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The effect of the thermodynamic closure on shock-to-detonation transition modeling in condensed-phase high explosives CARLOS CHIQUETE, MARK SHORT, STEPHEN VOELKEL, Los Alamos National Laboratory — The need for accurate prediction of detonation initiation and propagation in high explosives (HEs) has lead to various empirical constitutive models for the HE's equation of state (EoS) and reaction rate. These experimentally calibrated models are used at the continuum level where it is possible to efficiently calculate detonation wave motion at the engineering scale. A transition from the (solid) reactant to the (gas) product state occurs via a single irreversible reaction, requiring a closure condition between the two phases which must then coexist in a single material element. Different closures have been used in the past, for example, pressure-temperature equilibrium. However, analysis of more physical, explicitly 2-phase modeling approaches where each phase's thermodynamic state can evolve have shown that temperature equilibration occurs over a much longer time scale than the corresponding reaction zone scale. Nevertheless, this "nonphysical" closure has been shown to capture the shock-to-detonation-transition (SDT) for many HEs. To clarify this, we systematically vary the closure condition and isolate its effect by fixing the EoS models and reaction rate form. Computational results using the various closures will then be compared and contrasted with respect to SDT data.

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