

Combustion Modeling of Aluminum-Enriched Propellants Using a Surface Tension SPH Model

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Abstract

This study explores the mechanism of agglomerations and the interactions between the agglomerates and surrounding materials in aluminized solid propellants that experience both phase transitions and chemical reactions. A surface tension is modeled by including the cohesion and surface minimization for the reasons of (1) accounting for all three phases (gas, liquid, and solid), (2) combining chemical, physical, and geometrical aspects of agglomeration, and (3) representing the agglomeration and coalescence through the surface tension framework. The new surface tension model is incorporated in the momentum conservation that features a set of unique cohesion and surface minimization terms. To further analyze the reaction characteristics of the active materials, the in-house calorimetry is conducted, and the pre-exponential factor and activation energy are obtained. The overall practicality and applicability of the model are confirmed through the particle interaction simulations prior to performing the randomized solid propellant combustion, that revealed the material interactions in multi-phase flows and the coalescence occurring in the melt layer. Therefore, this research demonstrates the suitability of the novel surface tension modeling in the simulation of agglomerations and particle interactions with phase changes in aluminum enriched solid propellants.

1 Introduction

Due to the significant impact of agglomeration on the specific impulse of solid propellants [1], various studies have been conducted to elucidate the mechanisms of the agglomeration process in solid propellant combustion. Many experiments have focused on agglomerations occurring in the melt layer of aluminized solid propellants, comparing the combustion characteristics of aluminized propellants with those of other types of solid propellants [2,3].

Agglomeration models and numerical schemes can be classified into several categories [4]. The Empirical Model determines agglomeration parameters, which is practical due to its reliance on the empirical data. However, it is limited in its applicability to specific environments [5]. The Pocket Model incorporates statistical and geometric features of agglomeration by introducing the concept of a "pocket," which defines the agglomerate interface [6]. Although it is more precise over the Empirical Model, it cannot explain the physical properties of agglomerates. The Packing-based Model, an enhancement of the Pocket Model, estimates the agglomeration distribution [7]. However, its accuracy depends on the

parameters used, and it requires significant computational resources. To account for the physiochemical behavior in the melt layer, the Physical Model, which includes the physical features of agglomeration, was proposed in [8]. While it can analyze interactions between agglomerates and surrounding materials, it still falls short of precisely capturing the complex phenomena. The Condensed Layer Model provides a qualitative approach to modeling agglomeration in solid propellants, motivating the development of models that incorporate the advanced numerical methods [9]. Molecular Dynamics Simulation is a numerical method that focuses on the behavior of individual molecules and particles [10]. Although this model is useful for molecular-level analyses of chemical reactions and heat transfer, it is limited to a system that is small scale and at equilibrium state. The Monte Carlo Method is employed to address complex phenomena [11], and the Discrete Element Method is applied to simulate interactions between particles and surrounding materials [12]. Cluster Analysis is practical for investigating the geometric characteristics of agglomerates [13], while it cannot provide information on their physical and chemical properties.

It is crucial to calculate the formation of agglomerates, considering the physicochemical behavior, multiphase flows, and the complex dynamics occurring in the melt layer of a metal enriched propellants. By implementing the key and critical theories into the algorithm, it is possible to simulate the detailed mechanisms of agglomeration. The present research developed a surface tension concept, incorporating both cohesion and surface minimization into the momentum conservation law [14]. The algorithm developed here offers several distinctive advantages. First, the calculation can handle the multiphase flows, enabling simultaneous considerations of solid, gas, and liquid phases all together. Second, the computed results can represent both the physicochemical and geometrical characteristics of the agglomeration. Third, by incorporating the surface tension into the algorithm, the agglomeration phenomenon is shown quite pronounced and better compared with the experimental evidence.

This study simulates agglomeration occurring at the burning surface of aluminized solid propellants, with the surface tension force that includes cohesion and surface minimization, integrated into the momentum conservation equation. The chemical reaction kinetics of the metalized propellants are empirically obtained prior to conducting the simulations. In essence, the comprehensive two-dimensional aluminized solid propellant combustion simulation is presented.

2 Methodology

2.1 Governing equation

The governing equations include the continuity equation, momentum equation, energy equation, species conservation equation, and the deviatoric stress and strain conservation equations. The equations are formulated to account for all phases of the materials under two-dimensional conditions, as illustrated in Eqn. (1) and (2).

