

The Propagation of Detonation Waves in the Temperature Non-uniform Zone

Xi Liu, Tianbao Ma, Jian Li*

State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology
Beijing, China

1 Introduction

The research on the detonation propagation in the heterogeneous gas can provide necessary theoretical support for industrial safety protection and detonation propulsion system design. Under the premise of inhomogeneity, the explosion process of gases, including direct initiation, steady-state propagation, and failure mechanism, is highly complex, and many physical mechanisms are still unclear. Zhang [1] studied the effect of temperature non-uniform on detonation and pointed out that the temperature non-uniform can significantly affect the critical concentration gradient. Sharp and Short [2] conducted numerical experiments to study the effects of temperature gradient on detonation. Their result shows that the slower the exotherm, the smaller the gradient required for ignition. Gamezo [3] investigated the effect of initial non-uniform on detonation in the 2D plane. Dai [4-5] found that low-temperature chemical reaction mechanisms play an essential role in detonation propagation in the presence of a temperature gradient. Qi [6-7] studied the effect of temperature fluctuation amplitude on detonation and explained the effects of sinusoidal distribution temperature on direct ignition.

The present study aims to investigate the effect of temperature non-uniformity on the detonation that maintains the CJ state as a whole. More specifically, we focus on the change of the local detonation front subject to the periodic temperature distribution. Many studies have explored the influence of global gradients on detonation propagation. Thus, the global gradient will make the detonation no longer maintain the CJ state. However, in the present study, to ensure that the detonation is still near the CJ state and holds a planar front, the averaged state of the non-uniformity medium is equivalent to the homogeneous medium. With such a setup, we try to find the influence of periodical non-uniformity on the detonation front and its cellular structures by directly comparing it with the detonation front in a homogeneous medium.

2 Numerical model and initial condition

2.1 Governing equations

The governing equations used in this study are the two-dimensional reactive Euler equations. They have the following non-dimensional form:

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

where,

$$U = [\rho, \rho u, \rho v, E, \rho y_I, \rho y_R], F = [\rho u, \rho u^2 + p, \rho uv, u(E + p), \rho u y_I, \rho u y_R]$$

$$G = [\rho v, \rho uv, \rho v^2 + p, v(E + p), \rho v y_I, \rho v y_R], S = [0, 0, 0, 0, \omega_I, \omega_R]$$

Assuming a polytropic equation of state and an ideal thermal equation of state:

$$E = \frac{p}{\gamma - 1} + \frac{\rho}{2}(u^2 + v^2) - \rho y_R Q, p = \rho T$$

Where p is the pressure, ρ is the density, E is the energy per unit volume, u and v are the velocities in the x and y directions respectively, Q is the heat of the reaction, y_I and y_R are the process variables of the induction and reaction stages, respectively. A two-step reaction model is used to mimic the essential dynamics of a chain-branching reaction. The details about the model can be referred to [8]. In this study, the Mach number is 5.6, the specific heat ratio $\gamma = 1.44$, and the dimensionless induction and reaction lengths of the steady CJ detonation are 0.001 and 0.0036. The reaction parameters are chosen such that the detonation corresponds to a weak unstable mixture which we do not correlate to a specific real mixture. The qualitative conclusions obtained here help understand the actual experimental results.

2.2 Initial condition

As shown in Fig.1, a steady wave (shock, ZND or cellular detonation) propagates into the nonuniform zone from left to right in the channel. The channel width is set to 0.03 for shocks and ZND detonations, For cellular detonations, the channel width is set to 0.05, which is exactly 50 times the induction length or one cell size. The non-uniform zone is divided into three parts, one hot zone in the middle and two cold zones on the sides with an area ratio of 2:1:1. The temperature of the hot and cold zone T_{hot} and T_{cold} are set as $295 \text{ K} + \Delta T$ and $295 \text{ K} - \Delta T$, respectively. Note that in the following sections, we still use the dimensional temperature for convenience. The solid wall boundary conditions are used at the upper and lower walls. The Mach numbers of the three waves are all set to 5.6.

