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Toward a computational tool to simulate for the flame propagation in thermites powders

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Mixtures of metal/metal-oxide, commonly known as thermite, can burn in a self-sustained reaction with an ultra-high energy density [1-2]. The high combustion temperature, safety, and tunability of thermites make it possible to produce totally novel pyrotechnical devices for in-space maneuvers (stage separation, pulse power generation for extended space missions, ...) [3-4]. However, the effective transfer of thermites from research laboratories to industrial products faces a core challenge, which is the lack of realistic deflagration models to guide the system design. Thus, the customization of a thermite mixture is still guided more or less by empirical considerations mostly from observations in flame tube experiments or using the empirical "Edisonian" approach, based on trial-and-error. Both approaches are totally inadequate to explore the large number of possible metals and oxides, in which not only the chemistry but also the microscopic (particle scale) and mesoscopic properties (systems of particles) influence the macroscopic combustion. This paper presents a one-dimensional (1D) model that simulates Al reaction propagation when in contact with a strong oxidizer in a cylindrical tube. CuO was chosen as it is the widest used metallic oxidizer that decomposes below the reaction temperature. In addition to condensed phase theory [5], representations of the gas phase combustion at the different scale is implemented using a computational fluid dynamics scheme enabling to model multiphase physics and combined physico-chemical mechanisms [6] taking place during the thermite reaction which are all extremely important factors to account for.

The model is designed as a combustion tube as used for flame speed measurements, i.e. with rigid walls filled with homogenous mixture of Al and CuO particles. The Al particle richness, the powder density, the particles diameters, and stoichiometric ratio and heat loss through the wall define the main parameters of the system. The 1D heat flow equation is coupled with mass and momentum equations and both diffusion and advection are considered. The calculated values of flame velocity show a reasonable compatibility with the experimental data.

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