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Slow N-O chemistry in detonating oxygen balanced mixtures[1]

NIR GOLDMAN, SORIN BASTEA, Lawrence Livermore Natl Lab — The chemical evolution and states of matter of energetic materials under detonation conditions remains an open question despite decades of research. Reaction zones for many energetic materials are inferred from hydrodynamic measurements to be anywhere between nanosecond to microsecond time scales. However, the molecular level processes that govern these reaction zone lengths are poorly understood for many organic materials and composites. To this end, we have conducted quantum molecular dynamics simulations of zero and positive oxygen balance mixtures of hydrogen peroxide/nitromethane under detonation conditions to close to equilibrium time scales. We observe the formation of metastable nitrogen oxide intermediates that effectively act as an oxygen "trap" by directly slowing the formation of the equilibrium products CO_2 and N_2. This is in sharp contrast to the decomposition mechanism of carbon-rich, negative oxygen balanced energetic materials, where N-O chemistry equilibrates extremely rapidly, and carbon condensation and carbon-oxygen bond chemistry are the rate limiting steps to achieving chemical equilibrium. Further work is underway to fully determine the kinetic parameters for N-O chemistry under these conditions for possible use in hydrocode models.

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