Effect of Cellular Instabilities on the Detonation Transmission of Weakly Unstable Detonations

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1 Introduction

When a detonation wave propagates from a channel into an unconfined space, the detonation could extinguish if the size of the channel reduces below a critical value. This value is defined as the critical channel height. Since its early discovery, extensive experimental and numerical investigations have been conducted to understand the diffraction phenomena [1-5]. Lee [6] attributed the failure mechanism for stable mixtures to the excessive curvature of the attenuated detonation wave, and for unstable mixtures to the failure of the formation of re-initiation bubbles. Numerically, the study by Jones et al. [1] shows that $H_2/O_2/Ar$ detonation without any cellular structure failed when transmitted into a large volume. However, the high-resolution simulations by Arienti and Shepherd [7] indicates that for a channel with a fixed height, the reignition of a planar detonation diffraction would occur if the activation energy dropped below a critical value. Due to the constrain of computational capability, their simulations were limited to a planar detonation wave propagating in a short inlet channel. The channel length is of 33 half-reaction length (*hrl*) approximately. Also, the zero-gradient boundary condition was applied at the end of the inlet channel. This constraint arouses two major concerns on – (1) how the cellular instabilities inside the channel can affect the re-initiation mechanisms when the detonation wave is diffracted into an unconfined space, and (2) whether the critical channel heights predicted are the same by using a planar detonation wave or a cellular detonation wave.

In the present paper, the 2D simulations are performed to determine the critical channel heights for planar/cellular detonation diffraction. The re-initiation mechanisms are then analyzed.

2 Numerical Set-up

The simulation domain consists of a long inlet channel, with its right end connected to the unconfined space (Fig. 1). The length of the channel is 800 *hrl*, which allows the initial over-driven planar detonation wave to decay into a steady Chapman-Jouguet detonation, and the cellular detonation wave structure to be fully

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developed near the channel exit. The simulations are terminated when the shock front along the symmetry line propagates 800 *hrl* beyond the channel exit. The height of the region corresponding to the unconfined space ranges from 600 to 800 *hrl*. Reflective boundary conditions are used at the symmetric line and the walls.

For the planar detonation diffraction case, the detonation is ignited by a uniform high pressure and high temperature strip. For the cellular detonation diffraction case, the detonation is ignited by a perturbed high pressure and high temperature region with the same thermodynamic conditions as planar detonation. Variables are non-dimensionalized with respect to the state of the unburned mixture. The one-step Arrhenius reaction model is used. Considering the longitudinal instability in detonation propagation for a mixture with high activation energy [8], the activation energy selected is slightly smaller than the neutral stability boundary and the gas parameters studied are: $Ea = 24, \gamma = 1.2, Q = 50$.

The second-order a-α CE/SE scheme [9-15] is implemented together with the Massage Passing Interface (MPI) for high resolution computations. Considering the exceptionally large simulation domain for the diffraction problem, grid convergence has been verified on the long-term cellular dynamics in a narrow channel. The grid resolution of 24 pts/*hrl* is used and the total mesh number is around 410 million.

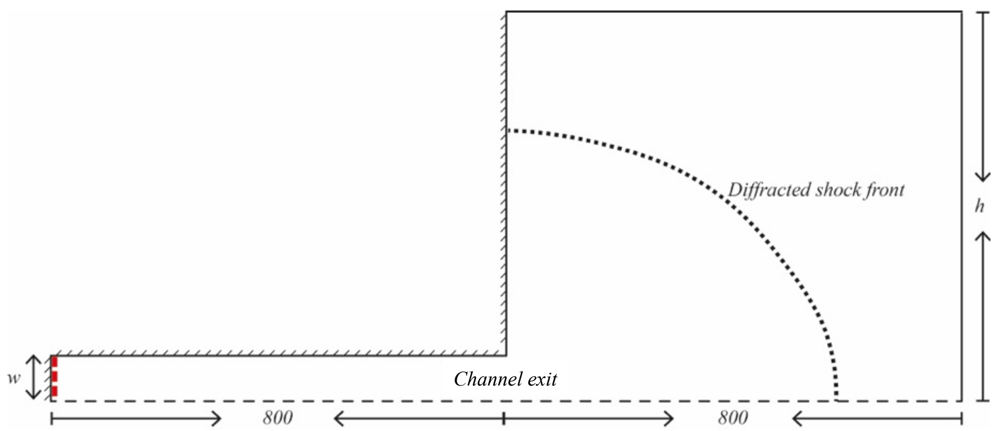

Figure 1. Configuration of the simulation domain.

