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An equilibrium-based reactive boundary layer model for burning aluminum particles

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In point-particle descriptions of reactive solid fuel particles, the mass and heat transfer rates between a particle and the carrier gas are commonly obtained from a boundary layer model that implements an idealization of the gas phase and surface chemical reactions. Focusing on burning aluminum particles, we aim to lift the restrictive assumptions of previous boundary layer models by enforcing thermodynamic equilibrium throughout the boundary shell enveloping a spherical particle. Compared to the passive boundary layer and the thin flame approximation, this has the advantage that both the oxidation of nitrogen during combustion in air and the endothermic dissociation of oxide smoke can be consistently accounted for. Additionally, gas phase oxidation reactions and surface chemistry may occur simultaneously in the equilibrium-based model and are not restricted to sequential combustion stages. Formally, our boundary layer formulation involves a nonlinear system of equations for the species mass fractions and enthalpy at the particle surface, the radial species and temperature gradients at the surface as well as the surface element concentrations. Here, the necessary conditions for thermodynamic equilibrium and the corresponding radial derivatives are complemented by gas-particle interaction conditions that constrain the element and enthalpy flow rates through the boundary layer. For a given particle temperature, we specifically assume that elemental nitrogen is not absorbed, whereas the mass flow rate of elemental aluminum adjusts in such a way that the gas composition at the particle surface is in equilibrium with bulk liquid aluminum. The transfer of elemental oxygen across the gas-particle surface, by contrast, is restricted to the species O, O_2 and Al_2O_3(l). In order to close the system of equations, the element mass fractions and the specific enthalpy at the particle surface are linked to their free-stream counterparts and associated flow rates by the integral element and enthalpy conservation laws. Finally, the species-specific mass transfer rates and the conductive heat flow rates both at the surface and across the far border of the boundary layer are obtained in a post-processing step.

In view of the collective behavior of reactive particles in a dust cloud, the equilibrium-based boundary layer formulation is incorporated into a population balance model for an aluminum particle dispersion. Along with the drag law, the mass and heat transfer rates obtained from the boundary layer model provide the kinetic link between the population balance equation and the balance laws governing the state of the carrier gas. After analyzing the ignition temperature of a monosized homogeneous dust cloud and the pollutants emitted during combustion, we proceed to investigate the spatially one-dimensional propagation of a reaction front through a homogeneously dispersed dust. The corresponding flame speed predictions are contrasted with the flame speeds obtained for a passive boundary layer and the thin flame approximation, respectively, and validated by comparison with existing experimental measurements.