Propagation laws and direct initiation for quasi-steady curved detonations with chain-branching kinetics

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Abstract

Propagation laws are derived for quasi-steady, near-CJ, weakly curved detonations for a chain-branching reaction model having two components. The first is a thermally neutral chain-branching induction stage governed by an Arrhenius reaction with a large activation energy, which terminates at a transition layer where conversion of fuel into an intermediate species (chain-radical) occurs. The second is an exothermic main reaction layer (or chain-recombination zone) having a temperature-independent reaction rate.

For cylindrically or spherically expanding waves, a multi-valued detonation velocity-curvature relationship is found, similar to that found previously for a state-sensitive one-step reaction. The change in this relationship is investigated as the length of the main reaction layer is changed. We also discuss the implications that chain-branching reaction kinetics has on predictions of critical detonation initiation energy based on detonation-velocity curvature laws. Finally we conduct some calculations that illustrate the important effect that transverse flow variations may have on the quasi-steady propagation of nonplanar detonation fronts. Such variations may be important for the propagation of cellular gaseous detonation fronts and for the axial propagation of detonations in a cylindrical stick of condensed phase explosive.

Introduction

Detonations are high-speed, shock driven, reaction waves. Generally they propagate at the Chapman-Jouguet (CJ) velocity D_{CJ} for which the reaction zone solution passes through a sonic point in a frame of reference attached to the detonation shock (Fickett & Davis 1979). Planar Chapman-Jouguet detonation waves are seldom observed, but curved fronts are. Examples include detonations propagating axially in cylindrical sticks of high explosives (Bdzil 2000), detonations in systems that undergo an area change, detonations diffracting around corners and the local fronts of cellular detonations (Klein, Krok & Shepherd 1994). Consequently there is substantial interest in understanding how the propagation speed of a detonation varies with the geometry of the non-planar

front, i.e. in the derivation of intrinsic surface propagation laws for the motion of curved detonations.

Much of the work on detonation shock dynamics for slowly evolving or quasi-steady waves has been conducted for simple one-step reaction mechanisms of the form

$$Fuel \rightarrow Product.$$

The rates may be either state-insensitive or state-sensitive, with the sensitivity controlled by the activation energy of the reaction. For example, for a reaction rate

$$r = k(1-\lambda)^{\nu}, \tag{1}$$

where k is the rate constant, $\nu < 1$ is the order of the reaction and λ is the reaction progress variable, it is found that the detonation velocity D_n depends on the shock curvature κ ($\ll 1$) in an essentially linear fashion such that

$$D_n = 1 - \alpha\kappa + O(\kappa^{1/\nu}), \tag{2}$$

where α (> 0) is a constant that depends on an integral through the entire reaction zone structure (Stewart & Bdzil 1988).

On the other hand, for a highly state-sensitive reaction rate of the form,

$$r = \epsilon(1-\lambda)^{\nu} \exp\left[\frac{1}{\epsilon}\left(\frac{1}{c_0^2} - \frac{1}{c^2}\right)\right], \tag{3}$$

where c_0 is the one-dimensional steady sound speed at the shock, and $\epsilon \ll 1$ is the inverse activation energy, the detonation velocity-curvature relation takes the form

$$D_n^{(1)} + \frac{\alpha_2}{a\alpha_1} \ln\left[1 - a\kappa^{(1)} \exp(bD_n^{(1)})\right] = 0, \tag{4}$$

where $D_n = 1 + \epsilon D_n^{(1)}$, $\kappa = \epsilon\kappa^{(1)}$ and a, b, α_1 and α_2 are constants. Here the curvature and detonation speed are related by the scale $D_n - 1 = O(\kappa) = O(\epsilon)$. The nonlinear relation (4) gives a multi-valued response; there is a critical value of curvature beyond which no solutions exist which pass smoothly through a sonic point.

Thus far, little work has been conducted on propagation laws for nonplanar detonations with more realistic chemical reaction pathways. In the present work, we study a two-step chain-branching reaction sequence, a model motivated by the three-step chain-branching model previously studied by Short & Quirk (1997) and Short, Kapila & Quirk (1999). A schematic of the reaction model is shown in figure 1.

The model has two components: a thermally neutral chain-branching induction zone and an exothermic main reaction layer or chain-recombination layer of finite extent. We note that this mimics the actual structure of detonations not only in gaseous systems but also in condensed phase explosives. The extent of the induction zone is controlled by a reaction rate of Arrhenius form, but no heat is released due to reaction. This mimics the fact that chain-initiation and chain-branching reactions typically liberate only a small amount of heat, while the length of the induction zone is a sensitive function of the shock state. The end of the induction zone corresponds to the point where a rapid conversion of fuel into radical species occurs as in Short & Quirk (1997). The reaction rate in the

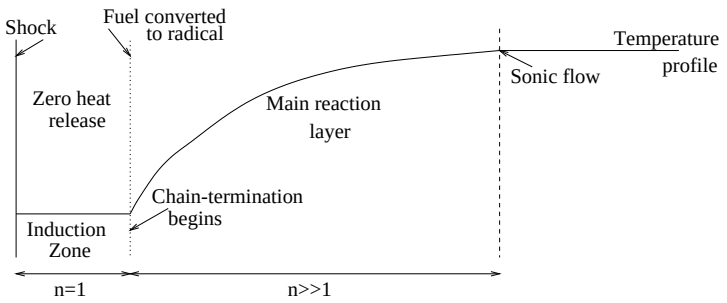

Figure 1: A schematic of the steady detonation structure for the two-step chain-branching reaction model.

