Two-Dimensional Numerical Simulations of Cellular Detonation Diffraction in Channels

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1 Introduction

Diffraction of detonation waves from tubes or channels to a larger open area is a classical problem in detonation research [1, 2]. When a detonation wave propagating down a rigid round tube expands abruptly into open space filled with the same reactive mixture, the detonation will fail if the tube has a diameter less than some critical value, referred to as the critical diameter, d_c. For common fuel-air mixtures, results from a number of experiments had confirmed the universal relationship for the critical tube diameter problem to be $d_c = 13\lambda$ where d_c is the critical tube diameter and λ is the characteristic detonation cell size [3, 4]. Although this empirical correlation appears to be quite adequate for most gaseous combustible mixtures, it is shown to be invalid for special cases such as mixtures with high argon dilution where the scaling can be up to $d_c \sim 25\lambda$ [5, 6]. Recent experiments were also reported by Meredith et al. [7] for detonation diffraction from a thin annular channel into free space, resulting essentially a cylindrical expansion of the detonation wave. Critical widths for the successful transformation of a planar to a cylindrical detonation are measured in two different stable and unstable mixtures, i.e., 70% argon diluted C_2H_2–O_2 mixture and undiluted stoichiometric C_2H_2–O_2 mixture, respectively. For the unstable mixture, the critical channel width over detonation cell size is found to be about 2.74–3.80. It agrees with the earlier studies by Benedick et al. [8] and Liu et al. [9] using rectangular channels that w_c/λ is about 3 for unstable mixtures. However, for highly argon-diluted mixture with regular cellular pattern, the non-dimensional critical width w_c/λ is determined to be as much as 12. The breakdown in the scaling between stable and unstable mixtures thus indicated that the detonation stability or cell regularity plays an important role in the detonation undergoing a sudden expansion into open space [10].

A number of numerical studies on the detonation expansion abruptly from a two-dimensional channel to a large one can be found in the literature, e.g., [11-14]. Obtaining reliable numerical results for any detonation phenomenon generally requires simulations to be performed with high degree of numerical resolution and hence, most of the previous numerical studies were conducted using the reactive Euler equations with one- or two-step chemical kinetics. Although numerical investigations using multi-component formulation with detailed chemistry are becoming more apparent, however, most reported results are often obtained with low and possibly insufficient numerical resolution

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generating discrepancy with experimental observations. Furthermore, in most studies the initial condition is a planar ZND detonation wave propagating in a channel with an abrupt area increase.

In this study, a series of high resolution, two-dimensional numerical simulations using the reactive Euler equations with a three-step chain-branching reaction model are performed to investigate the evolution of the cellular detonation wave expanded from a small channel to a larger open space in a stable mixture with highly regular cellular pattern, to another mixture where the effect of detonation instability becomes apparent. The goal of this numerical study is to look at again different wave dynamics and instability during the detonation expansion, or otherwise the mechanism responsible for the successful transmission for the different types of reactive mixtures. The numerical results are also used to establish and examine different scaling relationship previously determined from experiments for the critical channel width.

2 Numerical details

Numerical simulations were performed using the ideal detonation model, as in most previous studies, see [15]. The flow is governed by the reactive Euler equations with a three-step chain-branching chemical kinetic model [16, 17]. The governing equations are non-dimensionalized using the unburned flow properties. The heat release $Q = 8.22$ and $\gamma = 1.2$ are used for the present study. The chemical kinetic scheme involves two temperature-sensitive radical producing reactions and a temperature-independent exothermic chain-termination reaction. It is represented by the following three stages:

$$\mathrm{F} \rightarrow \mathrm{Y} \qquad k_I = A_\mathrm{I} \exp\left(E_I \left(\frac{1}{T_I} - \frac{1}{T} \right) \right)$$

$$\mathrm{F} + \mathrm{Y} \rightarrow 2\mathrm{Y} \qquad k_B = A_\mathrm{B} \exp\left(E_B \left(\frac{1}{T_B} - \frac{1}{T} \right) \right)$$

