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A detailed flame structure and burning velocity analysis of aluminum dust cloud combustion using the Eulerian–Lagrangian method

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Abstract

Aluminum particle dust cloud combustion with oxygen is numerically simulated using an Eulerian–Lagrangian two-phase approach. A single aluminum combustion model containing detailed aluminum combustion phenomena (melting, the heterogeneous surface reaction, alumina shell growth, combustion heat distribution, etc.) is suggested and applied to a three-dimensional, compressible CFD in-house code. High order space discretization and field variable interpolation for particle technics are employed to reduce grid dependency. Flame propagation is simulated in a slip-wall bounded open duct with well distributed aluminum particles in an O_2–N_2 mixture. The flame structure shows a flame zone that is longer than the pre-heating zone. This is unlike a gas phase flame, and it is due to the long combustion time needed for solid particles. The temperature behaviors of the gas and particle phase are captured reverse as the temperature rises. The dust cloud combustion model is validated by comparing burning velocities with the Bunsen burner experimental data in various oxygen and dust concentrations. Additionally, flame structure analysis is accomplished for better understandings on the behaviors of burning velocity in different conditions.

Keywords: Aluminum combustion; Burning velocity; Dust cloud combustion; Flame structure; Two-phase simulation

1. Introduction

Aluminum particle has been in the spotlight for more than a half-century in the defense and aerospace industries owing to its high energy densities and non-toxic combustion products. The high volumetric and gravimetric energy densities [1] make this fuel significantly more advantageous than the hydrocarbon fuel. Especially for a solid rocket, aluminum additives improve specific impulse and dampen acoustic instability. The boron and beryllium have higher energy density but aluminum has advantages in non-toxicity of combustion products and difficulties of ignition and combustion [2]. Due to these advantages, aluminum has

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been used in various applications. For instance, it has been used as an additive or main energy source for propulsion systems and as an energetic material for pyrotechnics and explosives. In most of the applications, the aluminum particles form a scattered dust cloud. As such, modeling aluminum dust combustion is important. Additionally, dust explosions also constitute a large safety issue in terms of particle storage, mining, and manufacturing. Thus, a fundamental understanding and detailed modeling of dust combustion are required to improve the performance of propulsion system and to prevent dust explosions.

Various fundamental experiments and analytical studies have been conducted on aluminum dust cloud combustion using Bunsen burners [3,4] and other methods [5]. These studies have provided a fundamental understanding of the combustion process, including flame speed data for different dust and oxidizer concentrations. Several studies in the literature have also looked at aluminum dust combustion using computational fluid dynamic (CFD). Kuhl et al. [6] studied an Eulerian–Eulerian two phase simulation using a fast-chemistry model. They found that this method was computationally efficient but had limitations regarding dust combustion modeling. The Eulerian–Lagrangian approach was used by Balakrishnan et al. [7] for dust explosions, and Najjar et al. [8] used it for a solid rocket motor. They modeled a simple form of an aluminum reaction rate using experimental correlations. Recently, Bidabadi et al. [9] predicted laminar dust flame speed by treating aluminum as a heat source. They demonstrated good feasibility for a detailed simulation using the Lagrangian approach.

The main purpose of the present study is to develop a numerical model for aluminum dust combustion capable of simulating real applications such as propulsion systems. The single particle combustion model suggested in this study includes detailed physics for a detailed simulation. It is applied to an Eulerian–Lagrangian CFD code in order to create dust flame propagation. The burning velocities of the premixed $Al–O_2–N_2$ mixture are calculated and compared to experimental data to validate the grid dependency and combustion model. The structure of the aluminum dust flame is analyzed to enhance understanding on the dust combustion.

2. Theoretical modeling

2.1. Governing equations for fully coupled two-phase flow

The finite volume method (FVM) is used to solve fully compressible Navier–Stokes equation with species transportation using an in-house-code. Three dimensional solver is used to directly calculate the governing equations since a dust flame has a complex heterogeneous mixture and reactions by scattered particles. A turbulence model is not adopted because this study only treats laminar flame propagation. The 2nd and 4th order central schemes and a TVD 3-stage Runge–Kutta scheme are used for spatial discretization and temporal advancement, respectively. Multiple species with a polynomial profiled specific heat, viscosity, and conductivity are solved.

The dynamics of the dispersed particles are modeled using the Lagrangian approach. $dx_p/dt = u_p$ is used for particle location and $dV_p/dt = F_p/m_p$ is used for particle velocity, where x_p, u_p, and m_p represent the instantaneous particle location, velocity, and mass, respectively. Due to the simple laminar flow, the only force acting on the particle body is surface drag. This drag force is modeled as $F_d = 1/8 \cdot C_d \rho \pi d_p^2 |u_r| u_r$, where d_p and u_r represent the particle diameter and relative velocity between the gas and particle. The criterion for the drag coefficient are calculated as presented in the literature [10].

2.2. Aluminum particle combustion model

2.2.1. Phenomenological aluminum combustion

Aluminum particles follows diffusion controlled combustion mechanism for large micro particles whereas it follows kinetically controlled mechanism for nano particles [11]. The reason is that diffusion speed of oxidizer become faster than a chemical reaction rate as particle diameter decreased. The critical diameter value which this phenomenon happens is about 100 μm for 1 atm [12]. At the pressure of 1 atm, particles larger than 100 μm have a constant ignition temperature of 2327 K because ignition occurs after the melting of alumina oxide shell. However, ignition temperature reaches close to 933 K as the particle size decreased less than 100 nm because ignition physics changes from melting of a shell to shell spallation by molten aluminum core [13]. Sizes between 100 nm and 100 μm are assumed to constitute a transition region. Thus, a heterogeneous surface reaction (HSR) and decreased ignition temperature coexist.

This paper uses 5.4 μm aluminum particle for the dust flame propagation. Especially for particle diameter less than 10 μm, chemical kinetics is significant on the burning time [14]. Therefore, this paper models combustion of 5.4 μm particle under the assumption of kinetically controlled regime. The combustion modeling is divided into a pre-heating stage and a quasi-steady combustion stage distinguished by the ignition temperature.

2.2.2. Pre-heating stage

In the pre-heating stage, convection and the HSR are the major parameters heating up particles. Convection is related to aerodynamics. Hence, the total diameter, d_p, which includes the alumina, is