Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Shock Simulations of Single-Site Coarse-Grain RDX using the Dissipative Particle Dynamics Method with Reactivity[1] MICHAEL SELLERS, U.S. Army Rsch Lab - Aberdeen, MARTIN LISAL[2], Institute of Chemical Process Fundamentals of the ASCR, IGOR SCHWEIGERT, U.S. Naval Rsch Lab - Washingon DC, JAMES LARENTZOS, JOHN BRENNAN, U.S. Army Rsch Lab - Aberdeen — In discrete particle simulations, when an atomistic model is coarse-grained, a trade-off is made: a boost in computational speed for a reduction in accuracy. Dissipative Particle Dynamics (DPD) methods help to recover accuracy in viscous and thermal properties, while giving back a small amount of computational speed. One of the most notable extensions of DPD has been the introduction of chemical reactivity, called DPD-RX. Today, pairing the current evolution of DPD-RX with a coarse-grained potential and its chemical decomposition reactions allows for the simulation of the shock behavior of energetic materials at a timescale faster than an atomistic counterpart. In 2007, Maillet et al. introduced implicit chemical reactivity in DPD through the concept of particle reactors and simulated the decomposition of liquid nitromethane. We have recently extended the DPD-RX method and have applied it to solid hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) under shock conditions using a recently developed single-site coarse-grain model and a reduced RDX decomposition mechanism. A description of the methods used to simulate RDX and its tranition to hot product gases within DPD-RX will be presented. Additionally, examples of the effect of microstructure on shock behavior will be shown.

[1]Approved for public release. Distribution is unlimited.
[2]Additional Affiliation: Department of Physics, Faculty of Science, J.E. Purkinje University, Czech Republic

Michael Sellers
U.S. Army Rsch Lab - Aberdeen

Date submitted: 28 Jan 2015 Electronic form version 1.4