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A comparative study of chemical kinetics models for HMX in mesoscale simulations of shock initiation due to void collapse NIRMAL RAI, Univ of Iowa, IGOR SCHWEIGERT, Theoretical Chemistry Section, US Naval Research Laboratory, H.S. UDAYKUMAR, Univ of Iowa — The development of chemical kinetics schemes for use in modeling the reactive mechanics of energetic materials such as HMX has been an active area of research. Decomposition, deflagration and detonation models need to predict time to ignition and locations of onset of chemical reaction in energetic materials when used in meso- and macroscale simulations. Modeling the chemical processes and development of appropriate kinetic law is challenging work because of lack of experimental data. However, significant work has been done in this area. Multistep kinetic models by Tarver and Tran, Henson and Smilowitz have provided plausible chemical kinetic rate laws for HMX. These models vary in the way they model the details of the decomposition process. Hence, a comparative study of different models will provide an understanding of the uncertainties involved in predicting ignition in HMX. In the current work, hot-spot ignition due to void collapse in shock compressed HMX has been analyzed using several reaction rate models, including the Tarver-Tran 4-equation model, the Henson-Smilowitz 7-equation model, and a new rate model that combines the condensed-phase decomposition rates measured by Brill et al and the detailed mechanism of nitramine flame chemistry due to Yetter et al. The chemical models have been incorporated in a massively parallel Eulerian code SCIMITAR3D. The variations in the predicted thresholds due to differences in the rate models will be discussed.

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