

Propagation limit of gaseous detonations governed by yielding confinement and Arrhenius kinetics

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1 Introduction

The question, namely whether an inviscid-flow simulation can describe the essential propagation mechanism of a gaseous detonation wave, remains baffling. Radulescu argued that turbulence arising from the wave complex associated with a detonation front, i.e., triple-point interaction of shock waves and hydrodynamically unstable slip lines, plays a non-negligible role in the detonation-driving reaction zone. [1] It is conjectured by Radulescu that, as a significant amount of reactive gas is processed by a cellular shock front at an insufficient strength to trigger adiabatic ignition, turbulent transport assists in releasing energy from the resulting large pockets of slowly burning gas. If this conjecture is true, then simulations of an inviscid flow based on the Euler equations, which do not describe transport phenomena, are inadequate to capture the complete mechanism of energy deposition in a detonation-driving zone. For a highly irregular detonatable mixture, a greater amount of weakly shocked gases is present than that arising from relatively regular mixtures. Following Radulescu's argument, the energy release of a highly irregular detonation should more rely on turbulent burning, thus, inviscid flow simulations must result in a more inefficient burnout for an increasingly unstable mixture.

Some recent simulations based on an inviscid flow have been performed by Reynaud *et al.* [2] and Mi *et al.* [3] to probe the propagation limit of cellular detonations responding to losses due to yielding confinement. Both studies have demonstrated that, for an increasingly unstable mixture (i.e., an increasingly greater activation energy), the minimum thickness of the reactive layer required for a self-sustained detonation increases, suggesting a decrease in resistance to losses. This qualitative dependence of detonation resilience on activation energy contradicts the experimental findings—a more unstable mixture is more robust against losses. [4,5] These contradictory results from the simulations and experiments seem to support Radulescu's conjecture that, without the assistance of turbulent transport in an inviscid flow, a less efficient energy deposition process more likely yields to losses. The findings of Reynaud *et al.* and Mi *et al.* are, however, still far from conclusive: In their studies, only the cases governed by single-step Arrhenius kinetics with a relatively low activation energy, i.e., $E_a/RT_0 < 40$, have been examined. [2,3]

To further explore whether simulations of inviscid flow can capture the combustion mechanisms underlying an unstable detonation wave, one must perform Euler-based simulations invoking a more realistic reaction model. To this end, two different sets of two-dimensional, Euler-based simulations of cellular detonations governed by yielding confinement are performed in the current study: (1) Cases governed by single-step Arrhenius kinetics with a greater activation energy than those considered in previous studies, i.e., $E_a/RT_0 \geq 40$; (2) Cases governed by two-step induction-reaction kinetics with parameter values obtained by fitting to the detailed chemical kinetics of both regular and highly irregular mixtures. The resulting critical thickness of the reactive layer from cases with various extents of instabilities will be compared.

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 with flow and state variables non-dimensionalized with respect to the pre-shock, initial state. For the first set of simulations, the reaction rate $\dot{\omega}$ is governed by single-step Arrhenius chemical kinetics as follows,

$$\frac{\partial Z}{\partial t} = -\dot{\omega} = -k(1 - Z)\text{Exp}(-E_a/T) \quad (1)$$

where Z is the dimensionless reaction progress variable that varies from 0 (unreacted) to 1 (completely reacted), k is the pre-exponential factor, and E_a is the activation energy non-dimensionalized with respect to the pre-shock, initial state. The spatial coordinates for the cases with single-step Arrhenius kinetics are non-dimensionalized by the half-reaction-zone length $l_{1/2}$ of the ZND solution.

For the second set of simulations, a two-step induction-reaction model is considered [6]. The induction and reaction rates are governed by the following equations, respectively,

$$\frac{\partial Z_i}{\partial t} = \dot{\omega}_i = -H(Z_i)k_i\text{Exp}\left[-E_i\left(\frac{1}{T_s} - \frac{1}{T}\right)\right] \quad (2)$$

$$\frac{\partial Z_r}{\partial t} = \dot{\omega}_r = (1 - H(Z_i))k_r(1 - Z_r)\text{Exp}(-E_r/T) \quad (3)$$

where $H(Z_i) = 0$ for $Z_i \geq 1$ and $H(Z_i) = 1$ for $Z_i < 1$. The activation energies for induction and reaction processes, i.e., E_i and E_r , are normalized by RT_0 . These activation energies can be alternatively scaled by the temperature jump δ at the leading shock of the corresponding Chapman-Jouguet (C-J) Mach

number as $\epsilon_i = E_i/\delta$ and $\epsilon_r = E_r/\delta$. The spatial coordinates for the cases with two-step kinetics are non-dimensionalized by the induction-zone length Δ_i of the ZND solution. As shown in Fig. 1(a), a fully developed cellular detonation wave rightward propagates into a domain wherein the upper part is an inert, yielding confinement, and the lower part is a layer of reactive gas. The thicknesses of the inert and reactive layer are h_I and h_R , respectively.

