SHOCK19-2019-000631

Abstract for an Invited Paper
for the SHOCK19 Meeting of
the American Physical Society

Mirrored continuum and molecular scale simulations of deflagration in a nano-slab of HMX[1]

D. SCOTT STEWART, Mechanical and Aerospace Engineering, University of Florida

We (Chaudhuri, Joshi, Lee and Stewart) have developed a continuum modeling approach, grounded in classical physical chemistry, based on the following assumptions that the states in the material can be represented by local stationary averages of the pressure (stress), temperature, and mass fractions computed from atomistic simulation, and that the mixture has well-defined molecular components, each with a complete equation of state. The continuum model, "Gibbs formulation", applies to near-atomic length and time scales, which we identify as the scales where the lowest frequency, high energy phonons equilibrate in molecular mixtures, (about six atomic radii and six to ten vibrational periods). Phase changes and chemical changes due to reaction are not in (asymptotically, long-time) equilibrium, and changes are assumed to occur on much longer time scales than those required for stress and temperature equilibration.

Recently in the Journal of Chemical Physics, J. Chem. Phys. 144, 184111 (2016), we carried out both atomistic molecular dynamics (MD) simulations and "mirrored" continuum simulations to model, thermal ignition of a nano-sized cube of explosive RDX. The CVE simulations of a constant volume explosions of RDX were performed using reactive molecular dynamics (RMD), that used REXAFF to model chemical changes in the MD simulation. The MD simulation was regarded as the exact molecular system. The continuum simulation was regarded as an interpretation and measurement of the average chemical changes between a set of identified chemical components of that molecular system.

In this work we extend these ideas to include spatial averaging to study wave propagation and spatially distributed transport, combined with chemical reaction. Joshi and Chaudhuri used RMD to simulate a sustained spatially distributed deflagration in a nano-scale slab of HMX; Journal of Physical Chemistry C, 122, 14434-14446, (2018). Those RMD results are binned for macroscopic properties using the CV formulation by spatially averaging 20 bins. Mirrored continuum simulations considered only two components, reactant and product. Both atomistic and continuum simulations show a hot spot ignition followed by a structured deflagration that propagates through the HMX slab and are compared with good to excellent agreement.

[1]GRANT: Supported by Office of Naval Research, Code 35