$$\mathrm{Y} \rightarrow \mathrm{P} \qquad k_C = 1$$

where F, Y and P correspond to the amount of reactant, radical and product, respectively. The chain-initiation and chain-branching rate constants k_I and k_B have an Arrhenius temperature-dependent form, while the chain-termination reaction is assumed to be first order, independent of temperature and to have a fixed rate constant k_C. In present work, the values used for the activation energy of the initiation and chain-branching steps are respectively $E_\mathrm{I} = 37.5$ and $E_\mathrm{B} = 10$. The cross-over temperature for the chain-initiation is fixed at $T_\mathrm{I} = 3T_{shock}$ and the chain-branching cross-over temperature T_B is used as a bifurcation parameter to control the detonation instability of the mixture. For a highly stable case, $T_\mathrm{B} = 0.75T_\mathrm{shock}$ and for a weakly unstable case, $T_B = 0.85T_\mathrm{shock}$.

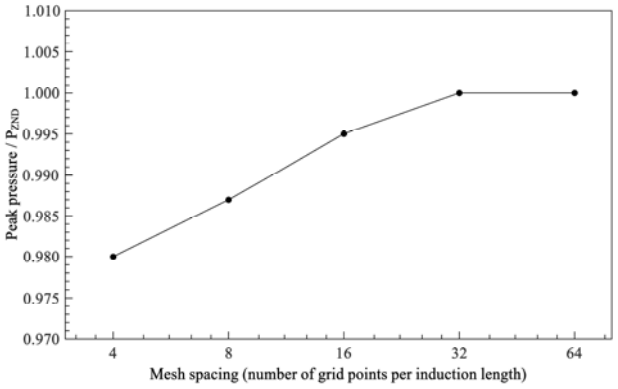


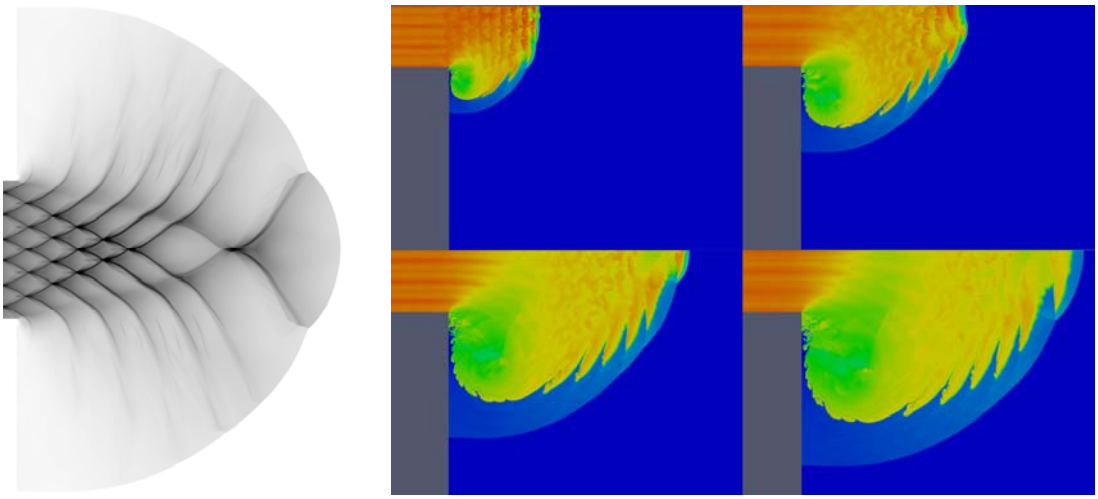
Figure 1. Peak pressure as a function of relative mesh spacing with $T_\mathrm{B} = 0.75T_\mathrm{shock}$