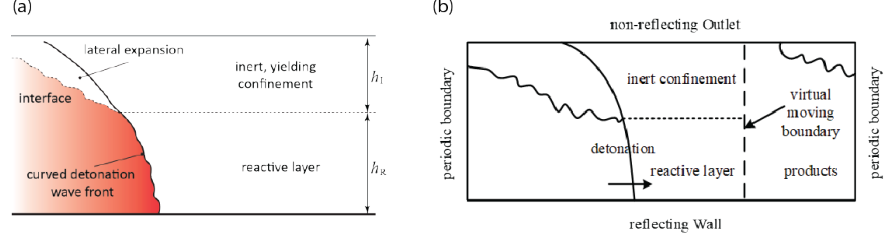


Figure 1: (a) A conceptual illustration of a cellular detonation wave with yielding confinement and (b) a schematic illustration of the computational domain.

In this work, the simulations with single-step Arrhenius kinetics are for the cases with $Q = 50$ (the dimensionless heat release normalized by RT_0), $\gamma = 1.2$, and $E_a = 10, 20, 30, 35$, and 40 . For the simulations with two-step kinetics, two scenarios, i.e., a weakly unstable mixture with $\epsilon_i = 4.8$, $\epsilon_r = 1.0$, $\gamma = 1.44$, and $Q = 19.7$, and a highly unstable mixture with $\epsilon_i = 5.414$, $\epsilon_r = 1.0$, $\gamma = 1.32$, and $Q = 21.3$, are considered.

3 Numerical methodology

Figure 1(b) schematically illustrates how the problem is computationally tackled in this study. In order to optimize the usage of computational resource, the left and right boundaries of the domain are connected via periodic boundary conditions, so that the detonation wave always propagates periodically in the calculation zone. The position of the leading wave surface is detected every certain number of time steps, and then reinitialize a fresh zone of a certain length (i.e., $30l_{1/2}$ or $30\Delta_i$ away from leading wave surface) in front of the leading wave surface with initial parameters. It can be understood as that there is a virtual boundary in front of the leading wave, the detonation wave propagates forward a certain distance, and the virtual boundary also moves forward a certain distance at the same time. The simulation code used to solve the two-dimensional reactive Euler equations is based upon uniform Cartesian grids. The AUSMPW+ scheme with a third-order MUSCL extrapolation [7], and a third order Runge-Kutta algorithm were used to approximate numerically the solution of the governing equations.

4 Results and discussion

4.1 Wave structure

For the simulations with single-step Arrhenius kinetics, the wave structure resulting from the cases with $E_a = 10$ and 40 are shown in Figs. 2 and 3, respectively. For the simulations with two-step kinetics, the results of wave structure for the weakly unstable mixture and highly unstable mixture are presented in Figs. 4 and 5, respectively. In all of these cases, the detonation wave front is curved due to a laterally expanding

flow behind the wave front. For the cases with a small E_a and a weakly unstable mixture, the wave front is smoothly curved, and the reaction zone exhibits a laminar-like structure. The globally curved wave front resulting from the cases with a large E_a and a highly unstable mixture exhibits a highly irregular structure. As shown in Figs. 3 and 5, large pockets of unreacted material are detached from the leading shock wave. A more significant amount of unreacted pockets can be found near the interface between the inert and reactive layers.

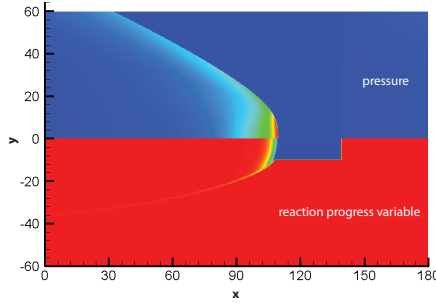


Figure 2: Sample result showing the wave structure resulting from the case with single-step Arrhenius kinetics of $E_a = 10$ and $h_R = 10$.

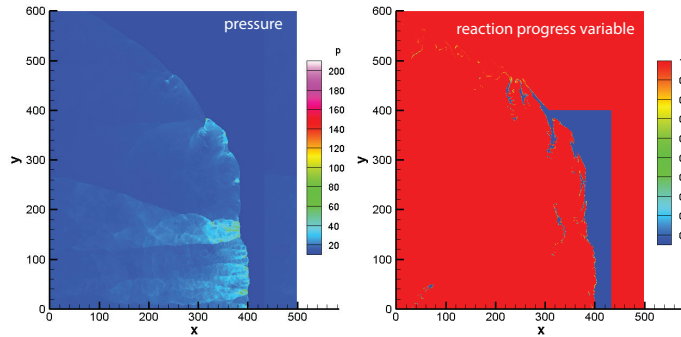


Figure 3: Sample result showing the wave structure resulting from the case with single-step Arrhenius kinetics of $E_a = 40$ and $h_R = 400$.

