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Propagation and failure mechanism of cylindrical detonation in free space

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ABSTRACT

Cylindrical detonations propagating in free space characterized by different activation energies were computationally studied. It is found that unstable detonations with the 2-D cellular structure have more velocity deficit than those without the cellular structure computed with the 1-D simulation. The weakening is due to lengthening of the detonation structure and the unreacted pocket behind the cylindrical front, while propagation sustenance depends strongly on the re-amplification and regeneration of transverse shocks and triple points. For low activation energies, cellular detonation can be initiated in free space through the subcritical initiation path due to absence of unreacted pockets, and the propagation is not very sensitive to the attenuation of transverse waves and triple points. However, for high activation energy the unreacted pocket aggravates initiation such that even a cellular detonation first established is prone to quench due to the lack of re-amplification of the transverse wave and the triple point. When considering confinement, it is demonstrated that a detonation that quenches in free space can be reinitiated in confined space.

1. Introduction

Detonation waves are intrinsically unstable, exhibiting complicated three-dimensional cellular structure that consists of triple-shocks, transverse shocks and turbulent shear layers [1–8]. The extent of the instability–stable, mildly unstable and highly unstable, has been found to depend sensitively on the (global) activation energy, E_a, of the underlying reaction mechanism. Specifically, with increasing E_a, the propagation of a planar detonation without cellular instability respectively exhibits no pulsation, regular pulsation, and irregular pulsation; while for propagation with cellular instability the front takes regular, mildly irregular and highly irregular patterns. Furthermore, the pulsation is enhanced when the front has a positive curvature, which could lead to significant changes in the initiation and self-sustenance of the propagation [9–11].

He and Clavin [10] studied theoretically and numerically the direct initiation of cylindrical and spherical detonations by a localized energy source, and found that successful initiation requires a larger energy source relative to that for the planar detonation. Watt and Sharpe [12] performed a 1-D linear stability analysis of the weakly curved, quasi-steady detonation, and showed that even weak curvature has a significant destabilizing effect. Ng and Lee [13] found that intrinsic instability can suppress successful detonation initiation, as further reported in the 1-D simulation of Watt and Sharpe [11]. Eckett et al. [14] also observed that, for direct initiation with near-critical initiation energy, the initial overdriven detonation first decays to be quasi-steady, and then rapidly quenches by pulsating instability. He and Clavin [10] theoretically showed that there exists a critical initiation radius below which the generalized Chapman–Jouguet solution does not exist, while a subsequent study [14] showed a non-uniqueness of the critical initiation energy, and as such suggested that their quasi-steady assumption could be the limitation for direct initiation. Short et al. [15] demonstrated theoretically the existence of quasi-one-dimensional, quasi-steady, self-sustaining convergent detonation waves by using a two-step sequential reaction mechanism, with the second stage being endothermic, and compared these theoretical results with the direct numerical simulation of imploding detonations in cylindrical and spherical geometries.

Experimental and numerical studies [16–19] have also shown that regular and irregular cellular patterns correspond to stable and unstable detonations. For mixtures with regular cellular detonation patterns, corresponding to low activation energies, the gas

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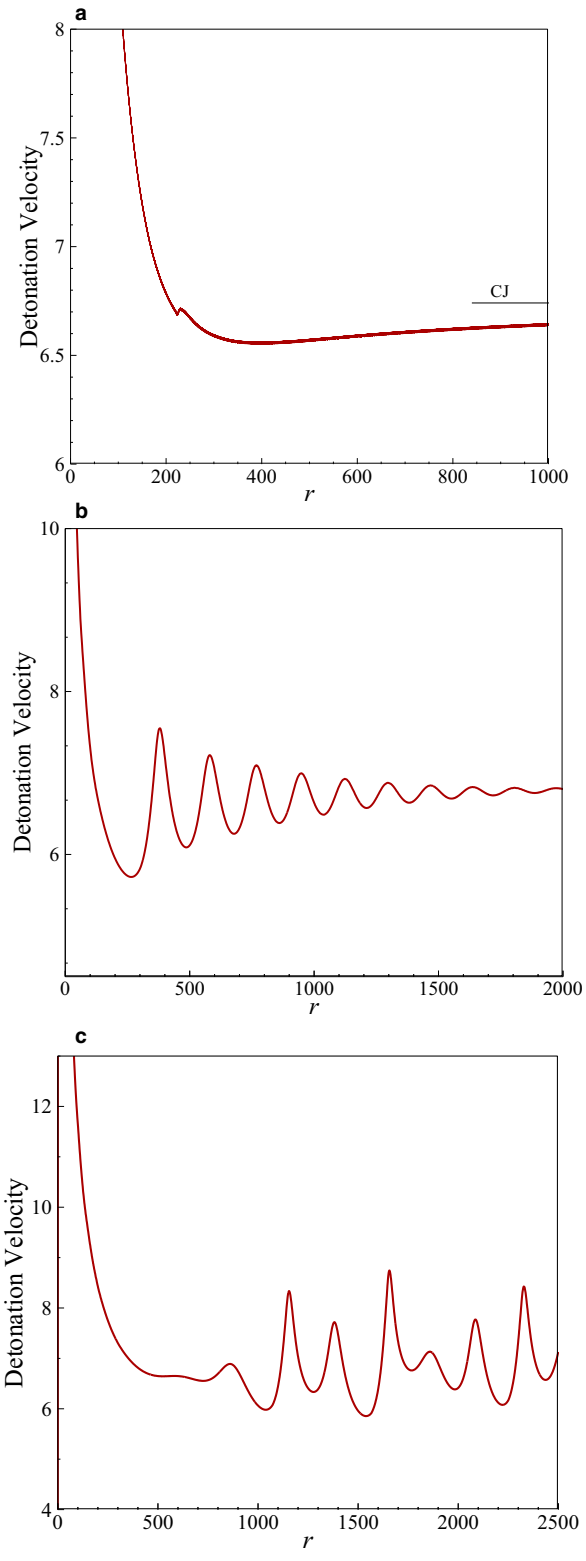

