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Non-equilibrium dynamics due to moving deflagration front at RDX/HTPB interface[1] SANTANU CHAUDHURI, KAUSHIK JOSHI, NAIDA LACEVIC, University of Illinois — Reactive dissipative particle dynamics (DPD-RX), a promising tool in characterizing the sensitivity and performance of heterogeneous solid propellants like polymer bonded explosives (PSXs), requires further testing for non-equilibrium dynamics. It is important to understand detailed atomistic chemistry for developing coarse grain reactive models needed for the DPD-RX. In order to obtain insights into combustion chemistry of RDX/HTPB binder, we used reactive molecular dynamics (RMD) to obtain energy up-pumping and reaction mechanisms at RDX/HTPB interface when exposed to a self-sustaining deflagration front. Hot spots are ignited near and away from the heterogeneous interface using the thermal pulse. The results show that the hot spot near interface significantly delays the transition from ignition to deflagration. We will present the mechanical response and the combustion chemistry of HTPB when the propagating deflagration front hits the polymer binder. We will discuss our efforts to incorporate this RMD based chemistry into the DPD-RX which will enable us to perform such non-equilibrium dynamics simulations on large-length scale with microstructural heterogeneities.

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