# HYDODYNAMIC INSTABILITIES AND UNREACTED GAS POCKETS IN CELLULAR DETONATIONS

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# Abstract

The role played by transverse waves and hydrodynamic instabilities mainly, Richtmyer-Meshkov instability (RMI) and Kelvin-Helmholtz instability (KHI) in consumption of unburnt gas pockets in detonation structure is studied in the present work using two-dimensional numerical simulations. The computations are performed for both high and low activation energy mixtures, characterized by their highly turbulent and laminar reaction zone structure, respectively. Results reveal that, upon collision of triple points a pair of forward and backward facing jets is formed by the mechanism of Richtmyer-Meshkov instability. Interaction of the backward jet with unreacted gas pockets causes the unreacted gas pockets break into to smaller pieces. As the structure evolves, the RMI grows dramatically and the size of the jets increases. The growth rate of the forward jet found to be much higher compared to that of the backward jet. In comparison to the role of RMI, KHI found to be less important in consumption mechanism of unreacted gas pockets either in stable or unstable detonations. Moreover, it is revealed that KHI and RMI to have more substantial role in propagation mechanism of irregular structure detonations. The present results indicate that the transverse waves do not play substantial role in ignition mechanism of unreacted gases. Transverse waves are solely a carrier of the triple points. In fact, this is the collision of the triple points that produces high-pressurized regions, resulting in formation of large vortical structure. These large vortices have profound role in consumption of unburned gas pockets, thereby supporting the self-sustained propagation of irregular detonations. In regular detonations, the lead shock ignites all the gases passing through it, hence, no noticeable unburnt pocket form behind the main shock. Therefore, the transverse waves and hydrodynamic instabilities do not play crucial role in propagation and ignition mechanism of such stable detonations.

# Introduction

Experiments have revealed that all self-sustained detonations are unstable with three-dimensional transient cellular structure that is formed by an ensemble of interacting shock waves[1]. The leading shock involves Mach stems and incident waves. Shear layers and transverse shocks extend from the cell boundaries into the reaction zone behind the leading shocks. Triple points exist at the intersection of the leading shock front and the transverse waves. The transverse shocks sweep laterally across the leading shock surface and collide with each other. They also interact and sometimes couple with the shear layers [2]. When a detonation propagates in a tube with soot-coated wall, the track of the triple point creates the boundaries of detonation cell [1]. Depending on the cell regularity on the smoked foil the detonations are classified into regular and irregular cellular structure [1]. Schlieren visualizations and numerical simulations of the reaction zone structures in irregular structure detonations indicate that the shock front cannot ignite all the gases that are passed through it and pockets of unreacted gas detach from the front [3-4]. On the other hand, in regular structure detonations intense chemical activity is observed behind the lead

shocks, where very little sign of unreacted pockets are found [3, 5]. Numerical simulations (e.g. [3]) and experimental observations (e.g. [2, 4]) pointed out that in irregular structure detonations, hydrodynamic instabilities, mainly Richtmyer-Meshkov instability (RMI) and Kelvin-Helmholtz instability (KHI), forms a turbulent mixing zone of hot reacted gases and cold unreacted materials.

Investigating deflagration to detonation transition (DDT) phenomenon (e.g. [6]), it was found that repeated interactions between shocks and flames lead to RMI, which distorted the flame surfaces, promoting localized mixing and enhancing the burning rates. In [6] it was pointed out that the origin of the large-scale turbulence is RMI induced by repeated shock-flame interactions. Besides, KHI in small-scale was found to be another source of turbulence. However, it was found that KHI to be less important than RMI in promoting the turbulent mixing and disrupting the flame surface [6]. The evolution and growth of RMI was put forward both theoretically and numerically in numerous investigations (e.g. [7]). In such numerical investigations, a shock is interacted with an interface separating two fluids of different density. Any perturbation initially present on the interface is amplified following the refraction of the shock. The basic mechanism for the amplification of perturbations at the interface is baroclinic vorticity generation resulting from the misalignment of the pressure gradient of the shock and the density gradient across the interface. As the interface between the two fluids becomes more distorted, secondary instabilities, such as the Kelvin-Helmholtz instability, develop and produces a region of turbulent mixing.

The present study, using high resolution numerical simulations, attempts to elucidate the growth and the evolution of the Richtmyer-Meshkov and the Kelvin-Helmholtz instabilities in detonation structure. Consequently, the mechanism by which the unreacted gas pockets are burnt is then examined. Subsequently, the role of transverse waves in ignition and propagation mechanism of detonations is identified.