3 Results and Discussion

First, we solve the problems in the planar scenario, the numerical soot foils obtained for planar detonation diffraction at the ends of simulations (t=173 for w=110 case, and t=221 for w=100 case) are given in Fig. 2. Notably, $t = 0$ is defined when the shock wave reaches the inlet channel exit. It is noticed that for both cases, the disturbance angle (22.45°) agrees well with the prediction from Skews' construction [7, 16]. The re-initiation does not occur along the disturbance line. In the w=110 case, the re-initiation is established at the location (x=1250, y=220) (Fig. 2a) where a maximum pressure occurs. It is interesting to note that the high pressure region near the same location is also recorded for the w=100 case (Fig. 2b), but the local exothermicity is comparably weak, the re-establishment of detonation wave is unsuccessful. Figure 3 shows the pressure and temperature contours for w=110 case during the formation of the hot bubble that re-initiates the cylindrical detonation. The pressure wave formed at t=90 quickly overtakes the leading shock, and heat release is found intensive behind the transmitted shock (Fig. 3c).

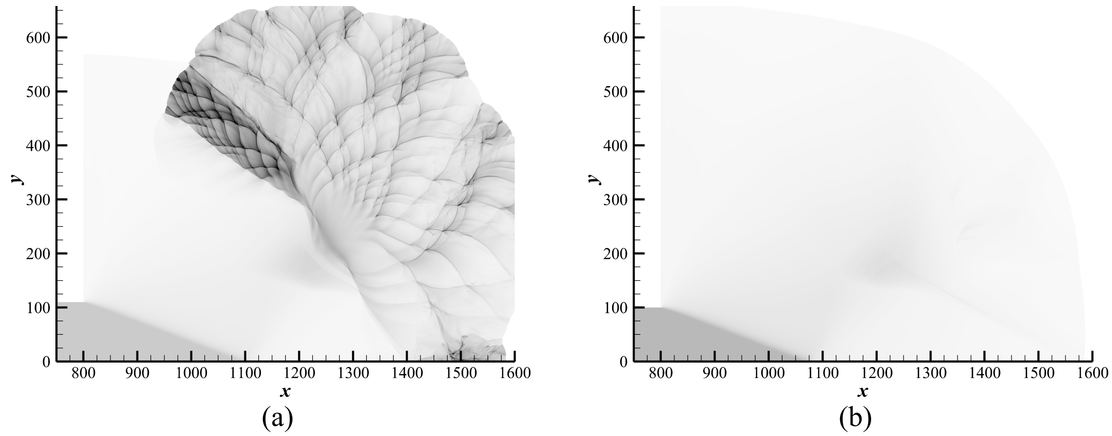

Figure 2. Numerical soot foil for planar detonation diffraction. (a) w=110, t=173; (b) w=100, t=221.