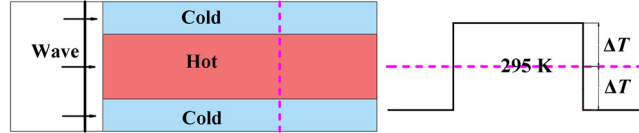


Figure 1: Setup of numerical simulations

3 Results and discussion

3.1 Propagation of shock waves in the temperature non-uniform zone

Geometrical Shock Dynamics (GSD)[9] is a simplified model for nonlinear shock propagation for which the front evolution is governed by a local relation between the geometry of the shock and its velocity. Based on the GSD model, we first examine the case of shock wave refraction at a planar interface separating two gases with different constant sound speeds (or equivalently the temperatures). As shown in Fig.2, the wavefront bends and distorts as it adjusts to the fluid non-uniformities, but the degree of bending is different and highly depends on the sound speed ratio. In the cold zone, two triple-wave structures appear on the wavefronts. In the hot zone, the front becomes convex because of the effect of expansion waves. Horizontal line AB is the temperature interface. Line AC and line AE are the trajectories of the two triple-points. Line AF is the head trajectory of the expansion fan. As shown in Fig.3, it is observed that the angle $\angle BAC$, $\angle BAE$, and the inclination angle of the two oblique shocks ED and BE all increase with the increase in sound speed ratio. It suggests that the increased sound speed ratio results in a more curved wavefront because of the increase in the velocity difference across the

interface. However, the sound speed ratio almost has no influence on the $\angle BAF$ which indicates the effect of the expansion wave.

Figure 4 shows two numerical smoked foils obtained from the numerical simulation of inert shocks, in which the initial evolution of the front structure is similar to Fig.2. However, the numerical results indicate that the Mach stem (or the oblique shock) asymptotically evolves into a steady state ($x > 0.1$) and its length finally becomes a fixed value, which is depicted by the horizontal line DE as shown in Fig.4. Line CD is the trajectory of the triple point of the Mach stem, which generates from the reflection on point C. The Mach stem elongates and meets the lower oblique shock. Depending on the strength of the oblique shock, two possible steady structures exist on the shock front, namely a weak and a strong one, as shown in Fig. 6. In the weak structure, the oblique shock smoothly connects to the Mach stem, becoming a slightly concave front in the cold zone. However, the strong structure has an oblique shock and a planar shock separated by a triple-point in the cold zone. As it propagates into the non-uniform media, the shock first goes through an unsteady state with the presence of two triple-wave structures in the cold zone, while as the asymptotical steady state is reached, the above weak and strong structures appear in the cold zone. Thus a broadened hot zone and two narrowed cold zone separated by the triple-point attached to the oblique shock makes up a typical smoked foil in the case of inert shocks.