### Mathematical model and numerical details

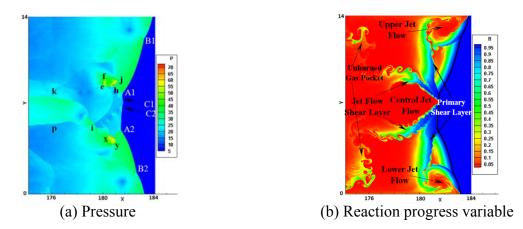
The two-dimensional reactive Euler equations with a single step Arrhenius kinetics model are integrated to simulate the structure of idealized gaseous detonation. The gases are assumed to be perfect, and the product and reactant gases are assumed to have the same specific heats. The dependent variables are non-dimensionalized with respect to the unburnt mixture properties. Density is non-dimensionalized with  $\rho_0$ , and pressure with  $\gamma p_0$ . For the velocity, the sound speed of the unburned mixture,  $C_0$ , is used as the reference. The characteristic length scale  $L_c$ , is the length traveled by a fluid particle (in the detonation frame of reference) from the leading shock to the position where  $\beta = 0.5$  in a ZND structure, the so-called half-reaction length (*hrl*). Due to the presence of intense reactions near the shock front, it is necessary to use very fine meshes in this region. To fulfill this requirement, a simple version of the adaptive mesh refinement of Berger and Colella [8] is utilized in the present work. The above methods were used extensively in previous numerical simulation of gaseous detonations (e.g. [3, 9]). The thermo-chemistry parameters are chosen as:  $E_a/RT_0=10$  and 20,  $Q/RT_0=50$  and  $\gamma=1.2$ . These data have been used extensively in past numerical simulations of detonation waves [3, 9-10].

For initiation of detonation a strong blast wave is located at x=5.0, moving to the right and forming a one-dimensional detonation. The one-dimensional detonation is then perturbed by adding a disturbance in the ambient density. The domain width in the y-direction is 14 and 12 for the activation energies of 20 and 10, respectively. This permits to have two detonation modes in the computational domain. In order to ensure that the structure is independent of the initial conditions, it is allowed that the detonation to propagate to 400hrl. In the present numerical

simulation, resolution of 320 points in hrl is employed to capture properly the evolution of the hydrodynamic instabilities in both low and high activation energy mixtures [3]. A scalable parallel reactive Euler code is developed to carry out the heavy two-dimensional computations. The details of the governing equations, nondimensionalizing, the numerical methods and parallelization strategy were discussed in depth in [10-11].

# **Detonation with irregular structure**

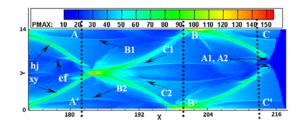
Typical structure of a self-sustained detonation, in a mixture with  $E_a/RT_0=20$  is shown in Fig. 1. Contours of pressure and reaction progress variable are produced here. In Figs. 1a and 1b, the primary triple points A1 and A2 move toward each other. The secondary triple points B1, B2, C1 and C2 are also seen in these figures. In Fig. 1b, the central jet flow is generated due to collision of two primary triple points at the start of a new detonation cell cycle. The upper and lower jet flows, as well, are created due to collision of the primary triple points with the upper and lower boundaries, respectively at the end of the first half of the detonation cell cycle. The secondary triple points are created due to interaction of the jet flows with the shock front [3, 12]. The upper and lower jet flows, cause the appearance of B1 and B2, respectively. The central jet flow is responsible for the formation of C1 and C2. Interaction of the primary transverse waves corresponding to the triple points A1 and A2 with the shear layers, results in generation of reflected waves hi, ef and xy. The existence of the additional shock waves hi, ef and xy along the transverse waves indicates that the transverse waves in such mixture is of strong-type [13]. Furthermore, the interaction of the transverse wave associated with the triple point A2 with the "central jet flow shear layer" at point i generates two weak shocks k and p. These observations indicate that, although the transverse waves in irregular structure detonations are of strong-type, however, their interaction with the unreacted pockets boundaries, scatter these waves into a system of shocklet waves. Thus, as it is seen the resulted weak shocks (hj, ef, ei and xy) are not strong enough to participate in consumption of unreacted gas pockets inside the shear layers. Also interesting to note is that, although, faint chemical activity is observed at the shear layerstransverse waves interactions (i.e. points h, e and x in Fig. 1a), however, the interaction of the transverse wave with these unreacted layers does not even alter the unreacted pockets morphology (Fig. 1b).