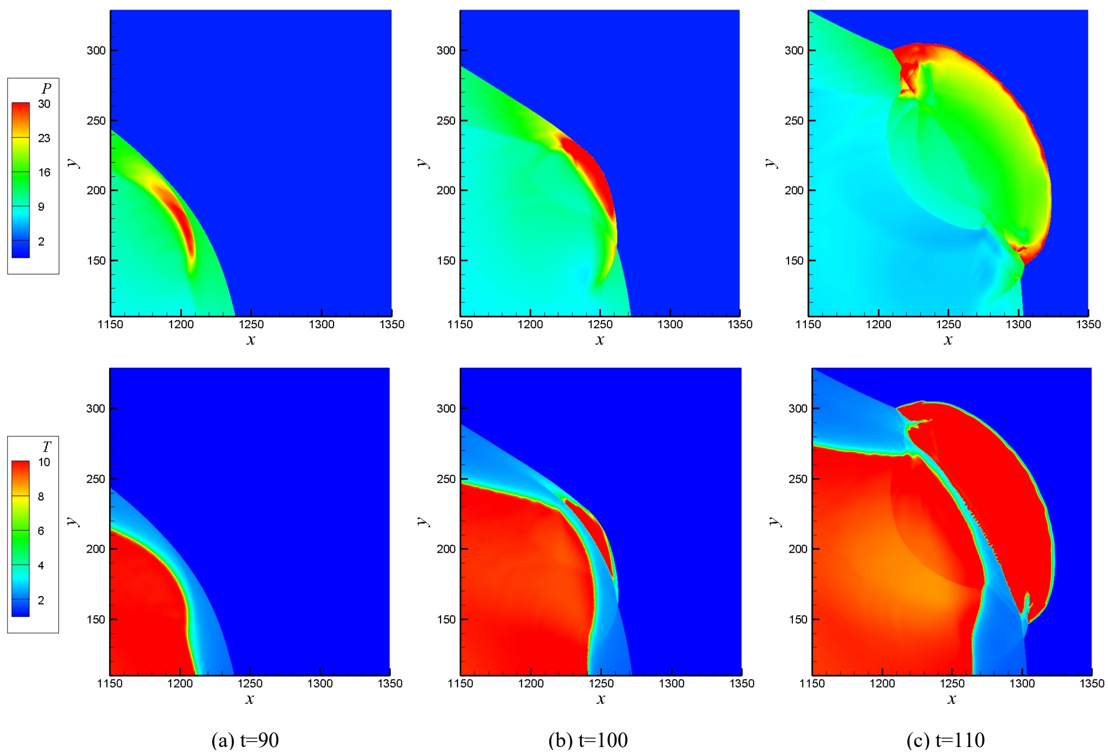

Figure 3. Local explosion for w=110.

In the cellular detonation diffraction scenario, detonation fails to proceed when there are not enough strong transverse waves collisions before the shock/combustion decoupling phenomenon (w=75 in Fig. 4a). Contrarily, successful re-initiation happens, with multiple hot bubbles formed where the collision of transverse waves happens in opposite directions (w=85 in Fig. 4b). The successful transmission for w=85 case can be explained by the frontal structures of the diffracted wave (Fig. 5). Collisions of transverse waves create local over-driven waves to sustain continuous shock-ignited reaction.

The planar and cellular detonations were found to have values of the critical channel height around 100~110 and 75~85 *hrl*, respectively. The re-initiation mechanism of the cellular diffraction contrasts with that of the planar diffraction. In the cellular diffraction, continuous detonation is self-sustained by energetic transverse wave collisions. For the planar case, before the re-initiation (formation of hot bubble), there is a stage when the shock is totally decoupled from the flame front (presence of large area between the disturbance line and the re-initiated structures, shown in soot foils in Fig. 2(a)), if the channel height is near the critical value. Although these calculations were performed in a weakly unstable mixture using a simplified chemical kinetic, the re-initiation results show many similarities to those observed in the experimental work of Mehrjoo et al. [13], in which suppression of cellular instability using the porous wall near the channel exit causes a significant increase of critical pressure limit. This is equivalent to the effect on the critical channel height in the present paper.

