Triple Points Collision in Unstable Detonations

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1 Abstract

In the present work, the detonation structure in high activation energy mixture, which is characterized by its irregular structure, is investigated numerically. The process of transverse wave and triple point collision at the end of the both, first and second half of detonation cell cycle is then examined by a very high-resolution simulation of 600 cells per half reaction zone length. Consequently, the origin of large unburnt gas pockets behind the front is determined. During the reflection in the first-half cell, as the triple point collides with the upper wall, the transverse shock interacts with the unreacted pocket and after reflection of the triple point, the transverse wave collides with the wall. In the second-half cell, the triple point and the transverse wave, collide simultaneously with the wall. In second half-cell, the detonation structure after reflection is single-Mach configuration, but the strong transverse wave switches from primary triple point before collision, to a new one after reflection. In the first half-cell, however, the structure is Double-Mach configuration and does not change before and after reflection. Upon reflection in both first- and second-half, cell due to the detachment of the jet flow and shear layer, the reaction zone decoupled from the shock. After some time a new jet, forms and the reaction zone sticks to the shock front again. The tongue-like unreacted gas pocket detaches from the front, during the reflection process at the end of the first half-cell. The simultaneous interaction of triple point and transverse wave with the wall at the end of the first half-cell produces high-pressurized region at the boundary, which results in formation of large vortices via Richtmyer-Meshkov instability. Thus, in the second half-cell, where the shock strength decreases substantially, the heat resealed via ignition of this pocket due to large vortices helps the self-sustenance propagation of detonation wave.

2 Introduction

Previous experimental research has established that the self-sustaining gaseous detonations are unstable and have a three-dimensional non-steady cellular structure [1]. The leading wrinkled shock consists of alternate weak incident shocks, stronger Mach stems and transverse waves that are interact at so-called triple points. Two types of detonation structure, weak and strong, are observed in experiments [1]. In the weak structure, the transverse wave is relatively weak and un-reactive. In the strong structure, a portion of transverse wave close to the triple point is so strong that may act as a detonation itself. The collision and reflection process of a triple point with the channel wall or another triple point that occurs in a small region and a very short time scale, cannot be captured in experiments. Therefore, numerical simulations are used to properly study the structure configuration in such process (e.g. Lefebvre and Oran [2], Sharpe [3] and Hu et al. [4]). In summary, these numerical

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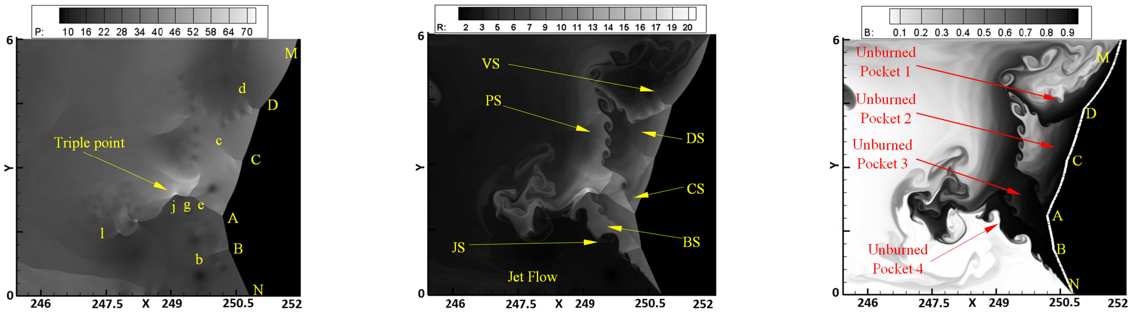
simulations, determined the structure configuration at the end of the first half of the detonation cell in low activation energy mixture, which characterized by its regular structure. They concluded that, the single-Mach configuration that appears after the collision, is changed quickly to a double-Mach configuration. At the first half of a cell, the strong Mach stem sweeps across the channel, at the decaying portion of the cell, a weak incident wave forms the leading shock. Therefore, it seems that the structure configuration during the collision processes, at the end of the first half-cell differs from that at the end of the decaying portion of the cell cycle. Besides, experimental and numerical observations indicate the existence of two different types of structure in mixtures with different activation energies. Irregular structure with the existence of un-reacted gas pockets behind the front, for high activation energy mixtures; and regular cellular structure with no noticeable un-reacted gas behind the front observed for low activation energy mixtures [5]. Unburnt pockets are one of the important phenomena that have been observed both in experiments and in numerical simulations [5-9]. These investigations pointed out that in high activation energy mixtures turbulent mixing, produced by Richtmyer-Meshkov instability (RMI) as well as Kelvin-Helmholtz (KHI) play profound role in the the consumption of unburnt pockets. Nevertheless, the origin of the formation of unreacted pockets, as well as, the burning mechanism of these unreacted pockets and their role in ignition and propagation mechanism of detonations, are not still well resolved. In the present study, using a very high-resolution numerical simulation, i) the structure configuration of unstable detonations are studied during the collision and reflection processes of triple point and transverse wave with the channel walls, at the end of the first as well as the second half of detonation cell. ii) The origin and the mechanism by which unburned pockets form behind the front, are investigated. iii) The role of RMI and KHI, and the transverse waves in consumption of these pockets are clarified.