**Figure 1**. Detonation structure in a channel with two triple points in a mixture with  $E_a/RT_0=20$ ,  $Q/RT_0=50$ ,  $\gamma=1.2$  and N=320cell/hrl. (a) contour of pressure, (b) contour of reaction progress variable. Solid line indicates the shock position.

It is seen in Fig. 1b that the unreacted gas pockets, which are produced in the previous cell cycle, are dragged into the rolling zone of the jet flows and consumed via mixing of hot and cold materials. Besides, the upper and lower jet flows, extract the gases from the primary shear layers into their circulation zones, and facilitate the ignition of these partly burned gases. Moreover, the small-scale vortices are created along the shear layers via the Kelvin-Helmholtz instability. Small-scale vortices distort the surface of the large-scale vortices and create smaller-scale turbulent motions. These turbulent zones, cause the mixing of hot and cold gases at pockets boundaries, and consequently, enhance the burning rate of the unburnt pockets. In Fig. 1b it is seen that the small-scale vortices are created along these small vortices is much smaller than those created via RMI. Besides, the size of these small vortices is much smaller than those created via RMI. Thus, the KHI has less important role in mixing of hot gases and cold materials.

The smoke-foil inscription is also numerically reproduced based on the maximum pressure in the flow field (Fig. 2). The tracks of the primary and the secondary triple points, as well as, the trajectory of the reflective waves along the transverse waves, xy, hj and ef are shown in this figure. ef is a reflected wave that is created due to interaction of the strong section of the transverse wave (i.e. hg in Fig. 1a) with the jet flow boundary.

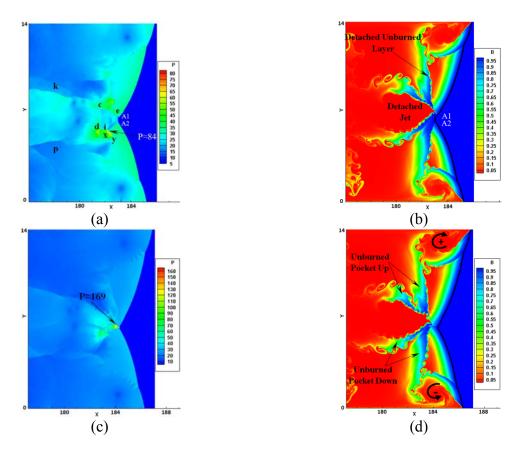


**Figure 2**. Numerical smoked-foil based on maximum pressure history in the channel in a mixture with  $E_a/RT_0=20$ ,  $Q/RT_0=50$ ,  $\gamma=1.2$  and N=320cell/hrl.

The region between AA' and BB' is referred to as a first half of a detonation cell, where the Mach stem sweeps the channel width. While, the region between the BB' and CC' is called the second half of the detonation cell, where the gases are processed by the weak incident wave. Hence, from AA' to CC' the leading front alternates between the Mach stem and the incident shock. In the following sections, in order to investigate the growth and evolution of hydrodynamic instabilities, the structure of detonation is investigated between section AA' and CC' (i.e. through the evolution of a complete cell cycle).

### Formation of unreacted gas pockets

To clarify the formation mechanism of unreacted gas pockets in detonation structure, a series of snapshot illustrating the contours of pressure and reaction progress variables is shown in Fig. 3. In these figures, two primary triple points A1 and A2 reflected off the upper and lower walls, respectively and moves toward each other.

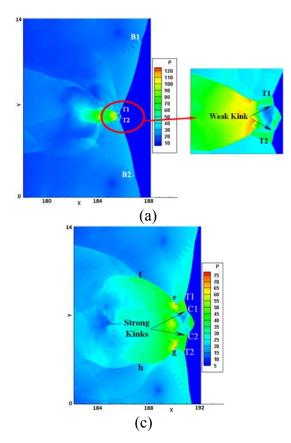


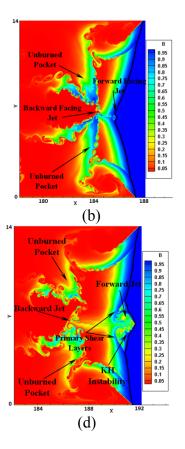
**Figure 3**. Detonation structure before and through the collision of two primary triple points in a mixture with  $E_a/RT_0=20$ ,  $Q/RT_0=50$ ,  $\gamma=1.2$  and N=320cell/hrl. (a) to (d) represent the structure before the collision of A1 and A2. (e) and (f) illustrate the collision of triple points A1 and A2. Right figures, contour of pressure and left figures are contour of reaction progress variable.

