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DPDE Based Mesoscale Simulations of Shock Response of HE Composites[1] PARVEEN SOOD, SUNIL DWIVEDI, NARESH THADHANI, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332, JOHN BRENNAN, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005, YASUYUKI HORIE, (Retired) Air Force Research Laboratory, Eglin AFB, FL 32547 — The dissipative particle dynamics with energy conservation (DPDE) method is extended to simulate the shock response of high explosive (HE) composites at the micron length scale. Originally developed for soft matter, DPDE has been successfully used to simulate polymeric and soft bio materials. However, the method has yet to be shown applicable to various mesoscale responses of HE composites, including intra-grain fracture, sublimation during reaction initiation, and coupling of the gas and solid phases. The long-term objectives of the present work are to develop the DPDE code and simulate the shock response of RDX at the micron length scale and later couple it with the finite element method for a generic computational approach. The statistical volume element (SVE) is composed of micron-sized RDX particles stacked in a simple cubic configuration whose interactions are simulated using the Lennard-Jones potential. The dissipative and random force contributions of the DPDE method are used to account for the heat transport phenomena. The artificial viscosity terms are added for the first time in the DPDE formulation to successfully damp out numerical oscillations. The results show that the shock propagation in the chosen SVE with wall-boundary conditions predicts the shock response of RDX in reasonable agreement with data available in the literature.

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