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{E}}{\partial x} + \frac{\partial \vec{F}}{\partial y} = \vec{S}(\vec{U}) \quad (1)$$

$$\vec{U} = \begin{bmatrix} \rho \\ \rho u_i \\ \rho E \\ \rho Y \\ \rho \tau_{ij} \\ \rho \varepsilon \end{bmatrix}, \quad \vec{E} = \begin{bmatrix} \rho u_x \\ \rho u_x u_i + P \delta_{ix} \\ u_x (\rho E + P) \\ \rho Y u_x \\ \rho \tau_{ij} u_x \\ \rho \varepsilon u_x \end{bmatrix}, \quad \vec{F} = \begin{bmatrix} \rho u_y \\ \rho u_y u_i + P \delta_{iy} \\ u_y (\rho E + P) \\ \rho Y u_y \\ \rho \tau_{ij} u_y \\ \rho \varepsilon u_y \end{bmatrix}, \quad \vec{S} = \begin{bmatrix} 0 \\ \sigma_{m,i} + \eta_i \\ \sigma_E + \rho Q \dot{Y} + \nabla \cdot (k \nabla \cdot T) \\ \rho \dot{Y} \\ \sigma_{S,ij} \\ \rho D \end{bmatrix} \quad (2)$$

The conservative variables ρ , u_i , E , Y , τ_{ij} and ε represent the density, velocity in the i -direction, total energy, mass fraction of chemical species, deviatoric stress in the ij -direction, and strain, respectively.

The pressure, P , is influenced by the Kronecker delta, δ_{ij} , while Q denotes the heat of reaction. The source term σ represents contributions to momentum, energy, and deviatoric stress, encompassing the first derivatives of the corresponding conservative variables. D denotes the plastic strain rate. The pressure is computed using the modified Tait equation of state (EOS) for solid and liquid materials, and the Noble–Abel EOS for gaseous materials .

2.2 Surface tension effect during agglomeration process

In the momentum equation illustrated in Eqn. (2), η represents the surface tension source term, which accounts for both cohesion and adhesion [14]. The details of surface tension are illustrated through Eqs. (3) to (6).

$$\eta_i = \nabla \cdot \frac{F_S}{A} \quad (3)$$

$$F_S = K(F_{co} + F_{cur}) \quad (4)$$

$$F_{co} = -\gamma\rho_i\rho_j C(d) \frac{d}{|d|} \quad (5)$$

$$F_{cur} = -\gamma\rho(n_i - n_j) \quad (6)$$

The relevant source term is described by the first derivative of the surface tension divided by the cross-sectional area, as shown in Eqn. (3). The surface tension is comprised of two components, namely cohesion (F_{co}) and a surface minimization term (F_{cur}). These terms are multiplied by a symmetrized correction factor to enhance the curvature near the material boundary. The first primary component, cohesion, is described in Eqn. (5). In this force, the surface tension coefficient and the densities of the two nodes subject to surface tension determine only the magnitude of cohesion, while a spline function governs both the magnitude and direction of the force. Because a repulsive force must be considered when two nodes are close to each other, the spline function transitions from attraction to repulsion when their distance becomes shorter than a critical threshold. Another main component is the surface minimization force, elaborated in Eqn. (6). This force is also influenced by the surface tension coefficient and the densities. In addition, local normal information is incorporated to determine the surface minimization term. By employing a Gaussian kernel function to evaluate the curvature near each node, the material boundary is rendered to be more rounded.

2.3 Reaction characteristics

To capture the chemical characteristics of the material, the Arrhenius equation was employed. The first derivative of the chemical species with respect to time is presented in Eqn. (7).

$$\dot{Y} = \nabla_t \cdot Y = Af(Y)\exp\left(-\frac{E}{RT}\right) \quad (7)$$

The reaction parameters, pre-exponential factor, and activation energy were obtained through the in-house calorimetry. This research focuses on the reaction characteristics of an aluminum–potassium perchlorate mixture at a 34:66 weight ratio, which corresponds to the stoichiometric condition for the $8Al + 3KClO_4 = 4Al_2O_3 + 3KCl$ reaction. The activation energy ranges from 100 kJ/mol to 180 kJ/mol, while the pre-exponential factor varies between $e^8 s^{-1}$ and $e^9 s^{-1}$. Both parameters increase gradually from the start of the reaction until it reaches approximately 70% completion, after which they decrease rapidly until the reaction ends.