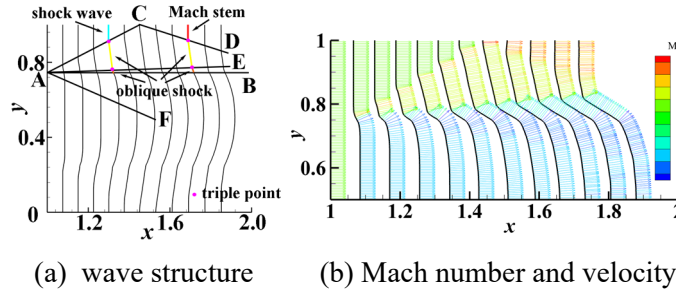


Figure 2: GSD results for a case with $c_{hot}/c_{cold}=1.4$

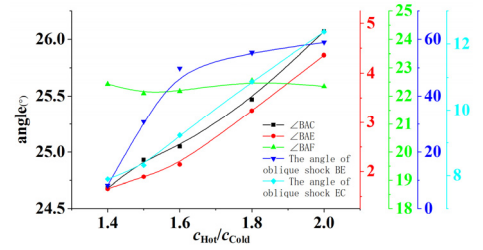


Figure 3: Inclination angles

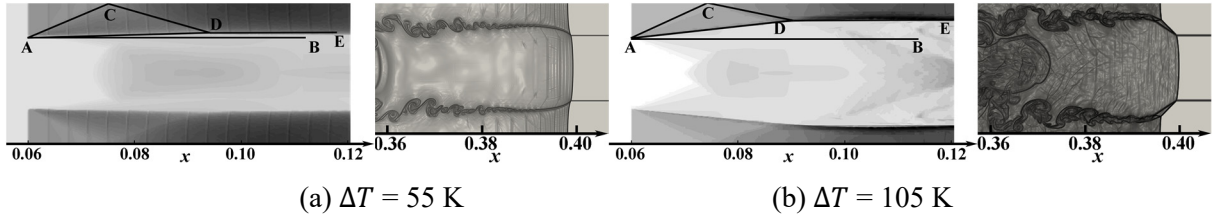
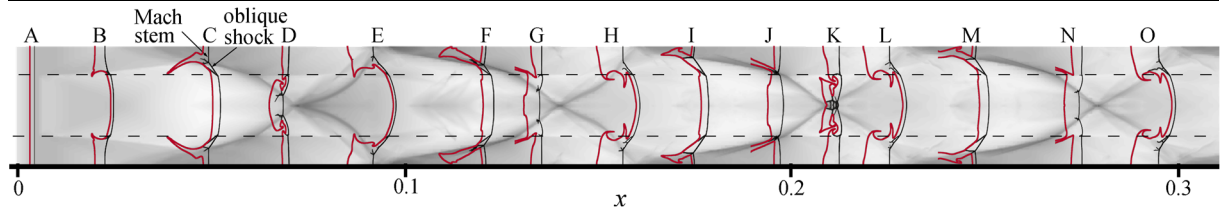


Figure 4: Numerical Smoked foils and asymptotical front structures of shocks in the non-uniform zone

3.2 Propagation of ZND detonation in the temperature non-uniform zone

We then study the propagation of ZND detonations in the non-uniform zone. Fig.5 shows the evolution of the ZND detonation when entering the non-uniform zone ($\Delta T = 55$ K). The black and red lines represent the shock and reaction fronts, respectively. When a ZND detonation initially travels into the non-uniform zone, the evolution of the wavefront is identical to the shock. Two triple-wave structures appear on the wavefront due to the velocity difference across the temperature interface. The reflected triple-point in the cold zone passes through the interface into the hot zone and collides with another reflected triple-point from the bottom wall, forming a cell in the channel.

However, compared to the shock, the non-uniformity triggers the generation of transverse waves. The transverse wave can highly influence the oblique shock formed by the temperature interface. It is observed that, in the case with small non-uniformity ($\Delta T = 55$ K), the smoked foil is different from that of the shock wave. The transverse wave dominates the evolution of the front structure, and the existence of non-uniformity and oblique shock only slightly disturbs the local structures and the cell shape.

Figure 5: Evolution of the ZND detonation in the non-uniform zone ($\Delta T = 55$ K)

When the non-uniformity is increased to $\Delta T = 105$ K, as shown in Fig.6, no evident triple-point trajectories (or cells) appear in the channel except for some faint traces created by extremely weak transverse shocks. It is observed that the smoked foil is similar to the case of inert shock, except the trajectory of the triple-point attached to the oblique shock is now fluctuated. It suggests the oblique shock near the interface is the dominant factor rather than the transverse wave, which is highly suppressed by the large temperature non-uniformity. Since the low temperature deeply slows down the chemical reaction rate in the cold zone, which causes the serious decoupling of the front and restricts the generation of transverse waves, as shown in Fig.6. In this stage, the fluctuation of the trajectory of the triple-point attached to the oblique shock is small. However, because of the hot spot explosion occurred in the shocked zone behind the decoupled shock front in the cold zone, the front accelerates and pushes the oblique shock back to the interface. The expansion of the front in the cold zone cannot sustain, and a new round of decoupling in the cold zone occurs. In the stage where $0.4 < x < 1.2$, the above process repeatedly appears in the propagation, causing the formation of highly perturbed triple-point trajectories. When $x > 1.2$, high-frequency weak transverse waves in the cold zone stabilize the reaction rate, thus the perturbing of the triple-point trajectories gradually decreases to a steady state.

