A Statistical Treatment of Hot Spots for the Reactive Burn Modeling of Solid Explosives

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1. Introduction

This paper describes a mechanistic burn modeling of solid explosives that combines the general purpose hot-spot model developed earlier (Yano et al. 2001) and a statistical treatment of energy localization that is thought to be the formation process of hot spots (spatially localized regions of high temperature). A primary motivation is to increase the predictive capability of burn modeling by using an explicit description of hot spot evolution, ignition and burn processes, and temperature-dependent kinetic equations. For proof-of-concept calculation the burn model is used to simulate shock initiation and detonation in one space dimension using the data for RDX.

2. Unifying Hot-Spot Model

The concept of hot spots has been used to describe the ignition of solid explosives by mechanical insults such as impact and shock loadings over the last fifty years. Primary mechanisms responsible for the creation of hot spots (energy localization) are thought to be void collapse, friction, and shear (e.g., Kang et al. 1992, Dienes 1995, and Frey 1981). These mechanisms transform overall mechanical energy into localized heating. But none of the models that are focused on a single physical mechanism has a universal appeal, because it is doubtful that any one mechanism dominates in vastly different ranges of mechanical loading (Khasinov, et al. 1996).

The new, unifying hot-spot model was developed to consider energy localization for various regimes of loading on a common framework by focusing attention on a mathematical abstraction of the fundamental features of three primary mechanisms: void collapse, shear banding, and friction. These features are, however, described without introducing the mechanism-specific traits. In this way, the issue of how to consider the localization as dependent on the state of the material is set aside temporarily. Instead, attention is focused on the parametric representation of the energy localization that is consistent with detailed mechanistic models.

In the new model the geometry of energy localization is simplified to a plane structure consisting of the following key features: a region of localized heating surrounded by material with a lower or zero heating rate; the existence or creation of a space next to the heated zone that is occupied by gases; energy transfer between the regions; and reaction chemistry within the gas, at the gas-solid surface, or both. What is important in this model is that attention is shifted from "hot spots" to "gas producing, hot interfaces." This feature is exploited in development of a statistical treatment of hot-spot evolution, incorporating a size distribution for energy localization.

3. Statistical Treatment of Hot Spots

A statistical treatment of hot-spot evolution is based on two main ideas. The first is a modified idea of Cochran (1986) and assumes that shock (or impact) loading creates a number of locally heated sites (they are thin bands in our model). For our initial attempt, we hypothesized that the size distribution for heated sites is exponential and the rate of production is proportional to the overall dissipated mechanical energy (e_d). The governing equations are solved by the method of moments. The result

is an analytic expression for the specific surface area of locally heated sites (f_A) where solids transform into gases at the appropriate conditions of temperature and pressure.

$$f_A = \frac{? _m f_N}{?}\left[1 - a_m \exp\left(-? \frac{e_d}{e_d^o}\right)\right],$$

where the product $? _m f_N$ represents the maximum area available for chemical reaction, and the parameters ?, a_m, and e_d^o are interrelated and depend on the conditions such as initial porosity, the saturation fraction of hot spots, and the corresponding energy input.

The major differences between our model and the Cochran's are (1) the source rate is a function of dissipated energy at the macrolevel in place of relative compression, and (2) the source rate is only concerned with the production of heated sites, and all the other mechanisms are treated mechanistically by the hot-spot model. So, for example, the ignition in our model occurs when self-sustained reactions are initiated in the above-mentioned reactant gases. The process is path-dependent. In the Cochran model, however, the ignition is preset to happen continuously at a specified rate as a function of pressure.

The second idea is that a collection of hot spots may be aggregated into a single, super hot spot through use of f_A for the heat and mass transport across the reacting solid-gas interface. The result is a scaled, localized heat flux $\hat{F}_{hs}$ for the super hot spot in terms of overall dissipated energy e_d.

$$\hat{F}_{hs} = \frac{M}{d}\frac{d}{dt}\left(\frac{e_d}{f_A}\right),$$

where M is the explosive mass in a representative volume (a computational cell) and d is the width of localized-heating sites. The product of d and f_A comprises the total volume

of locally heated sites. In our model, $\widehat{F}_{hs}$ is the expression that transforms the mechanical energy into localized heating and governs the ignition behavior. Once ignited, the chemistry drives the surface burning wave.

4. Model Calculations

To implement the burn model for hydrodynamic reactive flow calculations, We need a mixture rule and the equations of state for the unreacted solid explosives and the product gases. In this study we followed the formulation by Massoni et al. (1999). This approach assumes common particle velocities among constituents and mass based averaging for mass, momentum, and internal energy. Additionally, the equation of state for each constituent is written in a Mie-Grüneisen form. For the dissipated energy, we followed Kip (1987) and used the energy associated with the artificial viscosity.

One-dimensional hydrodynamic equations are solved for shock ignition and detonation using a standard leap-frog method and a two-term artificial viscosity-Materials parameters including chemical kinetics are those for RDX (Kang et al. 1992). This choice is historical in that the hot-spot model is first tested for RDX as a model material (Yano et al. 2001). The material is assumed to have an initial porosity of 1%.

Shock loading is initiated by a near, symmetric impact where the impactor is assumed to be an inert solid RDX. A thin buffer is added between the impactor and the reactive RDX to avoid a false ignition due to oscillations near the impact plane. Figure 1 shows a typical run-to-detonation behavior observed in simulation where the computational cell size was 10 μm.

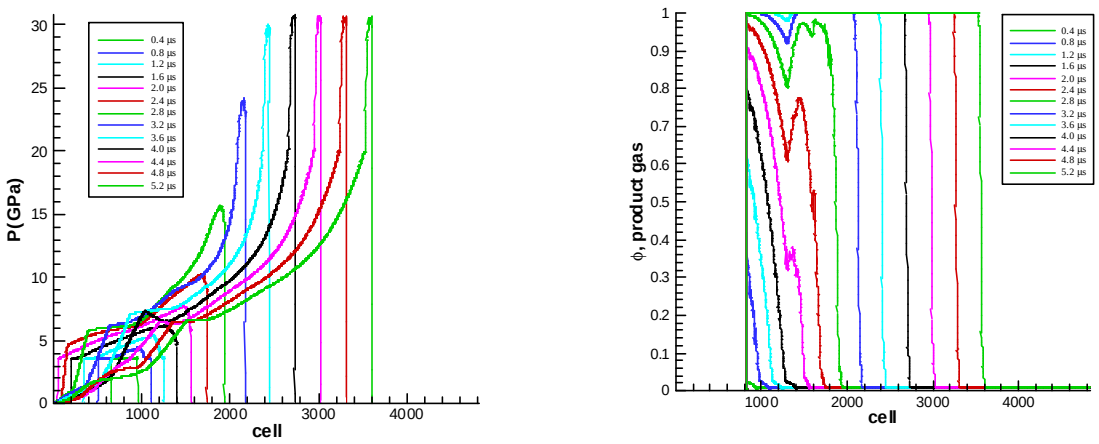

Fig. 1. Growth-to-detonation behavior is shown in (a) where the steady detonation propagates at the velocity of 8 km/s. The value in a LASL report is 8.6 km/s at 33.7 GPa (CJ state). Fractions of the product gas shown in (b) indicate an heterogeneous ignition.

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