Effect of Spatial Inhomogeneities on the Propagation Limit of Gaseous Detonations

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1 Introduction

Over the past 60 years, from the cellular imprints left on the smoke foils to the shadow patterns recorded on schlieren images, a substantial collection of experimental evidence revealing a transient, multi-dimensional wave structure of gaseous detonations has been uncovered [1, 2]. Using high-speed schlieren and self-emitted light photography, the spatial non-uniformities in the reaction zone of gaseous detonations have been visualized [3]. While there are regions of rapid reaction triggered by the adiabatic compression of strong Mach stems, weakly-shocked pockets of reactants may undergo a much slower burnout, likely via a turbulent flame-like process [3–5]. Given such a complex nature of detonation waves in gaseous mixtures, the well-established theoretical models are perhaps oversimplified to describe the key mechanisms underlying the detonation propagation behavior. Most theoretical models are developed on a basis of the steady, quasi-one-dimensional Zel'dovich-von Neumann-Döring (ZND) solution assuming a smooth wave front curvature and a laminar-like reaction zone structure. The question then arises as whether the wave propagation behavior is influenced by the self-developed non-uniformities in the detonation reaction zone.

Although numerical simulations seem to be an amenable approach to tackle the above-mentioned problem, researchers are further frustrated by the fact that, as shown for example by Mazaheri *et al*. [6, 7], a fully converged result cannot be obtained for a two-dimensional, cellular detonation wave structure at a numerical resolution of 10^3 to 10^4 computational cells per half-reaction-zone length. In this paper, a new approach will be used to computationally examine the effects of a spatially inhomogeneous reaction zone on the detonation propagation dynamics. Instead of exhausting the computational efforts to resolve the naturally developed instabilities, a non-uniform reaction zone can be induced by imposing spatial inhomogeneities to the initial reactive medium. This approach was recently used by Mi *et al*. [8, 9] to investigate the effect of

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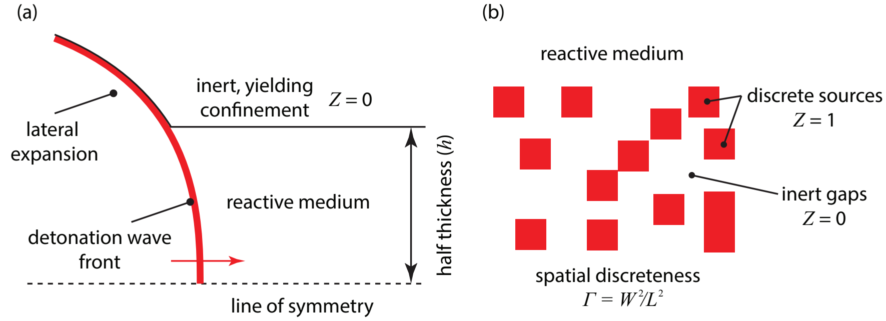

Figure 1: Schematic illustration of (a) a finite-sized detonable mixture with an inert, yielding confinement and (b) a reactive medium with randomly distributed discrete sources.

spatial inhomogeneities on the wave propagation velocity in adiabatic detonation systems. In this current study, spatially random distributions of inhomogeneities are introduced to a system of a mixture of detonable gases confined by an inert gas layer. In such a system, detonation waves experience losses due to the lateral expansion in the reaction zone, and there exists a critical thickness of the reactive mixture marking the propagation limit beyond which detonations extinguish. Simulations will be performed for both cases with a homogenous reactive medium and randomly distributed discrete sources. The critical thicknesses resulting from both cases will be compared in order to further elucidate the effects of a highly non-uniform reaction zone on the near-limit propagation of gaseous detonations.

2 Problem description

The reactive system consists of an inviscid, calorically perfect gas (i.e., with a constant ratio of specific heat γ). The gasdynamics of this system is described by the two-dimensional reactive Euler equations in a lab-fixed reference frame with flow and state variables non-dimensionalized with respect to the pre-shock, initial state. For a homogeneous reactive system, the specific total energy is defined as $e = p/(\gamma-1)\rho + (u^2+v^2)/2 + ZQ$, where Q is the specific energy release and Z is the reaction progress variable. In this study, the reaction rate $\Omega = \partial Z/\partial t$ is governed by single-step Arrhenius chemical kinetics as follows,

$$\Omega = -kZ \times \exp\left(-E_{\mathrm{a}}/T\right) \tag{1}$$

where k and E_{a} are the dimensionless pre-exponential factor and activation energy, respectively.