3 Results

The simulation is divided into two sections: verification of the surface tension model and its application. For the verification process, simulations are conducted for both single-particle and multi-particle cases. In the single-particle simulation, the goal is to verify the agglomeration of a liquid phase while the solid part remains stationary, thereby assessing the applicability of the surface tension model. The multi-particle simulation is performed to validate the range of forces and coalescence amongst multiple particles. Figures 1(a) and 1(b) illustrate the single-particle simulation, while Fig. 1(c) shows the outcome of the multi-particle simulation. These results confirm the functionality of the surface tension model and its applicability, as they replicate agglomeration behavior similar to that observed in combustion imaging experiments [3].

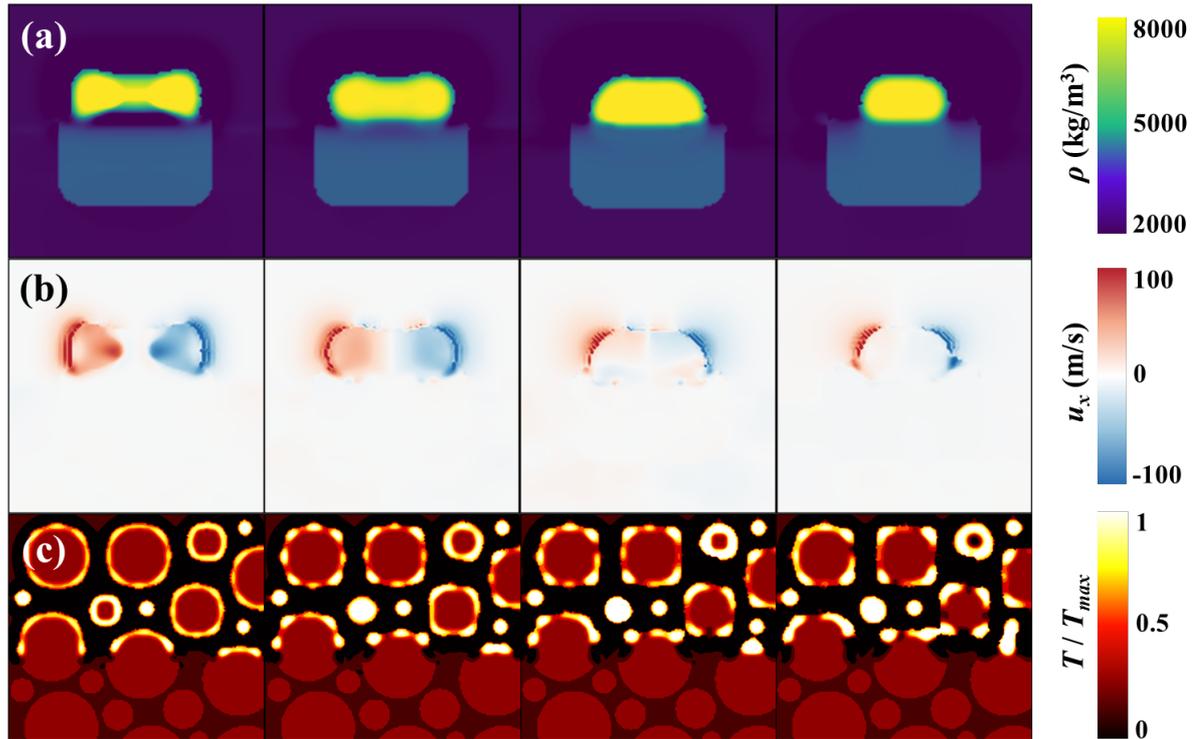


Figure 1: Single-particle simulation results for (a) density and (b) x-direction velocity, and multi-particle simulation results for (c) temperature