3 Computational Issues

Two-dimensional reactive Euler equations with a single step Arrhenius kinetics model are integrated to simulate the propagation of gaseous detonations in a 2D channel. The details of the governing equations, nondimensionalizing, and the numerical methods were discussed in depth in [9]. The half reaction length (hrl) of the steady structure of ZND detonation is considered as the length scale. The simulations are performed for mixture with thermo-physical properties, activation energy E_a/RT_0=20, specific heat ratio γ=1.2, and heat release Q/RT_0=50. The computational domain is considered such that half a cell (one mode) is formed in the channel width. All the computations are performed on a Beowulf cluster with six nodes. Each node contains clock speed of 3.0 GHz and 1GByte of memory. Typical computation for 600 computational cells per hrl takes about five weeks of the parallel system.

4 Detonation structure

In order to study the details of the structure of an unstable detonation, contours of pressure, density, and reaction progress variable of a mixture with E_a/RT_0=20 are shown in Figs. 1a to 1c. An extensive description of the structure is given by Mahmoudi and Mazaheri in reference [7]. However, the main features of the structure are introduced briefly here. In Fig. 1a the primary triple point (A) joins the primary Mach stem (AM), the primary incident wave (AN) and the primary transverse wave (Al). Secondary triple points B, C, D, which have their own transverse waves Bb, Cc and Dd, respectively, are clearly visible in Fig. 1a [10]. A jet flow that is developed due to RMI is shown in Fig. 1b. Js is a shear layer which separates the burned gases inside the jet flow with the gases that have passed through the segment BN of the incident shock. PS is the primary shear layer, and BS, CS and DS are the shear layers corresponding to the secondary triple points B, C and D, respectively. VS is the shear layer associated with the large vortex close to the upper wall. Al is the main transverse wave and the kinks e, j and g divide the primary transverse waves into different segments. The straight lines Ae and eg are weak and non-reactive section of the transverse waves. The line gj is the reactive segment of the transverse wave. jl is the rare segment of the transverse wave. It is seen that the detonation structure exhibits a double-Mach configuration of strong type, where a secondary triple point g exists along the primary transverse wave. Based on Fig. 1c, the reaction progress variable behind the segment MD of Mach stem is about β≈ 0.91, which is higher than the reaction progress variable behind the section DC, (β≈ 0.63) of the Mach stem. Unreacted gas pocket (1) behind the shock MD, is surrounded by shear layers VS and DS. The unburned pocket (2), with a lower value of β than pocket (1), is formed behind the stronger segment AD of Mach stem. Two unburned pockets (3) and (4) contain the partly burned gasses that have passed through the two portions, AB and BN of the incident wave, respectively. Therefore, in irregular structure detonations, most portions of the reactant remain as unburned gas pockets downstream of the main front.



(a) Pressure (b) Density (c) Reaction Progress variable

Figure 1. Detailed structure of detonation for mixture with E_a/RT_0==20, Q/RT_0=50 and γ=1.2.

