GRANULAR EXPLOSIVES AND INITIATION SENSITIVITY

Ralph Menikoff
Theoretical Division, Los Alamos National Laboratory
Los Alamos, NM 87544

Experimentally measured reaction rates are temperature dependent; usually, characterized by an Arrhenius rate law,

\[ R(T) = Z \exp(-T_a/T). \]

Yet for numerical simulations of detonation waves in plastic binded explosives (PBX) empirical pressure dependent reaction rates, such as ``Forest fire'' or the ``Ignition and Growth'' model, are typically used. The underlying reason for this disparity between fundamental chemical rate laws and empirical burn models is due to the fact that a PBX is a heterogeneous material consisting of small crystals of an explosive material held together with an inert binder material. Due to the strong temperature dependence, the overall reaction rate of a heterogeneous explosive is dominated physically by peaks in the temperature field, called hot spots. The hot spots occur on the length scale of the heterogeneities and are absent from continuum models based on homogenized constitutive properties. Consequently, the effective burn rate is not determined by the average temperature. Empirical burn rates represent ``sub-grid'' models which account for the short wavelength reaction phenomenon not resolved within a simulation.

Hot spots strongly affect the ignition process for a detonation wave. Experiments have shown that shock initiation is qualitatively different in a PBX than the thermal explosion theory describing a homogeneous explosive. Appropriately calibrated, burn models can reproduce important ignition characteristics such as run distance to detonation as a function of shock pressure. However, empirical burn rates are only effective for applications in which the hot-spot distribution is similar to that occurring in the experiment used to calibrate the burn model. In other words, currently available burn models have a limited domain of applicability.

The limitation of burn models is most severe for weak ignition, such as a deflagration-to-detonation transition. Simulations do capture qualitatively the evolution leading to a detonation wave but do not accurately predict the ignition threshold. This is
an important issue for explosive safety since accident scenarios typically involve weak stimuli and are in a very different regime from the prompt initiation for which explosive systems are designed and burn models are calibrated. In addition, accident scenarios frequently lead to damaged explosives. Damage is known to greatly increase the sensitivity of an explosive to initiation. In effect, damage introduces additional heterogeneities and exacerbates the effect of hot spots.

Compared to a homogeneous explosive, a granular explosive has two distinctive properties; a heterogeneous length scale from the grain size distribution, and an additional degree of freedom from porosity. These are key features of a damaged material. Consequently, a granular explosive is a suitable model, albeit simplified, for a damaged explosive. With a typical grain size on the order of 0.1 mm, the spatial and temporal scales relevant to hot-spots, microns and sub micro-seconds, respectively, are too small to observe experimentally with currently available diagnostic techniques. However, meso-scale simulations can be used as numerical experiments to gain an understanding of the mechanisms that generate hot spots and their subsequent evolution. In meso-scale simulations individual grains are resolved and the time evolution computed based on a continuum mechanics model.

Simulations of piston driven compaction waves in a granular bed of coarse grain HMX have been performed. Piston velocities from 200 m/s to 1000 m/s were chosen. This covers the range from weak ignition experiments that display a deflagration-to-detonation transition to prompt shock ignition. However, the focus of this study is on the mechanical behavior (the generation of hot spots), and the grains are treated as inert. Averaging the flow transverse to the propagation direction results in a smooth quasi-static wave profile. Weak partly compacted waves are fully dispersed while strong fully compacted waves have a wave width of 1 to 2 grain diameters. As expected the end states across a compaction wave obey the Hugoniot jump conditions. The temperature fluctuations behind the wave front are in the range that would affect ignition.

Hot spots can be much smaller than a grain diameter. They are affected by dissipative mechanisms. The simulations include plastic work, frictional heating modeled as shear viscosity and bulk viscosity. The hot-spot distribution behind the compaction wave is discussed. For weak initiation, material strength hence plastic work and shear heating are important for generating hot spots. In the regime of prompt shock initiation, void collapse is the dominate mechanism for generating hot-spots. The long term goal of this work is to develop an improved "sub-grid" burn model which is rationally based on the underlying physics of hot spots.