

DEVELOPMENT AND APPLICATION OF A MULTI-COMPONENT JWL EQUATION OF STATE

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An extension of the JWL equation of state (EOS) with chemical reaction has been developed for a gas-phase mixture undergoing detonation and post-detonation combustion. The formulation allows multiple component gases to be treated within a single equation of state in a manner analogous to standard ideal gas mixture relations. The component gases are tracked individually within the EOS using mass fractions and the mixture retains a single temperature, density and pressure across all the components. The formulation is built on a consistent energy basis through the use of NIST or JANAF thermochemical tables. It allows for temperature-dependent heat capacities, increasing the accuracy of temperature calculations over constant heat capacity methods. Reactions among component gases may be computed through the application of a kinetic rate law.

The development of this model was primarily motivated by the need to accurately compute post-detonation environments including fuel-rich scenarios with subsequent combustion of the detonation product gases with the surrounding atmosphere. Traditional hydrocode analyses would model the detonation products and air as separate materials with separate equations of state often built on differing energy bases. Moreover, the multi-material algorithms modeling the advection process may reduce to first-order accuracy at material interfaces. These factors make reaction modeling difficult and can reduce overall simulation accuracy. Combining the gases into a single material with a single EOS eliminates multi-material modeling while keeping the materials on a consistent energy basis and simplifying reaction modeling.

To demonstrate application of the extended JWL model, three simulations are presented. The first two involve detonations of fuel-rich explosives that include post-detonation combustion with air in an enclosed chamber. The third involves a PETN detonation with temperature measurement through absorption spectroscopy. Both constant and variable heat capacities are considered. The resulting pressures and/or temperatures are compared to each other and against experimental results. These comparisons are presented and show promise that this extended EOS can be advantageous in simulating a variety of blast and shock scenarios.