A finite-sized detonable mixture with an inert, yielding confinement (similar to that modeled by Li *et al*. [10, 11]) is schematically illustrated in Fig. 1. A rightward-propagating detonation is initiated by placing a high-pressure zone near the left end of the computational domain. The bottom boundary of the domain is a line of symmetry where a reflective boundary condition is applied. The half thickness of the reactive mixture is denoted as h. As shown in Fig. 1(a), the reactive medium is in the lower part of the domain with a layer of inert ($Z = 0$) gas as confinement in the upper part of the domain. A transmissive boundary condition is applied on the outer (top) boundary of the confinement.

The inhomogeneities are introduced into the system via initializing the value of Z as 1 in discretely located, square-shaped reactive regions and as 0 in the inert gaps. A spatially random distribution of reactive squares is schematically illustrated in Fig. 1(b). The side length of each square source is W, the average spacing between neighboring sources is L, and the spatial discreteness parameter can be defined as $\Gamma = W^2/L^2$ as indicated in Fig. 1(b). In order to maintain the average specific energy release Q the same as that in the homogeneous case ($\Gamma = 1$), the actual heat release associated with each discrete source must be increased according to the prescribed spatial discreteness Γ. Hence, for the inhomogeneous cases with discrete reactive sources, the specific total energy is formulated as $e = p/(\gamma - 1)\rho + (u^2 + v^2)/2 + ZQ/\Gamma$

3 Results

In this study, $Q = 50$ and $\gamma = 1.2$ fixed. For the cases with discrete reactive sources, the spatial discreteness is fixed as $\Gamma = 0.25$. Two sets of simulations, one with a relatively high activation energy $E_\mathrm{a} = 20$ and the other with a low activation energy $E_\mathrm{a} = 10$, have been performed. Note that the half-reaction-zone length for the homogeneous case is set to be unity by selecting the pre-exponential factor $k = 16.45$ and $k = 3.64$ for $E_\mathrm{a} = 20$ and $E_\mathrm{a} = 10$, respectively. For both homogeneous and inhomogeneous cases, the half thickness of the reactive medium h is varied. The results reported in this abstract are obtained from the simulations at a numerical resolution of 20 computational cells per half-reaction-zone length.

Sample wave structures resulting from the $E_\mathrm{a} = 20$ cases with a homogeneous reactive medium and randomly distributed sources are shown in Fig. 2(a) and (b), respectively. The top half of each subfigure is the contour plot of reaction progress variable Z; the bottom half is the contour plot of pressure. The red area in the plots of Z are the reactive regions where Z initially equals to 1. The white dash lines indicate the interface between the reactive medium and the inert confinement. In both cases shown in Fig. 2, the leading wave front is non-smooth and curved; the detonation products expand laterally into the confining gas behind an oblique shock attached with the leading detonation front at the confinement interface. For the homogeneous cases (Fig. 2(a)), the irregular wave structure, i.e., transverse waves interacting with leading shock front, are due to the intrinsic instabilities of the multi-dimensional detonation system with the selected parameters ($Q = 50$, $\gamma = 1.2$, and $E_\mathrm{a} = 20$). The more irregular wave structure resulting from the inhomogeneities (shown in Fig. 2(b)) are mainly due to the spatially random distribution of energy sources.

Sample wave structure resulting from the $E_\mathrm{a} = 10$ case with a homogeneous reactive medium is shown in Fig. 3(a). The resulting wave front exhibits a nearly smooth curvature. Figure 3(b) shows that the resulting wave structure becomes highly irregular in a medium with discrete sources of $\Gamma = 0.25$ and $L = 10$. While fixing the spatial discreteness $\gamma = 0.25$ and reducing the source spacing from $L = 10$ to $L = 1$, a slightly rough wave front with an identifiable global curvature is recovered as shown in Fig. 3(b).

4 Discussion

By tracking the leading shock position along the central axis and examining the propagation velocity history, whether a detonation wave can propagate at a given thickness can be determined, and the average propagation velocity V_avg can be calculated. For both homogeneous (blue squares) and inhomogeneous (red circles) cases with $E_\mathrm{a} = 20$, the averaged propagation velocity V_avg normalized by V_CJ are plotted as a function of the inverse of half thickness ($1/h$) in Fig. 4(a). For an infinitely large reactive medium, i.e., an adiabatic detonation system without losses, the average velocity resulting from a homogeneous case is exactly V_CJ. As the half thickness decreases, i.e., $1/h$ increases, the velocity deficit from the CJ value becomes greater

