Kinetic Flow Modeling of LX-17

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1 Kinetic detonation modeling of non-ideal, carbon-rich explosives

Detonation waves in non-ideal, insensitive carbon-rich explosives, such as those based on TATB, are believed to have multi-time scale regimes. The initial burn rate of LX-17 (92.5% TATB, 7.5% KLF) has a sub-microsecond time scale, while significant late-time slow release in energy due to diffusion limited growth of carbon clusters is likely to occur over a period of tens of microseconds. In the intermediate time scale of microseconds, the concentrations of product species may change from being in equilibrium to being kinetic rate controlled as the temperature and density drops in the reaction zone. We use the thermo-chemical code CHEETAH [1] linked to a multi-dimensional ALE hydrodynamics model to model LX-17 detonation waves. CHEETAH is a multi-phase first principle based equation of state model which uses as its starting point exponential 6 molecular dynamics modeling. For efficiency, CHEETAH maintains 2D and sparse multi-dimensional equation of state databases that are calibrated to experimental data. The linked CHEETAH-ALE model treats slowly reacting chemical species using kinetic rate laws, with chemical equilibrium assumed for species coupled via fast time-scale reactions. Typically greater than 30 species and phases are simultaneously treated. This results in a flexible, self-consistent treatment of the equation of state which allows for significant variations in concentrations of condensed and gaseous species with time. We present here a study of multi-time scale kinetic rate effects for detonation waves. Details of the EOS will be presented in a separate paper. In our rate equation modeling we include separate rates for the rapid transformation of the un-reacted explosive to product gases, for the slow growth of a small particulate form of condensed graphite to a large particulate form, and for intermediate time scale chemistry of species which dominate the detonation reaction zone. We present here results for detonation wave modeling of cylinder and rate-stick experiments.

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References

[1] Fried, L. and Howard, M., "Cheetah 3.0 Users Manual", LLNL UCRL-MA-117541, 2001.

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