Virtual DCMIC Seminar Series 2021

Nearly all materials and processes, whether natural or synthetic, are innately heterogeneous, where the heterogeneity is manifested at the microscale. While chemical reactivity is intrinsically an atomistic scale event, the initiation of chemistry often stems from mechanisms occurring at the microscale. As a computational means of investigating the role of chemistry on microscale mechanisms and material microstructure, we extended the Generalized Energy-Conserving Dissipative Particle Dynamics method [1] to include chemical reactivity, denoted GenDPDE-RX. GenDPDE-RX provides a means of simulating chemical reactivity at the micro- and mesoscales, while exploiting the attributes of density- and temperature-dependent many-body force fields. The GenDPDE-RX formulation considers intra-particle reactivity via a CG reactor construct. Extent-of-reaction variables assigned to each CG particle monitor the temporal evolution of the prescribed reaction mechanisms and kinetics. The GenDPDE-RX method is verified through comparisons to the Kramers theoretical model of reaction kinetics predictions. The GenDPDE-RX method is limited to intra-particle chemical reactivity. Neither inter-particle chemical reactions nor mass diffusion between particles can occur. Therefore, we consider activation-controlled reactions typical for energetic materials. Demonstrations of the GenDPDE-RX method are performed using constant-volume adiabatic heating simulations of three different reaction models. The reaction models include both reversible and irreversible reactions, as well as multi-step reaction mechanisms. Many-body force fields using analytical forms of the Lennard-Jones and Exponential-6 equations-of-state are used for demonstration.

[1] J. B. Avalos, M. Lísal, J. P. Larentzos, A. D. Mackie, and J. K. Brennan, Phys. Chem. Chem. Phys. 21, 24891, 2019

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Generalised energy-conserving dissipative particle dynamics with reactivity. A coarse-grain method for simulations of Energetic Materials

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