Equation of State Effects on a Chemically Based Reactive Flow Model of LX-17

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We link high-pressure chemistry models with hydrodynamics and kinetics to study the detonation of the non-deal explosive LX-17. For the equation of state we use statistical-based thermo-chemical equilibrium calculations based on an exp-6 (Buckingham potential) fluid, calibrated to high pressures (~ few Mbars) and high temperatures (~ 20000K). Included chemical species have multiple phases and include liquid water, water vapor, graphite, diamond, two phases of liquid carbon, and small- and large-scale graphite particulates among many others. We also include kinetic decomposition of LX-17 and some large molecules, which we discuss in a companion paper. In this paper, we study the influence of the equation of state of the primary constituents in the reaction zone on the kinetics and detonation properties of LX-17. In particular, the appearance of such large molecules such as HCNO in the high-pressure reaction zone can have a strong influence on the detonation properties. The appearance of these large molecules in the reaction zone depends on their assumed equation of state and non-equilibrium kinetic processes. We compare our kinetic and equation of state model to a wide variety of experimental data.

Auspices Statement:

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This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.