exothermic chain-recombination or main reaction layer is taken to be independent of temperature, typical of many chain-termination reactions. The ratio of the length of the induction layer to the main reaction layer is controlled by the rate constant k in the main reaction layer, and plays the role of the chain-branching cross-over temperature in Short & Quirk (1997). Although this model falls short of full reaction kinetics, in contrast to the classical one-step Arrhenius model it does retain some of the essential chemical dynamics of a real chain-branching reaction.

Results

Using the chemical model described above it is possible to derive a modified detonation velocity-curvature law for curved detonation waves that accounts for the presence of both a state-sensitive induction zone and a finite region of heat release. This law is obtained in an asymptotic fashion, by exploiting assumptions of quasi-steadiness, weakly curved fronts and a propagation velocity close to the Chapman-Jouguet velocity. The equation has a number of interesting features, which will be further explained during the talk.

For cylindrically or spherically expanding waves, the detonation velocity-curvature law generates a multi-valued response that can be used, for example, to provide a critical energy E_c for detonation initiation (He & Clavin 1994). Figure 2 shows one example of how the critical initiation energy of such a theory would vary as the ratio of the length of induction zone to main reaction layer changes, a factor controlled by the rate constant k in the main reaction layer, for a detonation which runs at a one-dimensional steady Chapman-Jouguet velocity of 1800m/s, initial density $\rho_0 = 1.1741$ kg/m^3, $\gamma = 1.2$ and induction zone activation energy 14, in which the main reaction layer extent is kept fixed at $5 \times 10^{-3} m$.

The conclusion is that the energy required to initiate a detonation would increase as the extent of the induction zone increased. This supplies valuable information on the required initiation energy of real chemical mixtures by examining the ratios of the induction to main reaction layer lengths in the steady planar detonation wave.

On the other hand, for non-cylindrically or -spherically expanding waves, we will show that transverse flow variations must generally be accounted for our two-stage reaction structure. Two situations where such variations may be important are the cellular structures observed in gaseous detonations and the axial propagation of a quasi-steady curved detonation in a cylindrical stick of high explosive (also known as a rate-stick

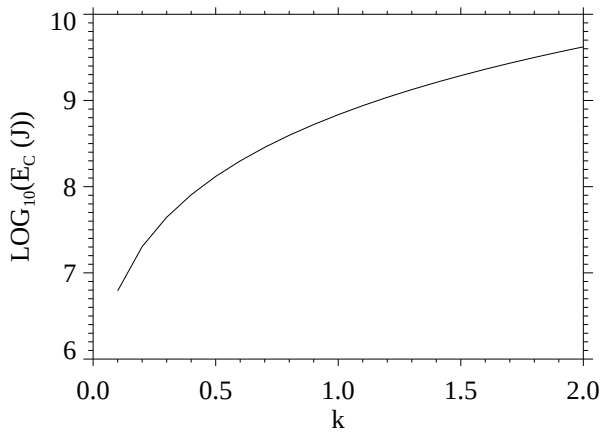

Figure 2: Variation of the critical initiation energy E_c (J) with rate constant k for a spherically expanding wave

(Bdzil 1981)). Our evolution equation predicts detonation velocity-curvature laws for such situations. The one example shown in figure 3 illustrates the velocity deficit $\epsilon D_n^{(1)}$ from the planar Chapman-Jouguet velocity caused by a curved detonation wave running down a cylindrical stick of condensed explosive, with symmetry conditions applied on the stick axis and conditions which determine the streamline deflection (a confinement condition) on the stick edge.

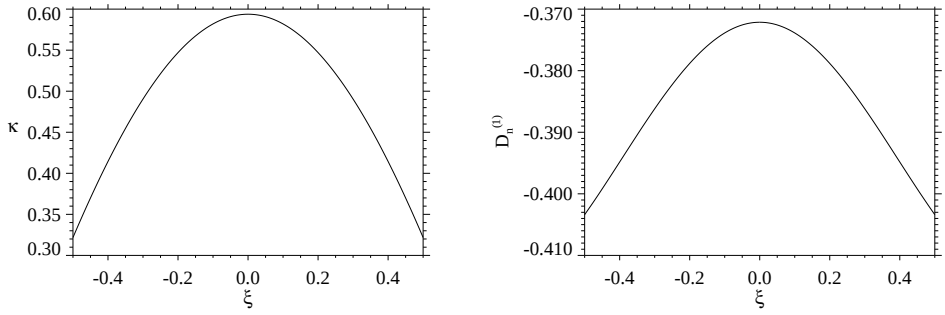

Figure 3: (a) Variation of curvature with radius along a detonation shock propagating in a rate-stick of radius $\xi = 0.5$. (b) Corresponding variation of $D_n^{(1)}$.

Substantial variations are observed, which can be explained by the model evolution equation, and will be compared with experimental data.

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