

Abstract Submitted  
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**Chemistry Resolved Kinetic Flow Modeling of TATB Based Explosives** PETER VITELLO, LAWRENCE FRIED, MIKE HOWARD, GEORGE LEVESQUE, CLARK SOUERS, LLNL — Detonation waves in insensitive, TATB based explosives are believed to have multi-time scale regimes. The initial burn rate of such explosives has a sub-microsecond time scale. However, significant late-time slow release in energy is believed to occur due to diffusion limited growth of carbon. In the intermediate time scale concentrations of product species likely change from being in equilibrium to being kinetic rate controlled. We use the thermo-chemical code CHEETAH linked to ALE hydrodynamics codes to model detonations. We term our model chemistry resolved kinetic flow as CHEETAH tracks the time dependent concentrations of individual species in the detonation wave and calculate EOS values based on the concentrations. A validation suite of model simulations compared to recent high fidelity metal push experiments at ambient and cold temperatures has been developed. We present here a study of multi-time scale kinetic rate effects for these experiments. Prepared by LLNL under Contract DE-AC52-07NA27344.

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