The governing equations are solved using the parallel AMROC code [18] built with block-structured adaptive mesh refinement (AMR). The entire computational domain was first covered by

coarse grids, and fine meshes were superimposed on the coarse grids in the vicinity of the front. A fractional steps method was used to decouple the hydrodynamic transport and chemical reaction numerically. The reactive Euler equations are solved with an explicit second-order Godunov type numerical scheme incorporating a hybrid Roe-solver-based method. In the present work, reflective boundary conditions are imposed on walls. Inlet and outlet boundary conditions are imposed on the left and right boundary, respectively. In present work, a maximum resolution of 50 points per induction zone length with four levels of Cartesian mesh adaptation with refinement factors (2, 2, 2, 4). A resolution test is shown in Fig. 1 which proves that the resolution used in present study is sufficient to resolve the peak pressure of a stable detonation ($T_B = 0.75T_{shock}$) and is expected to be reasonable as well for a weakly unstable case ($T_B = 0.85T_{shock}$).

3 Results and discussions

The numerical results obtained for the highly stable mixture with $T_B = 0.75T_{shock}$ are given in Figs. 2 and 3. The diffraction process is illustrated using both a sequence of temperature contour snapshots and the typical "numerical smoked foil" showing the time-integrated maximum pressure contour from the numerical simulation, which corresponds to the trajectories of the triple points. In this study, the channel width is varied so that for each case different number of detonation cells is initially present in the channel. It is important to point out that only half of the channel is considered for the computation and hence, the smoked foil figure includes also the mirror image to have the complete channel size. Figure 2 first shows the case where the channel width is below the critical value resulting in a detonation failure in the open area. The cellular structure in the channel before the divergence in the unconfined space can be seen to be highly regular. For the case where only 6 cells are observed at the frontal structure, the cellular detonation fails to transmit into the open area. The failure wave from the corner enters into the central axis and the resulting large curvature of the diffracting wave causes the continuous decoupling of the reaction zone from the diverging shock front. The failure is also indicated by the disappearance of cellular pattern.



(a) (b)

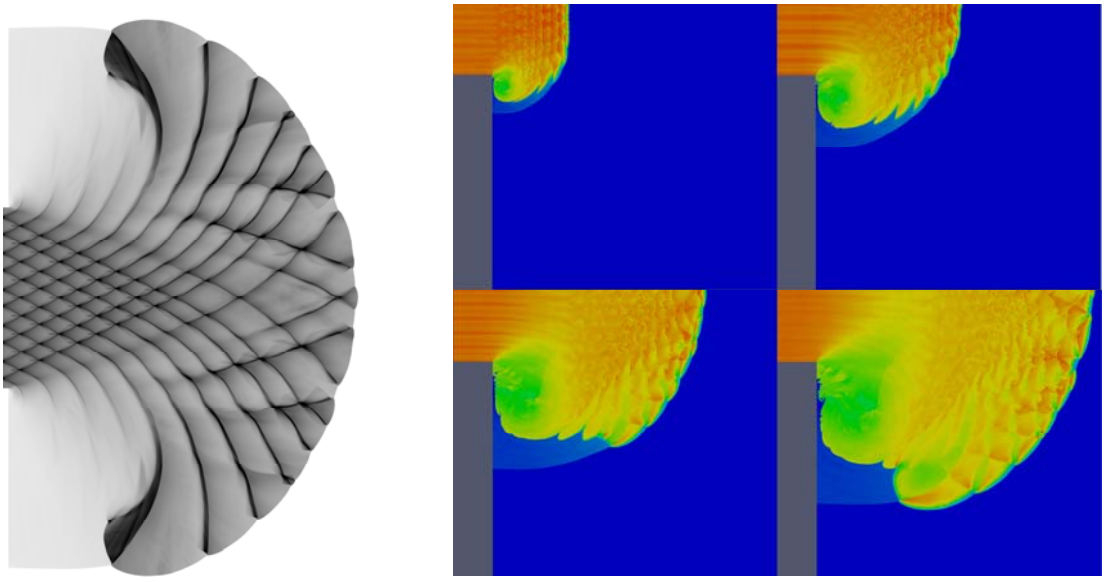
Figure 2. Numerical results a) smoked foil and b) sequence of temperature contour plots showing an unsuccessful transmission of the cellular detonation for the highly stable mixture with $T_B = 0.75T_{shock}$