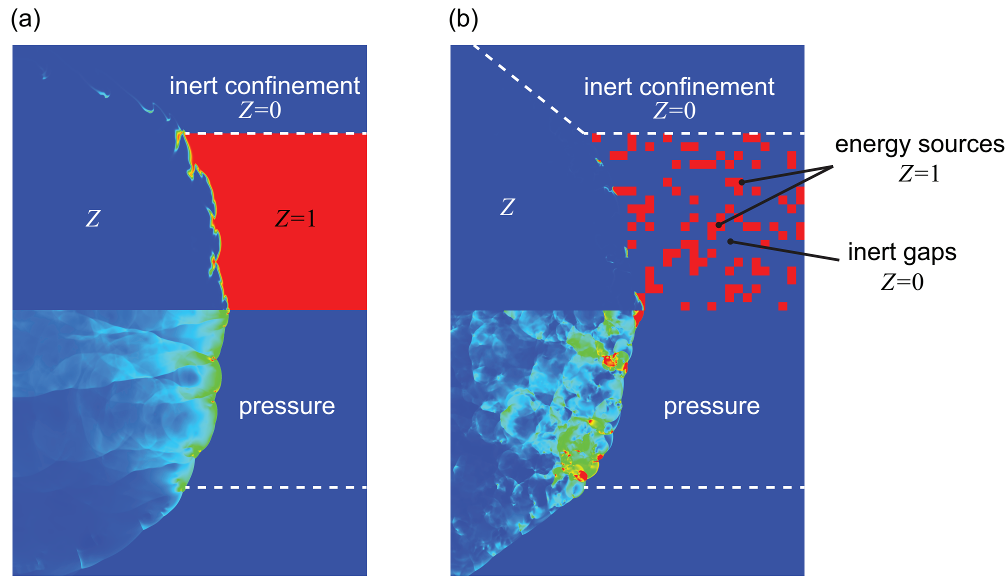

Figure 2: Wave structures (contour plots of reaction progress variable on top and pressure on bottom) for the $h = 100$ and $E_a = 20$ cases with (a) a homogeneous reactive medium and (b) an inhomogeneous medium with randomly distributed reactive sources ($\Gamma = 0.25$ and $L = 10$).

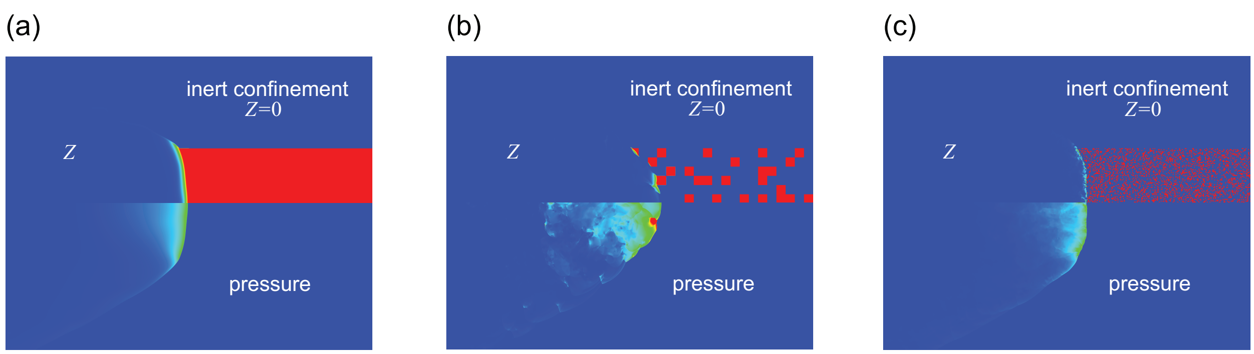

Figure 3: Wave structures (contour plots of reaction progress variable on top and pressure on bottom) for the $h = 30$ and $E_a = 10$ cases with (a) a homogeneous reactive medium and an inhomogeneous medium with randomly distributed reactive sources of (b) $\Gamma = 0.25$ and $L = 10$ and (c) $\Gamma = 0.25$ and $L = 1$.