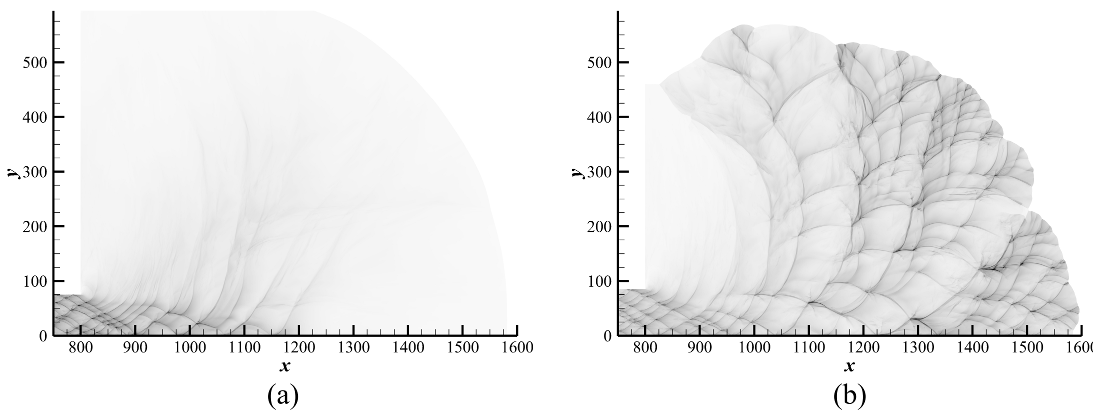

Figure 4. Numerical soot foil for cellular detonation diffraction. (a) w=75, t=210; (b) w=85, t=135.

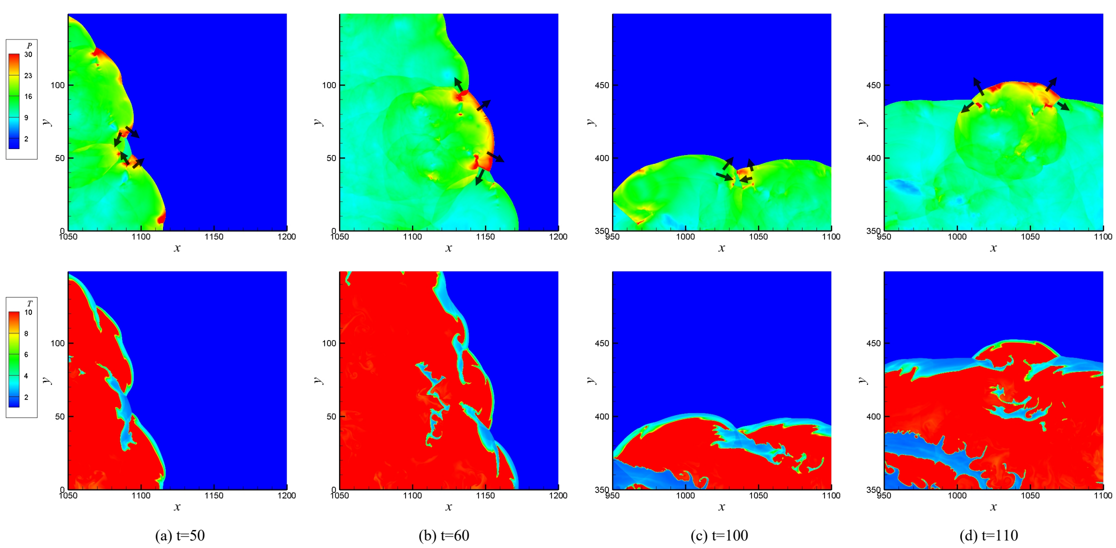

Figure 5. Transverse wave collisions for w=85.

6 Conclusions

In this paper, the diffraction of a weakly unstable mixture is numerically investigated. Two scenarios were examined – the diffraction of a planar detonation wave and the diffraction of a cellular detonation wave, respectively. First of all, a smaller critical channel height for a successful transmission is found for the cellular detonation case than that for the planar detonation case. For the planar detonation diffraction, re-initiation happens inside the shocked-unreacted zone. In the cellular cases, the transmission is greatly determined by the effective collisions of transverse waves with multiple randomly distributed hot sites, rather than only one hot bubble in the planar cases. It was demonstrated that the transverse waves can facilitate the successful transmission with a narrower channel.

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