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MESHFREE MODELLING OF COUPLED MECHANICAL-THERMAL-CHEMICAL PHENOMENA IN ENERGETIC AGGREGATES AT MULTIPLE LENGTH SCALES

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Energetic aggregates are a complex class of materials that produce exothermic chemical reactions with varying degrees of violence when exposed to dynamic mechanical impacts. The resulting energetic event (e.g., burning, explosive violent reaction, or full detonation) emerges from a sequence of coupled mechanical, thermal, and chemical processes that begin at heterogeneous features in the material's microstructure and subsequently evolve into a macroscale material response. The time-dependent, multi-physics and multiscale nature of this process poses many challenges for continuum models to be both predictive and physics-informed. Additional modelling challenges arise due to the large deformations and pervasive material fracture that often accompanies these events.

To address these challenges, we present a multi-faceted modelling approach that leverages meshfree numerical techniques to model coupled mechanical-thermal-chemical phenomena in energetic materials at both the meso and continuum scales. Novel bonded particle methods have been developed and are used to directly model the material microstructure features during transient dynamic impact events at several different strain rates. These models account for complex microstructure morphologies (intra- and inter-crystalline pores, microcracks, polymer binders and interfaces) and are used to map out yield surfaces for the aggregate material and inform continuum constitutive model form choices. At the continuum scale, a multi-physics conforming reproducing kernel particle method has been developed to overcome the challenges associated with traditional finite element modelling in this large deformation regime. The method performs loosely coupled solves of the material momentum balance (stress and strain), energy balance (temperature), and temperature-dependent chemical reaction rates. Together, these methods are used to study the response of energetic aggregates to impact events and provide new continuum predictions that contain enhanced physical insight of the underlying mesoscale processes.

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