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A framework for propagation of uncertainties from meso- to continuum scale computational models for shock-to-detonation transition in energetic materials. OISHIK SEN, SIDHARTHA ROY, SANGYUP LEE, NIRMAL RAI, MIN-YEONG MOON, K.K. CHOI, H.S. UDAYKUMAR, University of Iowa — Predictive models of shock-to-detonation transitions in heterogeneous energetic (HE) materials must contend with uncertainties in the material properties, reaction kinetics and microstructural features of the material. These uncertainties affect the energy localization at hot-spots due to void collapse and other mechanisms at the meso-/grain scale of the material and are eventually propagated to the macro-/continuum scales, leading to variabilities in the run-to-detonation distances. This work presents a unified framework for propagating the uncertainties in constitutive and reaction models as well as in microstructural features across scales in an energetic material. The aforementioned uncertainties are fed as inputs to a Mesoscale-Informed Ignition and Growth (MES-IG) model, and their effects on the meso-scale hot-spot characteristics and reaction dynamics are studied by performing ensembles of high-fidelity reactive void-collapse computations. The uncertainties in the meso-scale hot-spot characteristics are propagated to the homogenized macro-scale model using a surrogate based Monte-Carlo method to determine the the uncertainties in the macro-scale run-to-detonation distances. The relative contributions of the individual uncertainties in the micro-structural features, thermo-mechanical models and the reaction kinetics to the overall uncertainties in the run distances are also quantified.

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