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Reactive Molecular Dynamics Study of TATB Detonation Products JASON QUENNEVILLE, Los Alamos National Laboratory, THOMAS D. SEWELL, University of Missouri - Columbia, TIMOTHY C. GERMANN, M. SAM SHAW, Los Alamos National Laboratory — Under shock conditions 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) reacts to form primarily gaseous N_2, H_2O, CO_2 and CO as well as solid carbon. In a previous study of TATB thermal decomposition based on molecular dynamics (MD) simulations using the ReaxFF reactive force field, we observed a large amount of amorphous (graphite-like) carbon but no diamond structures, even at high pressures. In the current study we focus in greater detail on the reaction products mixture to assess ReaxFF predictions of both the relative stabilities of diamond-rich and graphite-rich product fluids and the equilibrium stoichiometry of CO_2, CO and solid carbon at 3250 K and as a function of pressure. In these simulations, we vary systematically the initial phase of solid carbon (pure graphite vs. pure diamond), the initial oxidation state of the remaining gaseous carbon (balanced to either pure CO_2 or pure CO), and the material density. In this poster we will summarize the results of these simulations, compare the results with both experimental observations and previous theoretical models, and discuss more generally the extent to which results obtained using short-time MD simulations can influence our understanding of the long-time behavior of real high explosive product mixtures.

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