

Abstract Submitted
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Kinetics Modeling and Numerical Simulation of Reactive Materials¹ SUNHEE YOO, D. SCOTT STEWART, U. of Illinois, MechSE, DAVID E. LAMBERT, Air Force Research Laboratory-Munitions Dir. AFRL/RW, SUNJIN CHOI, U. of Illinois, MechSE — Simulations with reduced kinetic models are used to study shock ignition and detonation in reactive materials that may support non-classical detonation. Porous aluminum Teflon oxidizer mixtures that support combustion reactions in air are considered, as a member of a class of materials with intrinsic interest. We recast a phenomenological theory² with realistic kinetics with end products; AlF_3 , C and CO_2 . Intermediate products include at least thirty elementary reactions; a sub-set can be selected to simplify, but a hard problem remains. We use the multi-scale asymptotic “G-scheme” proposed by M. Valorani, S. Paolucci and reduce a dynamical system consisting of the intermediate reactions and rates, conservation laws and porosity evolution. Results of the multi-species evolution and its impact on rapid self-oxidizing combustion and possible detonation conditions and the computational methods are presented.

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²Yoo, S., D.S. Stewart, and D.E. Lambert, “Modeling a Supersonic Solid State Detonation in an Overdriven Porous Mixture of Aluminum and Teflon,” J. Mat. Sci. Forum V. 673, Explosion, Shock Wave, and High-Energy Reaction Phenomena, Sept 2010

D. Scott Stewart
U.of Illinois, MechSE

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