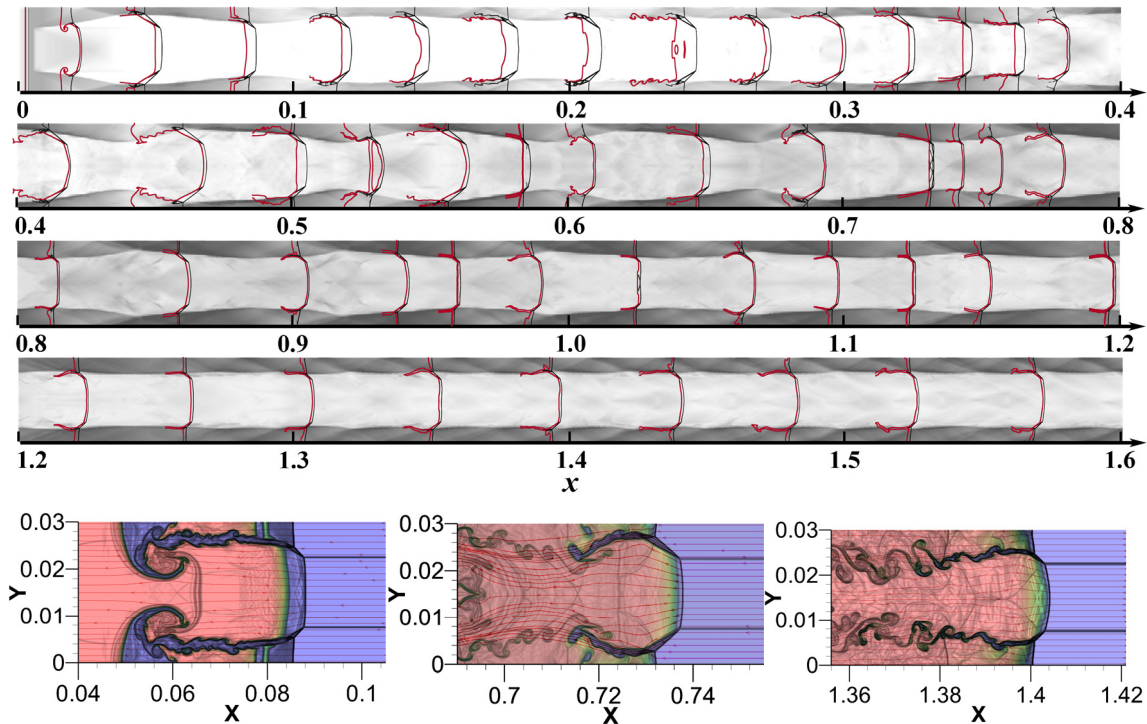
Figure 6: Smoked foil and wave structures of ZND detonation in the non-uniform zone ($\Delta T = 105$ K)

Figure 7 shows the front velocity of the ZND detonation when $\Delta T = 55$ K and 105 K. Due to the energy loss of the unreacted gas in the cold zone, the front velocity drops first. Subsequently, the velocity can increase to V_{CJ} or even higher because of the alternating overdrive of the cold zone and hot zone wavefront. Finally, the shock velocity approaches a value close to V_{CJ} . For the case with large non-

uniformity, i.e., $\Delta T=105$ K, the frequency of oscillation is large, and the amplitude is small compared to the case with $\Delta T=55$ K, indicating the effect of non-uniformity.

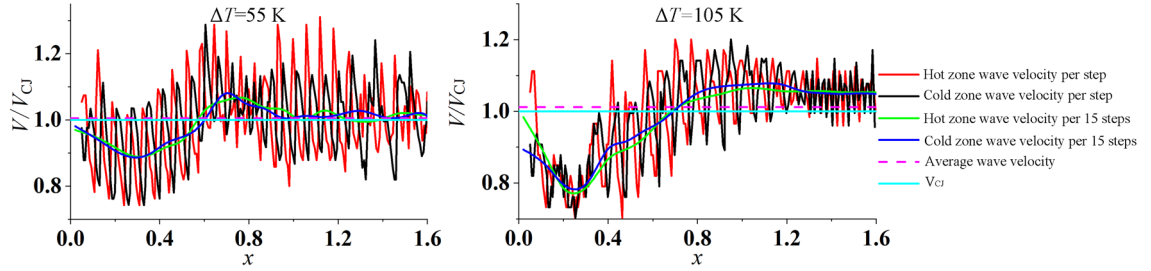


Figure 7: Front velocity of the ZND detonation ($\Delta T=55$ K, $\Delta T=105$ K)

3.3 Propagation of cellular detonation in the temperature non-uniform zone

To get closer to reality, we study cellular detonation in the non-uniform zone at last. As shown in Fig.8, the smoked foils clearly show the influence of different non-uniformities. For the case with small ΔT , the dominant factor is transverse waves, and the oblique shock formed by the temperature interface has a limited effect. However, in the case with large ΔT , the oblique shock created by the temperature interface dominates the evolution of the front, and the high frequency weak transverse waves only cause small fluctuations. Fig.9 shows the front velocity of the cellular detonation. Compared with the front velocity of ZND detonation shown in Fig.9, the initial decay state disappears due to the presence of cellular structures. However, the initial decay state is still present in the case with $\Delta T=105$ K, suggesting the cellular structures postpone the effect of non-uniformity compared to the ZND detonation.