For the successful transmission as shown in Fig. 3 where the number of cells in the channel is increased to 10, the rarefaction waves first cause an enlargement of cells at the diffracting front. Nevertheless the cellular structure re-establishes globally at further distance once the effect of curvature becomes less severe. Both the sequence of the temperature contour plots and the numerical smoked foil indicate the transmission is a global event showing the re-coupling of the reaction zone

with the diverging front and continuous evolution of the cellular structure rather than a local event of which transmission is originated from a hot spot where instabilities manifests.

One interesting feature as previously observed and discussed by Arienti and Shepherd [13] is the formation of a fold or kink in the diverging shock front which propagates toward the corner wall. This folding results from the interplay of transverse rarefaction waves with the accelerating detonation front near the channel central axis. Although this distinct feature may appear to be driving force for the re-initiation, it is important to note that new transverse waves must be generated to keep the average spacing (cell size) the same as the surface area of the diverging front increases. If transverse waves are not generated, the cylindrically diverging detonation still fails as it continues to expand.

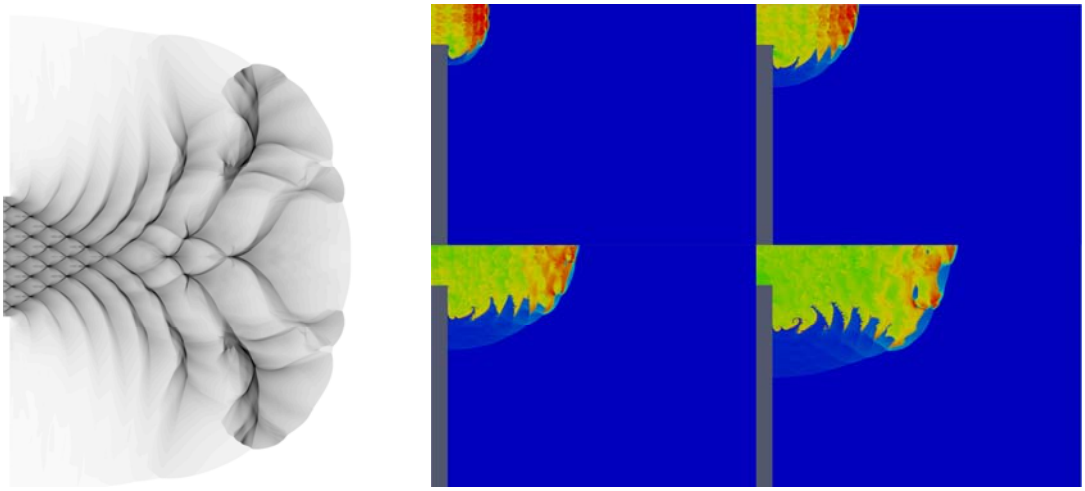
It is worth noting that from the present numerical study, the scaling of critical channel width over cell size, w_c/λ, required for the detonation to re-initiate and continue to propagate in the unconfined volume is about 10. Taking into account the simplicity of the numerical model using the Euler equations and the chemical reaction mechanism, the resulting numerical w_c/λ ~10 are in quite good agreement with the experimental value of about 12.



(a) (b)