5 Collision with lower wall at the end of second half-cell

In this section the collision and reflection processes of triple points with the channel wall at the end of the decaying portion of the detonation cell is investigated. The contours of pressure and reaction progress variable are shown in Fig. 2. Referring again to Fig. 1a it is seen that the primary triple point A moves downward and is about to collide with the triple point B. After a while, triple point A catches up with the secondary triple point B and moves downward as combined triple point AB, Figs. 2a and 2b. Also, Fig. 2b shows that the shear layers associated to these two triple points combine to each other and create a new shear layer corresponding to triple point AB. The triple point B is produced due to interaction of the lower jet flow with the front. Since the position of the jet is fixed, hence, the position of the triple point B is not changed in the structure; therefore, the interaction of triple point A with B is not similar to collision of two triple points, which move toward each other. Hence, such collision results in a small-pressurized region. Shown in Fig. 2c and 2d are the structure of the detonation when the triple point AB collides with the lower wall. The shear layer corresponding to triple point AB merges with the shear layer of the jet flow and create a single “detached shear layer”, which is shown in Fig. 2d. Due to interaction of the AB and the transverse waves with the wall, produces high-pressurized region at lower boundary, which produces a region whose pressure is p≈72. Interesting to note is that, before the collision, the incident shock propagates like an oblique shock (Fig. 2b), while, as Fig. 2d shows, the incident shock propagates as a normal wave. Furthermore, the jet flow detaches from the shock front and consequently, the reaction rate behind the incident wave decreases dramatically. Thus, in comparison to Fig. 2a, where the length of reaction zone is about L1≈0.11, the reaction zone length behind the normal incident wave increases in Fig. 2d (L1≈0.33). Referring again to Figs. 2c and 2d, since, the collision occurs inside the hot and burned gases of the jet flow, hence, it does not affect the reaction rate of the unburnt gases outside the jet flow. Besides, based on Fig. 2d, as the triple point collides with the wall, the jet flow detaches from the front and fall behind it. Thus, the turbulent mixing of hot and cold gases at lower wall behind the incident wave decreases. Consequently, the length of the reaction zone behind this wave increases. The high-pressurized region at lower boundary creates compression waves. The interaction of these compression waves with the normal incident wave forces it to accelerate relative to the other portion of the shock and propagates as an oblique wave, Fig. 2e. Due to this acceleration, a kink (K) is created at lower part of the shock front, close to the lower boundary. This kink is a triple point, which has its own transverse wave (Kg), whose strength is about S=0.91 (Strength is defined as $S=P_2/P_1$ where P_1

and P_2 are the pressure across the transverse wave, [11]). Therefore, it is concluded that, before a new triple point reflects off the bottom wall, a triple point creates in the structure near the bottom boundary whose transverse wave is of strong-type (i.e. S=0.35). Thus, this triple point (K) acts as a primary triple point, after reflection. After some time, a new triple point (L) is formed at the bottom boundary below the triple point K. The triple point (L) is a secondary triple point, and its transverse wave is of weak-type. A pair of forward and backward jets creates at lower wall. The backward jet moves into the hot gases inside the detached jet flow, so it consumed quickly. The forward jet, however, moves toward the shock front and interact with the Mach stem, produces a new kink (L), Fig. 2f.

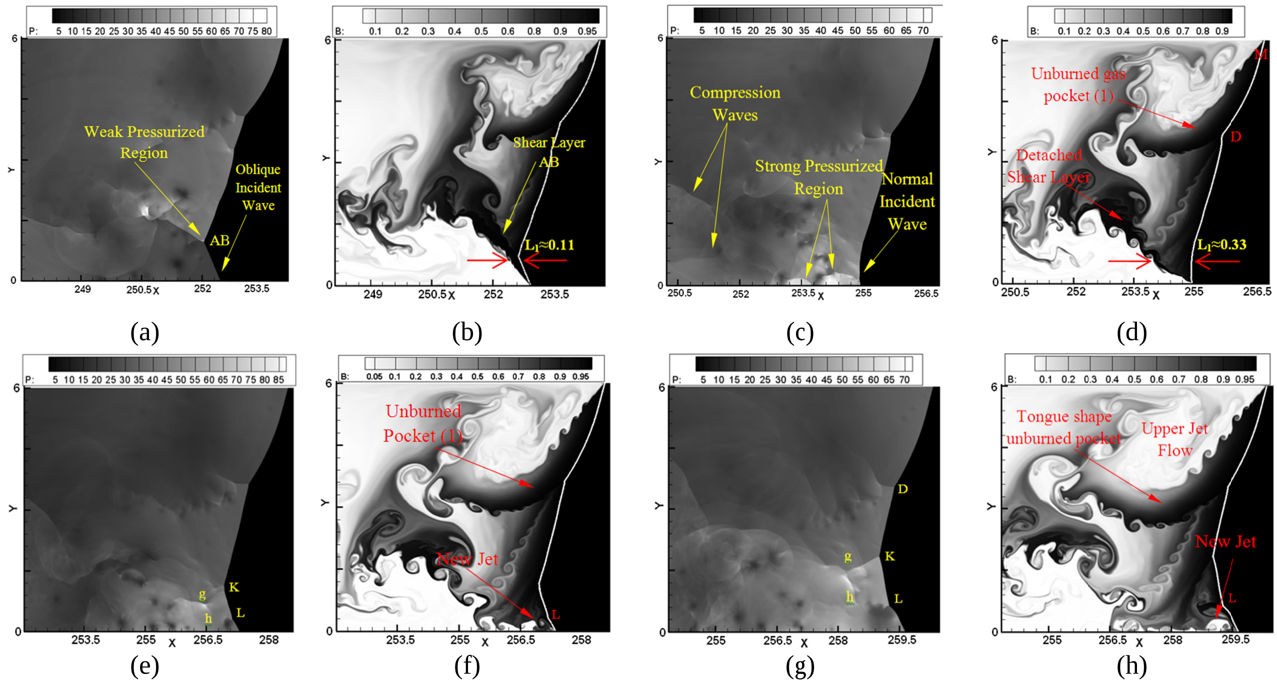


Figure 2. Detonation structure during the collision process with the lower wall, end of the second half-cell.

