (SGS) turbulence and combustion. The non-premixed nature of the multiphase aluminum particle combustion makes the reaction progress variable formulation an attractive modeling approach for this study.

The model presented is unique in that it combines a detailed mechanistic aluminum particle combustion model with a reaction progress variable formulation and a multiphase flow model. The combination of these allows the dynamics of the aluminum particle combustion, and the group combustion burning mode to be simulated. Additionally the multiphase flow model allows the phase interactions between the aluminum/alumina and gas products to be explicitly accounted for.

The remainder of this paper is organized as follows. First the two-phase flow model is presented, followed by the aluminum particle combustion model and reaction progress variable formulation. Next the numerical implementation is discussed, and results are presented. The results consist of isolated single particle cases, experimental comparisons to several tests conducted at the Explosives Components Facility (ECF) at Sandia National Laboratories, and sensitivity studies conducted to determine the effects of initial particle diameter and equivalence ratio on the model. Finally, conclusions are drawn from this study.

2. Mathematical formulation

2.1. Two-phase flow model

The multiphase system is formulated by phase-averaging of the instantaneous multiphase equations over a representative volume that is compactly defined by the filter function, $G(\boldsymbol{x}-\boldsymbol{x}')$, with the normalization property, $\int_{V_\infty} G\,dV = 1$ (Carrara and DesJardin, 2006). Application of the filtering operator and neglecting bulk phase molecular viscosity, conduction and diffusion processes results in the following system of equations for volume, mass, momentum and energy transport:

$$\frac{\partial \alpha_k}{\partial t} + \boldsymbol{u}_k \cdot \nabla \alpha_k = V_k^{\ddagger} + c_k^{\ddagger}/\gamma_k \tag{1a}$$

$$\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \boldsymbol{u}_k) = c_k^{\ddagger} \tag{1b}$$

$$\frac{\partial \rho_{i,k}}{\partial t} + \nabla \cdot (\rho_{i,k} \boldsymbol{u}_k) = \alpha_k \dot{m}_{k,i}''' + c_{k,i}^{\ddagger} \tag{1c}$$