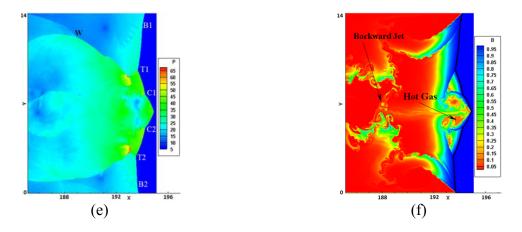
In Fig. 3a triple points A1 and A2 are about to collide with each other. At this moment, the maximum pressure behind the shock is pertinent to the interaction point (x or i,  $P\approx 84$ ). It is seen that before the collision of two triple points, the boundaries of the central jet flow and the primary shear layer corresponding to the triple point A1 break away from the front and form a pocket of unreacted gas (Fig. 3b). Hence, in contradict with what reported in [5, 10], current study shows the possibility of the formation of unreacted pockets before the collision of two triple points. After collision of A1 and A2 (Figs. 3c and 3d), a very high-pressure region is formed at the point of collision (P $\approx$ 169), in comparison to the pressure in Fig. 3a (P $\approx$ 84). By this time, the shear layers corresponding to triple point A2 is isolated from the shock front and creates an unburned gas pocket behind the front. Therefore, two groups unreacted gas pockets ("Unburned Pocket Up", and "Unburned Pocket Down") are formed behind the main shock. The clockwise flow circulation (+) inside the upper jet drags the upper portion of the unburned pocket into its circulation zone and the counterclockwise (-) flow circulation of the lower jet flow, extracts the lower portion of the unburned pocket into its rolling zone. Hence, the two unreacted pockets move toward the solid boundaries. In the next section, it will be seen that the two groups unreacted pockets persist to remain behind the shock during first half of a cell cycle, before the collision of the triple points with the sidewalls, occurs. Thus, it is speculated that the energy released via the consumption of these pockets can support the self-sustained propagation of the detonation front.

# **Evolution of Richtmyer-Meshkov instability**

Figures 4a and 4b represent the detonation structure shortly after the collision of two triple points A1 and A2. Enlargement of the structure near the collision point is shown in Fig. 4a. It is seen that after the collision, new triple points T1 and T2, as well as, two weak kinks are formed. In comparison to Fig. 3b it is seen that the size of the jet flows near the side boundaries are increased and the size of the two groups of unreacted pockets is decreased in Fig. 4b. The interaction of the upper and lower jet flows with the shock front forms the secondary triple points B1 and B2 (Fig. 4a). The interaction of two triple points produces a region of high pressure and temperature, significantly increasing the reaction rate in the unburnt gases that passed through the shock front, at earlier time. The high-pressure zone propagates in a pair of forward and backward facing jets by Richtmyer-Meshkov instability, involving the baroclinic  $\nabla p \times \nabla \rho$  vorticity production mechanism, which is clearly visible in Fig. 4b. The forward jet impacts on the new Mach stem, causing weak kinks in the Mach stem. The backward jet, however, travels back and interacts with the unreacted pockets, causing fragmentation of the pockets. Hence, one of the burning mechanisms of the unburned pockets is the interaction of the backward jet with the unburnt pockets, causes randomization of the unburnt pockets.







**Figure 4**. Detonation structure after collision of two triple points, illustrating the evolution of the RMI in a mixture with  $E_a/RT_0=20$ ,  $Q/RT_0=50$ ,  $\gamma=1.2$  and N=320cell/hrl. Left figures represent the pressure filed and right figures show the contour of reaction progress variable.

