

Abstract Submitted
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Reduced Order Models for Reactions of Energetic Materials EDWARD KOBER, Los Alamos National Laboratory — The formulation of reduced order models for the reaction chemistry of energetic materials under high pressures is needed for the development of mesoscale models in the areas of initiation, deflagration and detonation. Phenomenologically, 4-8 step models have been formulated from the analysis of cook-off data by analyzing the temperature rise of heated samples. Reactive molecular dynamics simulations have been used to simulate many of these processes, but reducing the results of those simulations to simple models has not been achieved. Typically, these efforts have focused on identifying molecular species and detailing specific chemical reactions. An alternative approach is presented here that is based on identifying the coordination geometries of each atom in the simulation and tracking classes of reactions by correlated changes in these geometries. Here, every atom and type of reaction is documented for every time step; no information is lost from unsuccessful molecular identification. Principal Component Analysis methods can then be used to map out the effective chemical reaction steps. For HMX and TATB decompositions simulated with ReaxFF, 90% of the data can be explained by 4-6 steps, generating models similar to those from the cook-off analysis. By performing these simulations at a variety of temperatures and pressures, both the activation and reaction energies and volumes can then be extracted.

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