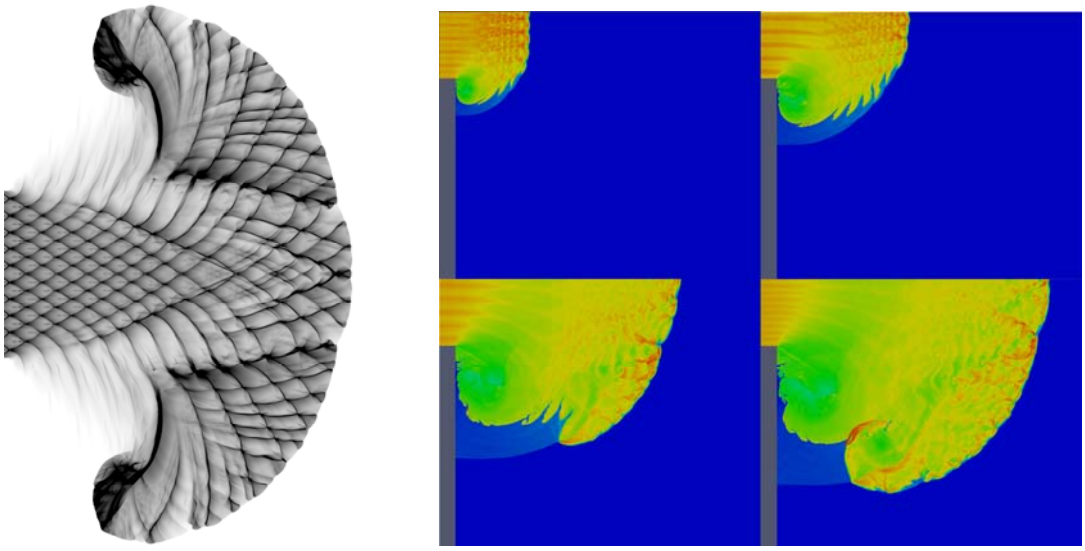
Figure 3. Numerical results a) smoked foil and b) sequence of temperature contour plots showing a successful transmission of the cellular detonation for the highly stable mixture with $T_B = 0.75T_{shock}$

To look at the effect of instability on the cellular detonation diffraction, simulations are carried out for a mixture with $T_B = 0.85T_{shock.}$ The increase of the chain-branching cross-over temperature makes the detonation more unstable with stronger dependence on transverse waves. Figure 4 shows the results where the detonation contains also initially 6 cells in the channel. The condition appears to approach to the critical one. Unlike the result shown in Fig. 2 where the wave fails globally with complete disappearance of cells, here it appears that at some local regions the wave attempts to re-initiate but is insufficient to re-establish the detonation further downstream. Such tendency thus suggests the fact that for more unstable mixtures, the instability will provide a mean to facilitate the transmission, reducing the number of cells required in the channel for successful transmission as evidenced by the experimental observation [7, 10]. For the weakly unstable mixture, the role played by instability becomes more apparent for the re-initiation. As shown in Fig. 5, the transmission is stimulated by a more spontaneous formation of transverse waves generating initially much finer cells.



(a) (b)

Figure 4. Numerical results a) smoked foil and b) sequence of temperature contour plots showing an unsuccessful transmission of the cellular detonation for the weakly unstable mixture with $T_B = 0.85T_{shock}$



(a) (b)

Figure 5. Numerical results a) smoked foil and b) sequence of temperature contour plots showing a successful transmission of the cellular detonation for the weakly unstable mixture with $T_B = 0.85T_{shock}$

4 Concluding remarks

In this study, two-dimensional numerical simulations are performed to look at the cellular detonation diffraction in stable and weakly unstable mixtures. The reactive Euler equations were considered together with a three-step chain-branching chemical kinetic model. For the highly stable case, the failure results from a continuous enlargement and subsequently disappearance of cells and the deceleration of the diverging wave due to curvature leads to the decoupling of the reaction zone with the leading front. For the successful transmission, the cellular structure survives and re-establishes at further distance. A distinct feature of shock folding or kink in the diverging shock front propagating toward the corner wall is also observed to stimulate the re-coupling between the reaction zone and the leading front for re-initiation. Comparison between the scaling w_c/λ obtained from the present numerical simulation and available experimental data shows rather good agreement despite the model simplification used for the computation. By increasing the chain-branching cross-over temperature T_B

making the detonation weakly unstable, the dynamics appear to be more dominant by the spontaneous formation of transverse waves generating initially fine cells and facilitating the transmission.

Acknowledgment

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