4.2 Critical thickness of the reactive layer

For the simulations with single-step Arrhenius kinetics, the failure of detonation propagation is captured in the cases with E_a greater than 20. For the cases with two-step kinetics, the failure of propagation is captured in both scenarios of weakly and highly unstable mixtures. The results of the detonation velocity normalized by the corresponding C-J velocity V_{CJ} are obtained from the simulations. A successful propagate is considered if the detonation wave can propagation over a distance of $3000l_{1/2}$ for single-step kinetics or $5000\Delta_i$ for two-step kinetics. For a case of successful propagation, an average propagation velocity V_{avg} can be measured over a distance of $1500-3000l_{1/2}$ and $2500-5000\Delta_i$ for single- and two-step kinetics, respectively. The critical thickness of the reactive layer below which a detonation fails to propagate can thus be determined. The results for both single- and two-stp kinetics are discussed. However, due to the limit in length, only the numerical results for the cases with two-step kinetics are reported in this abstract.

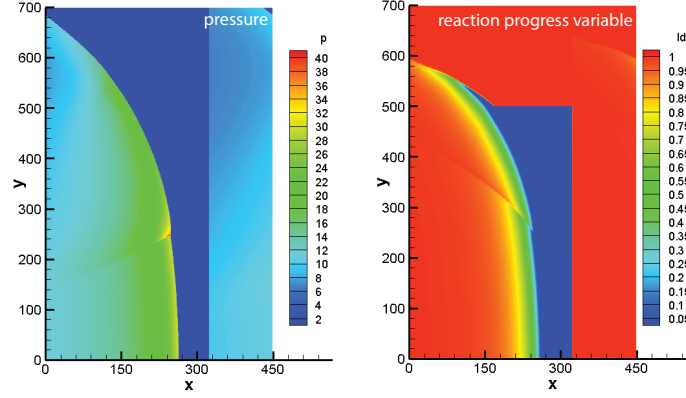


Figure 4: Sample result showing the wave structure resulting from the case with two-step kinetics for a weakly unstable mixture and $h_R = 500$.

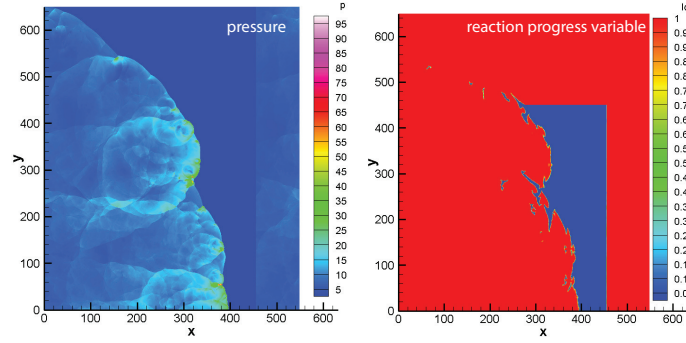


Figure 5: Sample result showing the wave structure resulting from the case with two-step kinetics for a highly unstable mixture and $h_R = 450$.

The numerical results obtained from the simulations with single-step kinetics are based on a resolution of 10 computational grid points per the ZND half-reaction-zone length, i.e., $l_{1/2}/\Delta x = 10$. For cases with $E_a = 10$ -30, the current results are compared to those of the same numerical resolution reported by Mi *et al.* [3]. It has been found that the current results fairly well agree with those in the literature except a slightly smaller (by approximately $10l_{1/2}$) critical thickness resulted from the case with $E_a = 20$. As E_a increases from 20 to 40, the critical thickness significantly increases. This trend is consistent with that found in both studies of Reynaud *et al.* [2] and Mi *et al.* [3].

The results of simulations with two-step reaction model are summarized in Table 1. These simulations were performed at a resolution of 5 computational grid points per the ZND induction-zone length, i.e., $\Delta_i/\Delta x = 5$. The critical thickness of the reactive layer for the weakly unstable mixture is between 450 and $500\Delta_i$ while that for the highly unstable mixture is between 400 and $450\Delta_i$. These results suggest that the highly unstable mixture is more resilient to losses due to lateral expansion than the weakly unstable mixture, which is qualitatively consistent with the experimental findings, but contradicts the results of the inviscid-flow simulations with single-step Arrhenius kinetics. More rigorous convergence tests and analysis on the effect of different reaction mechanisms will be carried out in the complete scope of this study.

Table 1: Average propagation velocity normalized by the C-J velocity resulting from the cases with two-step kinetics. The horizontal dash line indicates the critical value of h_R .

(a) Weakly unstable mixture

h_R	h_I	V_{avg}/V_{CJ}
550	200	0.8852
500	200	0.8520
500	300	0.8519
450	200	no-go

(b) Highly unstable mixture

h_R	h_I	V_{avg}/V_{CJ}
500	200	0.9578
450	100	0.9716
450	200	0.8911
450	300	0.8911
400	100	no-go
400	200	no-go

5 Concluding remarks

Two-dimensional computational simulations have been performed to model the dynamics of a detonation wave propagating in a layer of reactive gas under the confinement of an inert layer. For single-step kinetics with a sufficiently large activation energy and two-step kinetics, a critical thickness of the reactive layer below which the detonation wave propagation cannot be self-sustained has been captured. Qualitatively opposite relationships between the critical thickness and the stability of the reactive mixture have been obtained from the simulations with single-step Arrhenius kinetics and two-step induction-reaction kinetics. More in-depth investigation into these intriguing results will be done in future effort.

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