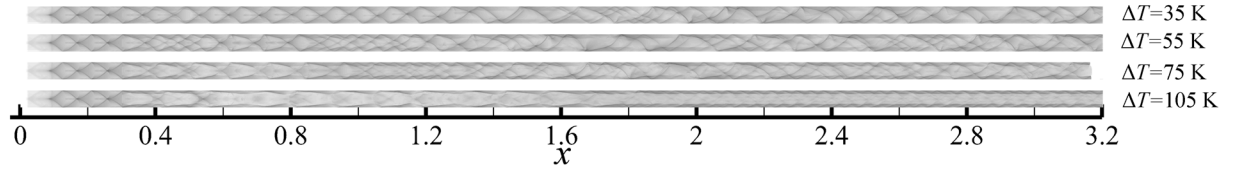


Figure 8: Smoked foils of cellular detonations with different ΔT

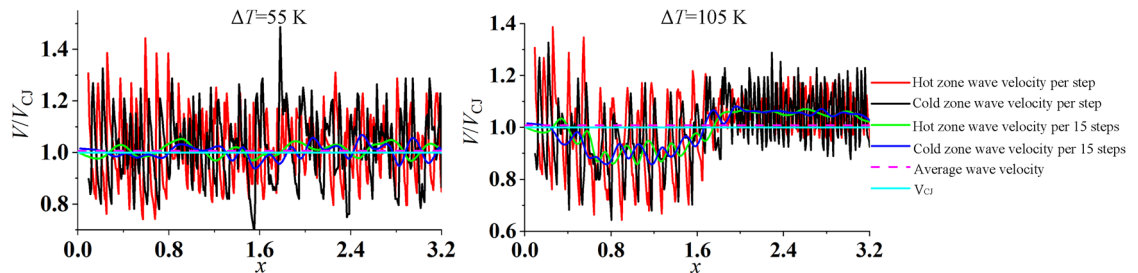
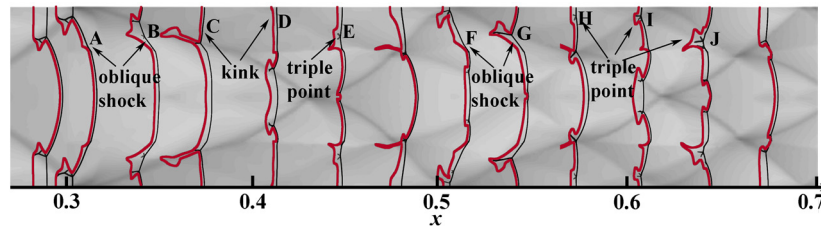


Figure 9: Front velocity of the cellular detonation ($\Delta T=55$ K, $\Delta T=105$ K)

Figure 10 shows the formation of new cells. When the detonation encounters the non-uniform zone at $x = 0.3$, an oblique shock wave (A and B) is formed on the wavefront. The reactive Mach stems merge into the oblique shock, and a kink (C and D) simultaneously appears on the Mach stem. The kink is enhanced by the reflection on the upper wall and becomes a stronger triple point (E). Identical to the above discussion, a new oblique shock is formed (F and G), and H, I, and J denote the new triple-point. The trajectories of the original triple points and the newly generated triple points collectively form the smaller cells.

Figure 10: Formation of new cells ($\Delta T=55$ K)

4 Conclusion

The presence of a temperature interface in the non-uniform zone causes the discreteness of the flow field and the wavefront, forming an oblique shock connecting the convex wavefront in the hot zone and a weaker wavefront in the cold zone. In the smoked foil, the trajectories of the triple points attached to the oblique shocks result in a broadened hot zone and two narrowed cold zones. If the wave is an inert shock, the triple-point trajectory is a horizontal straight line except in the initial transient stage due to the absence of chemical reaction and corresponding transverse waves. If the wave is a ZND detonation, the triple-point trajectory is fluctuated because of the disturbance of transverse waves. The triple-point trajectory is weak for cases with small non-uniformity, and the transverse waves dominate the propagation. However, for cases with large non-uniformity, the triple-point trajectory is strong, and the high-frequency weak transverse waves only cause small amplitude oscillation. In addition, the results suggest that the cellular structures postpone the effect of non-uniformity compared to the ZND detonation.

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