

Abstract Submitted  
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**Three-dimensional Microstructure-explicit and Void-explicit Mesoscale Simulations of the Detonation of HMX<sup>1</sup>** DANIEL OLSEN, CHRISTOPHER MILLER, YAOCHI WEI, MIN ZHOU, Georgia Institute of Technology — 3D microstructure-explicit and void-explicit mesoscale simulations of the shock-to-detonation (SDT) process of pressed granular HMX are performed. The overall size scale of the models are up to  $3 \times 3 \times 15$  millimeters. The models account for the heterogeneous material microstructure, constituent distribution, morphology, and voids. A viscoplastic constitutive law, the Mie-Grüneisen EOS, and the HVRB (History Variable Reactive Burn) chemistry model are used. Companion two-dimensional simulations are also carried out using cross-sections of the 3D samples to assess the differences between the 2D and 3D simulations in a fully consistent setting. Statistically equivalent microstructure sample sets (SEMSS) are generated and used, allowing the prediction of the statistical and probabilistic Pop plots (PP). The predictions are in agreement with available experimental data in the literature. It is found that both the microstructure (heterogeneous grain size, morphology, and distribution) and voids significantly affect the PP. These effects are systematically delineated and quantified via different combinations of simulations for homogenous material with no microstructure and voids and simulations that account for microstructure, voids, and both microstructure and voids.

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