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# On modeling the diffusion to kinetically controlled burning limits of micron-sized aluminum particles

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## ABSTRACT

Aluminum particle burn rates are known to be a strong function of particle size as the mode of burning transitions from diffusion to kinetically controlled. To better understand the rate dependent diffusion and kinetic processes, a fully compressible, one-dimensional, spherically symmetric particle burn model is developed. Several cases are studied to explore the burning of aluminum particles in air, carbon-dioxide and steam environments. Predictions of burn rates versus particle size reveal significant deviations from a diffusion controlled burning limit – highlighting the importance of accounting for finite-rate chemistry in modeling the burning of sub-micron aluminum particles. While overall agreement to data is satisfactory, the detailed model cannot be directly used in system level tools due to computational cost. Two reduced modeling strategies are therefore explored to account for finite-rate chemistry effects in simpler models for use in system level CFD analysis. The first is an augmented  $D^2$  – law where the finite-rate chemistry is treated as a perturbation to flame sheet approximation via augmented burn rate “constants”. Predictions using this approach of deflagration speeds in dusty aluminum-air gases agree well with experiments and show evidence of a maximum flame speed for a given mass loading. The second modeling approach uses a reduced numerical model and kinetics mechanism resulting in computationally efficient solutions. Results using this approach show up to two orders of magnitude reduction in computational effort while maintaining reasonable accuracy for predictions of flame structure, burn rates and burn times.

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## 1. Introduction

The use of aluminum particles continues to be of interest as an additive for propellants [1] and aviation fuels [2,3] to increase energy density and specific impulse. Recent studies have focused on the transition of diffusion to kinetically controlled burning with decreasing particle size [4–6]. One of the motivations for studying this transition is the potential of using sub-micron to nano-scale sized particles in fuels to shorten ignition times [7] and accelerate flame speeds [5].

The transition of diffusion to kinetically controlled combustion was studied by Bazyn et al. and Lynch et al. as a function of both particle size and pressure using a reflected shock-tube facility for O<sub>2</sub> and CO<sub>2</sub> environments [4,8]. For a pressure of 8.5 atm, the limit of a diffusion flame was observed to occur for particle sizes less than ~20 μm as reactions migrate closer to the droplet surface.

Aluminum particle combustion in the 2–20 μm range was studied by Badiola et al. by igniting particles generated using an electro-static aerosol generator and ignited with a CO<sub>2</sub> laser [9]. Using AIO emission measurements to determine burn times and average temperatures, Badiola et al. estimated the transition from diffusion to kinetically controlled combustion at ~10 μm in air.

Washburn et al. conducted detailed numerical simulations of aluminum particles in oxygen, carbon dioxide and steam environments [6,10]. Cases were conducted using 3–11 μm sized particles and compared to burn time data from Bazyn et al. [4,11]. Overall agreement was reasonable with some discrepancies observed for pressures below ~10 atm in CO<sub>2</sub> and H<sub>2</sub>O environments. Differences were attributed to the distribution of particles in the experiments which tends to skew burn time measurements at lower pressures.

Huang et al. conducted a study of flame speed of aluminum particle dust in air [5]. Model predictions of flame speed are compared to data using phenomenologically derived burn rate models. For larger micron-sized particles, ignition temperature is correlated with data and the overall mixture burn rate uses particle burn time

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## Nomenclature

|                |                                                                      |                                |                                                       |
|----------------|----------------------------------------------------------------------|--------------------------------|-------------------------------------------------------|
| $D$            | mass diffusivity ( $\text{m}^2/\text{s}$ )                           | $Z$                            | mixture fraction                                      |
| $D_p$          | particle diameter (m)                                                |                                |                                                       |
| $e_t$          | total energy (J/kg)                                                  | <i>Greek</i>                   |                                                       |
| $H_t$          | total enthalpy (J/kg)                                                | $\alpha$                       | thermal diffusivity ( $\text{m}^2/\text{s}$ )         |
| $h_{f,i}^0$    | heat of formation of species $i$ (J/kg)                              | $\gamma$                       | constituent density ( $\text{kg}/\text{m}^3$ )        |
| $h_{vap}$      | latent heat of vaporization of aluminum (J/kg)                       | $\nu$                          | mass based stoichiometric ratio                       |
| $K$            | burn rate constant ( $\text{m}^2/\text{s}$ )                         | $\rho$                         | mixture density ( $\text{kg}/\text{m}^3$ )            |
| $\dot{m}_i$    | mass flow rate (kg/s)                                                | $\rho_{air}$                   | density of ambient air ( $\text{kg}/\text{m}^3$ )     |
| $\dot{m}_i'''$ | mass source term of species $i$ ( $\text{kg}/\text{m}^3 \text{ s}$ ) | $\rho_u$                       | density of unburnt mixture ( $\text{kg}/\text{m}^3$ ) |
| $\dot{m}_F'''$ | mass consumption rate of fuel ( $\text{kg}/\text{m}^3 \text{ s}$ )   | $\phi$                         | constituent volume fraction                           |
| $m_o$          | initial mass of the particle (kg)                                    | $\Phi$                         | equivalence ratio                                     |
| $m_q$          | mass of quenched particle (kg)                                       |                                |                                                       |
| $\dot{m}_T$    | bulk mass flow rate in radial coordinates (kg/s)                     | <i>Subscripts/superscripts</i> |                                                       |
| $r$            | radial coordinate (m)                                                | $i$                            | $i$ th species                                        |
| $\dot{S}$      | flow rate of species towards the surface (kg/s)                      | $l$                            | liquid property                                       |
| $S_L$          | flame speed (m/s)                                                    | $q$                            | quenching limit                                       |
| $\tau_b$       | burn time (s)                                                        | $s$                            | particle surface                                      |
| $T$            | temperature (K)                                                      | $T$                            | total property                                        |
| $Y_i$          | species mass fraction                                                | $\infty$                       | ambient/far-field conditions                          |