Fig. 1. Change of average velocity as function of radius: (a) $E_a = 15$ and $E_s = 3000$; (b) $E_a = 24$ and $E_s = 12{,}000$; (c) $E_a = 27$ and $E_s = 30{,}000$.

entering the shock front is readily ignited through the classical shock ignition mechanism, leading to fast reaction rates. However, for mixtures with irregular cellular detonation patterns, corresponding to large activation energies and hence strong and local chemical rate sensitivities, small-scale chemical activity at the irregular front, as well as pockets of unreacted gas breaking away from the front, characterize the reaction zone structure [20–24]. Furthermore, new transverse waves are continuously generated from local instabilities in the reaction zone, producing complex dynamics. Consequently, transverse wave interaction is particularly relevant for the self-sustaining propagation of irregular cellular detonations when shock ignition is not sufficiently strong.

Recently, there has also been substantial interest on the role of the transverse wave in cellular detonation through confinement [11,21,25–27]. Specifically, Radulescu and Lee [21] conducted experiments in tubes with porous walls, and showed that while transverse wave interactions are essential in the ignition and propagation of irregular cellular detonations, they do not play significant role in the propagation of regular cellular detonations. This is because failure of these stable detonations is mainly due to the global curvature caused by the mass divergence into the porous wall. Furthermore, Mazaheri et al. [26] experimentally and numerically examined detonation propagation in a channel with porous walls, and identified the role of diffusive turbulent mixing and transverse waves in controlling the detonation limits. Jackson and Short [27] also examined evolution of the normal detonation velocity with local shock curvature for weakly unstable cellular detonations, and found that the curvature of the Mach shock is responsible for driving the cellular detonation.

Recognizing the above worthwhile studies, we nevertheless also note that they were mainly concerned with the sustenance and quenching mechanisms of weakly curved detonations in *confined* space, typically within channels and square tubes. However, the corresponding phenomena in *free* space [25,28], and the associated roles of the transverse wave in their propagation responses, have not been adequately studied and contrasted with those in confined space. In response to such a need, we have simulated cellular detonation in free space, and will show in due course the fundamentally different mechanisms governing the propagation and quenching of detonation in free and confined spaces. The simulation was conducted by using a high-resolution parallel code based on the WENO conservative finite difference scheme, and subsequently compared with the corresponding detonation in confined space to reveal the role of the re-amplification of the transverse wave and the triple point.

We now state the governing equations and the numerical method, and then present and discuss the results.

2. Formulation and numerical method

In the 2-D coordinate, the equations of mass, momentum and energy conservation as well as the heat transfer equation are as follows,

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} = S,$$

where the conserved variable vector U, the flux vectors F and G, and the source term S are given, respectively, by

$$U = (\rho, \rho u, \rho v, E, \rho Y)^T,$$
$$F(U) = \left(\rho u, \rho u^2 + p, \rho uv, u(E+p), \rho uY\right)^T,$$
$$G(U) = \left(\rho v, \rho vu, \rho v^2 + p, v(E+p), \rho vY\right)^T,$$
$$S(U) = (0, 0, 0, 0, \rho\omega)^T.$$

Here u and v are the Cartesian components of the fluid velocity in the x and y directions respectively, and ρ is the density, p the pressure, and T the temperature related through the ideal gas law, $p = \rho R_u T$, where $R_u = R/m$, m is the average molecular weight,

$$E = \frac{p}{(\gamma - 1)} + YQ + \frac{1}{2}\rho(u^2 + v^2)$$

is the total energy per unit volume, Y the reactant mass fraction, and Q the heat of reaction per unit volume and γ the specific