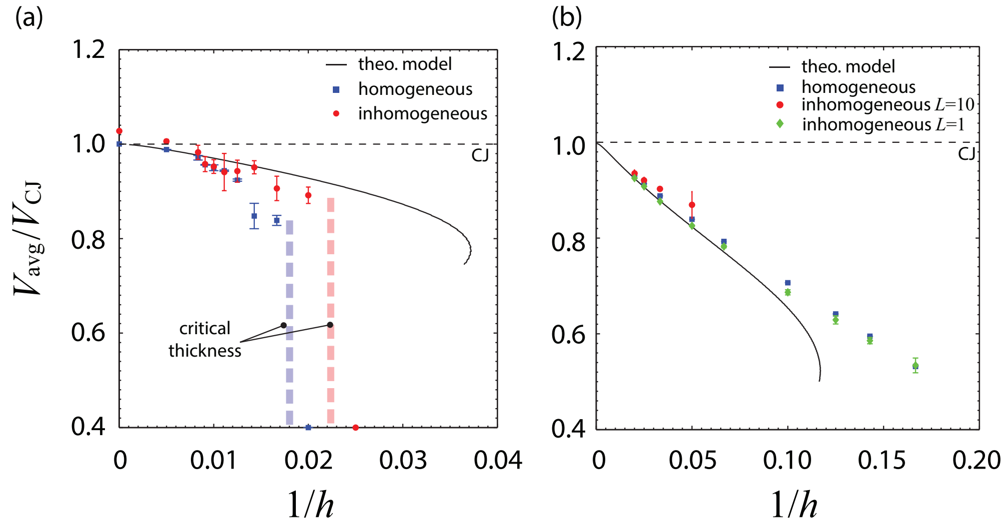

Figure 4: Average propagation velocity $V_{\rm avg}$ normalized by the Chapman-Jouguet (CJ) velocity $V_{\rm CJ}$ as a function of the inverse of half thickness $1/h$ for the cases with (a) $E_{\rm a} = 20$ and (b) $E_{\rm a} = 10$.

and greater until the propagation limit is encountered between $h = 60$ and $h = 50$ as indicated by the vertical blue dash line.

The solid red circles plotted on Fig. 4(a) are the average velocities resulting from the cases with discrete sources ($\Gamma = 0.25$ and $L = 10$). For the case with an infinitely large thickness ($1/h = 0$), the average velocity reaches a value that is approximately 3% greater than $V_{\rm CJ}$. The physical mechanism that is responsible for this super-CJ propagation velocity is discussed in [8, 9]. As the thickness decreases, the average propagation velocity decreases, but the average velocities are significantly greater than those resulting from the homogeneous cases at the same thickness. A critical half thickness (indicated by the red vertical dash line) between $h = 50$ and $h = 40$ is determined for the cases with inhomogeneities. Thus, the simulation results for the cases with a relatively high activation energy $E_{\rm a} = 20$ demonstrate that having an imposed spatially non-uniform energy release assists detonation waves to propagate beyond the limit encountered in the cases with a homogeneous reactive medium.

The results of $V_{\rm avg}$ normalized by $V_{\rm CJ}$ plotted as a function of $1/h$ in Fig. 4(b) are for the cases of a low activation energy $E_{\rm a} = 10$. As the reactive layer thickness decreases, the average velocity resulting from homogeneous and inhomogeneous cases decrease. The average velocities for the inhomogeneous cases with an average source spacing $L = 10$ (red circles), i.e., 10 times of the intrinsic half-reaction-zone length of the corresponding homogeneous medium, are slightly higher than those resulting from the homogeneous cases (blue squares). For the inhomogeneous cases with an average source spacing $L = 1$ (green diamonds), the resulting $V_{\rm avg}$ are very close to those for the homogeneous cases. The simulation results hence indicate that, for a relatively low activation energy, the effect of having spatially discretized energy release on detonation propagation limit is less significant than that in the cases with a high activation energy; for an average source spacing close to the intrinsic reaction zone length, the resulting propagation dynamics reverts to that of the homogeneous system.

The prediction of $V_{\rm avg}$ *vs.* $1/h$ relation using a theoretical model is plotted as the black curves in Fig. 4. This theoretical model consists of Wood and Kirkwood's quasi-one-dimensional model along the central streamline solving for the normal detonation velocity *vs.* front curvature relation (D_n-κ relation) [12], and the geometric construction of wave front first developed by Eyring *et al.* [13] More details about this model can be found in the Appendices of Ref. [11]. The model predicts a much thinner critical thickness than the simulation result based on inviscid Euler equations for an unstable detonation with $E_\mathrm{a} = 20$ (shown in Fig. 4(a)); the model prediction fairly well matched the simulation results with $E_\mathrm{a} = 10$ (shown in Fig. 4(b)) where the resulting detonation waves exhibit a smooth, laminar-like wave structure.

5 Conclusion

The effect of randomly distributed discrete sources, inducing reaction zone dynamics that resemble those resulting from a unstable mixture of detonable gases, on a detonation wave governed by an inert, yielding confinement has been examined via two-dimensional numerical simulations with a relatively high activation energy $E_\mathrm{a} = 20$ and a low activation energy $E_\mathrm{a} = 10$. In the cases with either a homogeneous reactive medium or discrete energy sources, the resulting detonation wave structure is transient and features a non-smooth wave front. The simulation results of the velocity deficit and the critical propagation thickness that have been obtained so far suggest that the imposed discrete sources in the reactive medium assist detonation waves to propagate significantly beyond the limit that is encountered in a homogeneous system for the cases with a high activation energy.

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