correlations developed by Beckstead [12]. For smaller nano-sized particles, the burn rates are assumed to follow that of a molecular limit using the chemical kinetics mechanism developed by Catoire et al. [13]. Flame speed predictions are shown to scale with decreasing particle diameter as  $\sim d^{-0.92}$ , consistent with  $D^2$  theory (see discussion regarding estimates of  $S_L$  in results section). For particles less than  $\sim 10 \mu\text{m}$ , however, further reduction in particle diameter results in a more gradual increase in flame speed, scaling as  $\sim d^{-0.52}$ , as the rate of burning becomes more kinetically controlled. Huang et al. estimate a maximum flame speed of  $5.82 \text{ m/s}$  as the particle diameter reaches a molecular asymptotic limit.

The transition from diffusion to kinetically controlled combustion is a recurring theme in the aforementioned studies and plays a crucial role in burning modes for decreasing pressures and particle sizes. In particular, particles that are  $\sim 10 \mu\text{m}$  and smaller exhibit a clear dependence on the rate limiting chemical kinetics. Relations between the Damköhler and Knudsen numbers have been made to help describe the mode of combustion of particles [14], but to date there have not been theoretical estimates of this transition as a function of particle size for aluminum particles, although estimates have been made for other energetic materials [15,16]. Typically, considerations of such a transition have been studied through the correlation of burn times versus pressure which exhibits a transition when pressure decreases and burn times increase. If pressure is held constant, burn rates will be a function of particle diameter and asymptotically approach a converged, diffusion-controlled burn rate as particle size increases.

Although experimentally derived empirical burn time relations have been developed to account for the burning behavior of aluminum particles for different burning regimes [17,8,18,9], they are limited to the select conditions of the experiment where the far-field temperature, pressure and oxidizer are held constant during the burning process. In system level applications using aluminum particulate (e.g., a rocker motor) the far-field conditions will most likely not remain constant. Detailed CFD models such as those by Washburn et al. [6,10] and Gallier et al. [19] do account for varying far-field conditions, however they are far too complex for use with system level simulations of multiphase flows involving billions of particles. An alternative description is therefore desirable which can balance complexity with accuracy of burn rates as the particle transitions from diffusion to kinetically controlled limits. Exploring

modeling strategies which can accommodate these constraints is a focus of this study.

The rest of the study is as follows. A fully compressible, one-dimensional, spherically symmetric model formulation is first presented that accounts for the full chemistry, differential diffusion, etc. using kinetic theory of gases. The purpose of the detailed model is to serve as the “exact” solution for which reduced approaches can be compared against. Validation is conducted using the experimental data and simulations of Bucher et al. [20] and also to measurements of Bazyn et al. [4] and numerical simulations of Washburn et al. [6] which span the diffusion to kinetically controlled burning transition regime. Two reduced modeling approaches are explored. The first relies on coupling burn rates in terms of a modified  $D^2$ -law where a normalized burn rate “constant” ( $K$ ) becomes a function of particle diameter and pressure to account for the effects of finite-rate chemistry. The normalized burn rate constants can be combined with eigenvalue based analytical solutions of the flame structure to account for effects of finite-rate chemistry. This model is used to compute flame deflagration speeds of aluminum-air dusty gases and compared to theory and data. The second reduced model is a simplified numerical model that employs quasi-steady assumption of mass transfer and reduced kinetics allowing for an efficient fully implicit formulation. Flame structure comparisons are presented using this model compared to the more general fully compressible formulation and errors in burn rates and flame structure are characterized.

## 2. Detailed model

The starting point for a detailed model is a spherically symmetric particle. The particle is assumed to have been heated sufficiently such that the aluminum oxide shell has fractured and collected on the particle surface to form the alumina cap. Assuming the Biot number is much less than unity, the aluminum particle in the molten liquid phase has a uniform temperature throughout. Since the focus of this study is not to explore multi-dimensional effects, a spherically symmetric configuration is the simplest geometry that needs to be considered for studying diffusion to kinetically controlled burning. The multiphase gas flow is considered one-dimensional, fully compressible and viscous resulting in the following set of transport equations for mass, species, momentum and energy conservation.

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