An additional shock wave (gh) is clearly visible along the transverse wave corresponding to triple point k. Indicating that the structure after reflection is like a double-Mach configuration of strong-type. The conclusion of the above study is that, at the end of the detonation cell, the structure is like a double Mach configuration, which interacts with the wall. After reflection, a weak triple point appears in the front and the structure is changed to a single Mach configuration. However, before the formation of this weak triple point, a strong triple point appears in the structure, near the wall, whose transverse wave is of strong-type. Shown in Figs. 2g and 2h are the detonation structure when the main triple point (K) moves further away from the wall. The secondary triple points g, D and L are clearly visible in Fig. 2g. Besides, the forward jet flow produced by RMI is now much larger than that at earlier time, Fig. 2f. Hence, the reaction rate behind the Mach stem increases and consequently the reaction zone length behind it decreases. Furthermore, the weak incident shock continuously engulfs gases with very long ignition delay time. This can be seen from the increasing size of unburned layer in Fig. 2h, which separates the burned gases inside the upper jet flow from that processed by the incident shock. The gases passed through the incident shock accumulate in a tongue-like shape, as can be seen in Fig. 2h.

6 Collision with upper wall at the end of first half-cell

Figures 3a to 3h show the detail of the structure of a detonation during the collision and reflection processes of a triple point and a transverse wave with the channel wall at the end of the first half of detonation cell. The contours of density and reaction progress variable are shown in Fig. 3. Before the collision, the triple point A caches up with the secondary triple point D and travels as combined triple point AD upward, Fig. 3a. The tongue-like pocket with $\beta \approx 0.97$ is seen in Fig. 3b that is in its maximum size, which extends far back into the hot gas behind the front. The primary shear layer (ps) and the shear layer corresponding to the upper jet flow (jsu), surround this pocket. Two weak localized high-pressure regions create inside this pocket. The interaction of reactive section of the transverse wave with jsu, causes the first high-pressure region. The first interaction creates the reflected shock waves R1 and R2. The interaction of shock R1 with ps generates the second high-pressurized region inside the pocket. However, Fig. 3b shows that the reaction progress variable does not alter at the interaction points, $\beta \approx 0.95$. Besides, these high-pressured region do not change the pocket morphology. As Fig. 3c shows, when the combined triple point AD collides with the upper wall, rapid pressure rise occurs at upper boundary, labeled by T.P collision in Fig. 3c. This collision produces a region whose pressure is $p \approx 70$. Although, at collision point, the pressure produced at upper wall is the same as that at lower wall (i.e. $p \approx 70$) , however, comparison of Fig. 3c with Fig.2c shows that, the high-pressure region produced at upper wall is much smaller than that at lower wall. By this time, the primary transverse wave engages with the unburned gas pocket and does not reach the upper wall. Based on Fig. 3d, the reaction zone length behind the front at upper wall is $L_1 \approx 0.08$ which is two times longer than that at earlier time, Fig. 3b ($L_1 \approx 0.04$). This indicates that, the shear layer is decoupled from the front. As the triple point reflects off the wall, due to interaction of the reactive section of the transverse wave with the wall, another strong pressure region occurs at upper wall (labeled by T.W collision in Fig. 3e) , and produces a region with pressure $p \approx 65$. As illustrated in Fig. 3f, the tongue-shape unburned pocket isolates from the main front and fall further behind the front. This pocket is triangular with a notch at its vertex. After reflection, the new primary triple point (A) and its associated shear layer (s) and transverse wave (Ag) are formed, Figs. 3g and 3h. Besides, the high-pressure region produces a jet flow, which interacts with the new Mach stem and produces the new kink (D), Fig. 3g.