Figure 2 shows the aluminized solid propellant combustion simulation for analyzing the agglomeration and coalescence within the melt layer of the solid propellant. It is also essential to examine how the coalesced particles interact with the surrounding elements such as outflow gas and molten particles. As illustrated in Fig. 2(a), three distinct particles emerge after a portion of the material is expelled as an outflow gas. Because alumina has a high latent heat of vaporization, a substantial amount of liquid alumina remains in the melt layer, thereby forming the agglomerates. The heat released by the reaction raises the temperature of alumina on the propellant surface, causing some of it to transition into the gaseous phase and to move into the outflow region. However, if there is insufficient heat to vaporize the liquid alumina, it remains on the burning surface, continually absorbing energy until it surpasses the latent heat of vaporization. As a result, the temperature (or total energy) in this region is relatively lower than in the surrounding areas, as shown in Fig. 2(b). In the gaseous region depicted in Fig. 2(c), the weight fraction of alumina varies based on the initial reactant ratio. Since the surface tension in this algorithm affects only the liquid elements, the distribution of alumina in the gas phase is random. In contrast, within the melt layer, the liquid alumina coalesces to form particles, demonstrating the process of coalescence and agglomeration overall.

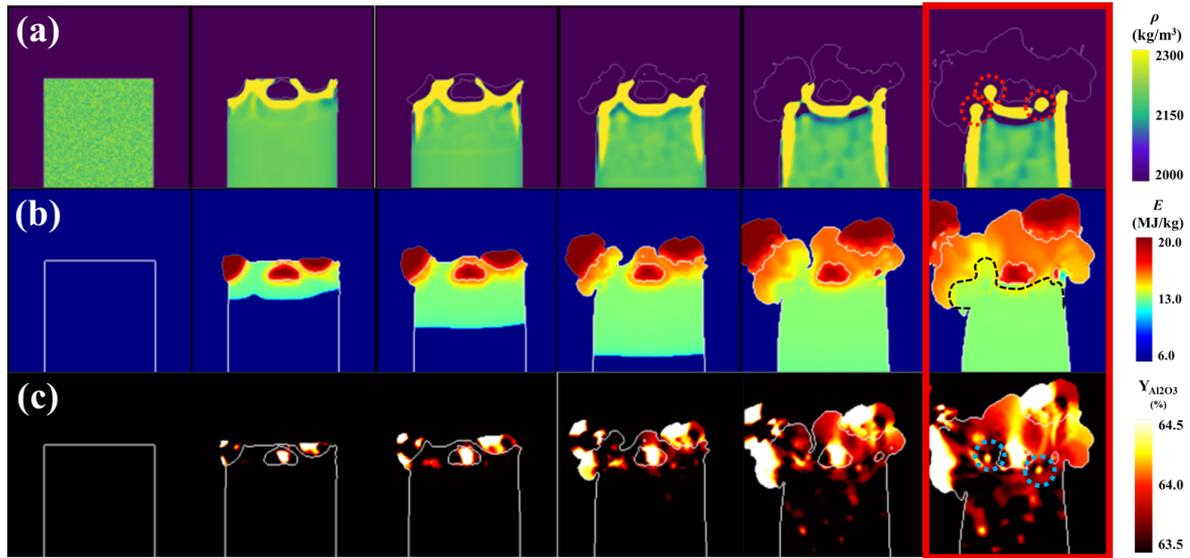


Figure 2: Surface combustion of the aluminized solid propellant shown via (a) density, (b) total energy, and (c) weight fraction of alumina evolutions.

The results provide evidence that the surface tension model as employed in the smoothed-particle hydrodynamics (SPH) simulations is also applicable to the present continuum domain as illustrated [14]. The present approach has significant potential not only for combustion simulations but also for all scenarios involving particle coalescence and agglomeration. To refine the parameters for surface tension, the future work involves validating these findings against experiments on the aluminized solid propellant combustion, which uses the same oxidizer, under similar environmental conditions [3].

4 Conclusion

This research developed a surface tension model for combustion simulation of solid propellants with randomly distributed particles of aluminum and potassium perchlorate. The surface tension model effectively replicated the processes of agglomeration and coalescence by incorporating both cohesion and surface area minimization term. Furthermore, it examined the interactions between coalesced particles and surrounding materials, which dynamically form and influence nearby regions. This interaction ultimately enhances our understanding of the agglomeration process. The novel findings facilitate a deeper interpretation of the complex physical and chemical phenomena that always occur at the burning surface of aluminum enriched propellants. Future work will involve validating the model against empirical data to further improve the surface tension parameters, which could then be utilized in various other applications.

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