Abstract Submitted
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Molecular Dynamics-informed RDX chemistry model and continuum static hot spot simulations[1] MICHAEL SAKANO, AHMED HAMED, Purdue University, ED KOBER, Los Alamos National Laboratory, BRENDEN HAMILTON, MD MAHBUBUL ISLAM, MARISOL KOSLOWSKI, ALEJANDRO STRACHAN, Purdue University — Reactive molecular dynamics (MD) simulations are able to describe the complex chemistry of high energy density materials and its coupling to mechanics. However, MD cannot reach the microstructural scales required to model hotspot formation and shock to detonation. Thus, we developed a multiscale model that uses MD simulations to inform a continuum model capable of reaching the microstructural scales. We developed a two-step reduced order chemistry model from reactive simulations of RDX and computed other critical physical properties like specific heat, thermal conductivity and equations of state. This information is used in a continuum model implemented in a finite elements code. We validate the continuum model via explicit MD hotspot calculations and then use it to characterize hotspot criticality for system sizes relevant to experiments.

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