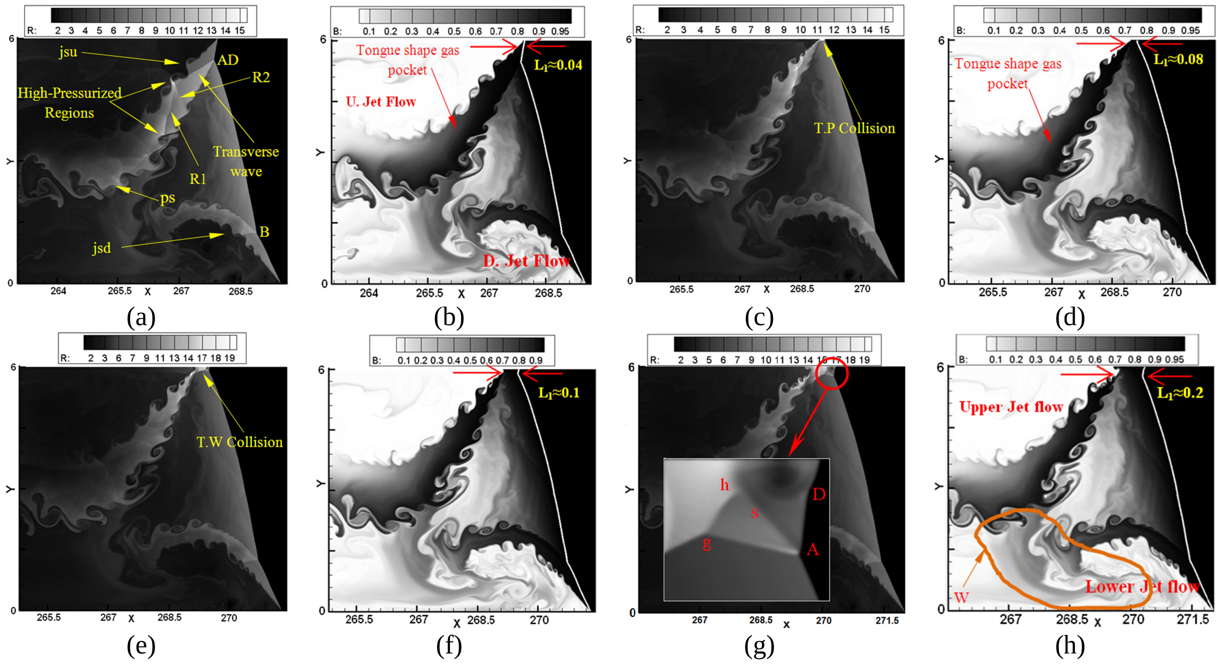


Figure 3. Collision and reflection processes with the upper wall at the end of the first half-cell.

The secondary triple point (g) and the shock wave gh, that are seen along the new transverse wave, indicates that the structure is like a double-Mach configuration. According to Fig. 3h, the upper jet flow recedes from the front, resulting in low reaction rate behind the new Mach stem, close to the upper wall. Consequently, the reaction zone length increases to $L_1=0.2$. Thus, in comparison to Fig. 3f, the reaction zone length is two times longer. Hence, before the reflection of a new triple point off the wall, the reaction zone becomes detached from the shock front. When the new triple point (A) propagates more toward the lower wal1, a structure like Fig. 1 appears. The new jet grows progressively, hence, the reaction zone length behind the Mach stem decrease. Thus, it is concluded that the genesis of the large tongue-like unreacted gas pockets is behind the Mach stem not incident wave. The conclusion of this section is that, in collision and reflection process with upper wall at the end of the first half of detonation cell, when the triple point collides with the wall, the transverse wave engages with the tongue-like pocket and does not reach the upper wall. While, at the end of the first half-cell, the triple point and the transverse wave, interact simultaneously with lower wall. Therefore, in collision with lower wall, the structure configuration is double-Mach before the collision and single-Mach after reflection. However, before the formation of weak triple point, a strong-type double Mach configuration forms near the wall. While, in reflection processes with upper wall, the structure is of strong-type double Mach configuration and does not change before and after collision. The Large-scale vortex produced by RMI drags the capsule of unreacted gas into it and facilitates the burning of the unreacted pocket. The secondary instability, Kelvin-Helmholtz instability develops along the large vortex boundary, which causes vortex roll-up in small-scales. Ultimately, a turbulent mixing zone develops between hot and cold gases. The present results show that, such turbulent zone leads to the consumption of the pocket during the second half of a cell cycle. Hence, the energy released via the consumption of the tongue-shape pocket within the second half of the cell, where the shock strength has decreased, support the lead shock and helps the self-sustenance propagation of the detonation.

7 Summary

The present work, based on a high-resolution numerical simulation of the Euler equations, has depicted the detonation structure evolution during the period of collision and reflection processes of triple points with the wall at the end of both, first- and second- half detonation cell-cycle. The origin and consumption mechanism of large un-reacted gas behind the front are studied.

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