It is seen in Fig. 4c that the kink points are now stronger than earlier time. These kinks are in fact new secondary triple points, which have their own transverse waves and shear layers (C1 and C2 in Fig. 4c). Figure 4d shows that as the triple points move away from each other, the backward and forward jets grow significantly. The result is that a "funnel" or "spike" of heavy materials (i.e. the unburnt gases) extends into a region of light material (i.e. the products). As the RMI develops, secondary instability (KHI) forms along the boundaries of large vortices. Interesting to note is that, the same as forward jet, the RMI of the backward jet develops progressively, however, the growth rate of backward jet is lower than that of the forward jet. This can be explained by two reasons:

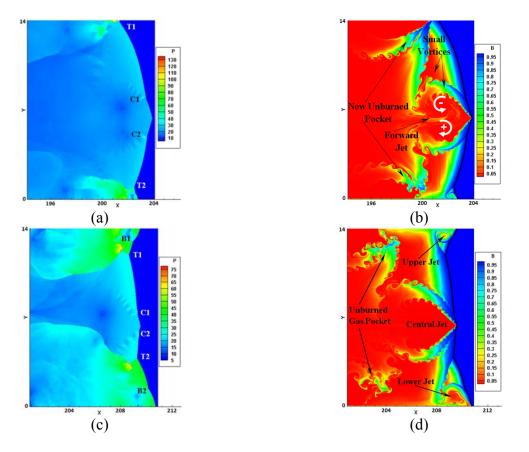
- 1- The direction of the collision of two triple points is in the direction of the detonation propagation, hence most portions of the hot gases as well as the compression waves, move forward. Consequently, the baroclinic vorticity production, which is due to misalignment of pressure gradient and density gradient, induces larger vortex in forward direction compared to backward direction.
- 2- The backward jet propagates into the hot and burned gases and is consumed shortly in the pool of hot products.

As the detonation propagates further, the primary triple points T1 and T2 move toward the boundaries (Figs. 4e and 4f). In Fig. 4f the forward jet is grown, while the backward jet is almost vanished. On the other hand, the size and the scale of the small-scale Kelvin-Helmholtz vortices along the surface of the central jet are decreased noticeably in Fig. 4f. Because, as the RMI grows, more and more hot burned gases are extracted into the jet flow. As a result the small-scale vortices generated by KHI are burned out by the hot gas inside the jet flow. It is observed that the unreacted pockets will be consumed during a half of a cell cycle. Thus, it is speculated that the energy released via the consumption of these unburnt gases augments the shock front and support the self-sustained propagation of the detonation front.

## Richtmyer-Meshkov in the latter portion of the detonation cell

This section deals with the role of RMI in consumption of unburnt gases in the second half of the detonation cell, where the shock strength decreases compared to that at the first half of detonation cell (i.e. region between BB' and CC' in Fig. 2). In Figs. 5a and 5b, the triple points T1 and T2

just reflected off the upper and lower boundaries and move toward each other. New unreacted gas pockets are formed due to the collision of the triple points with the upper and lower walls. The backward jet is completely disappeared in this snapshot. The forward jet, however, grows dramatically. As it is seen a pair of clockwise (+) and counterclockwise (-) circulation inside the central jet, extracts the unburnt materials into its rolling zone and facilitate the burning rate of the new unburnt pockets. Thus, it is deduced that in the first-half cell (Fig. 4), the jet flows near the side boundaries are responsible for the consumption of the unreacted pockets that are generated via collision of two triple points at the channel axes. In turn, in the second half-cell, the jet flow at the channel center sucks the unreacted pockets, which are detached from the front after the collision of the triple points with the sidewalls. Thus, another burning mechanism of the unburned pockets is the extraction of these pockets into the circulation zone of the forward jets and turbulent mixing of the hot and the cold materials inside the jet.

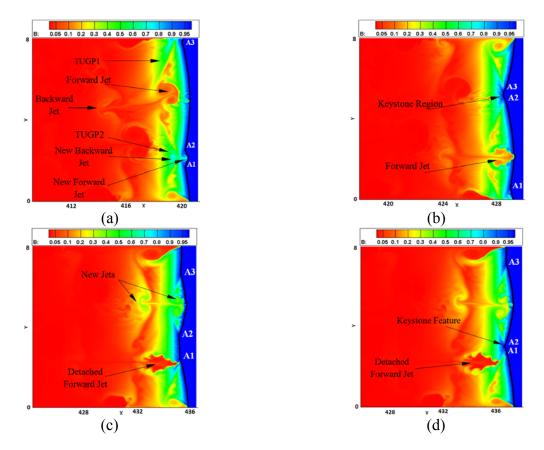


**Figure 5**. Detonation structure in the second half of detonation cell in a mixture with  $E_a/RT_0=20$ ,  $Q/RT_0=50$ ,  $\gamma=1.2$  and N=320cell/hrl. Left figures show the contour of pressure and right figures represent the contour of reaction progress variable.

Figures 5c and 5d illustrate the detonation structure some time after the reflection of T1 and T2 off the side boundaries. It is also seen that the central jet in Fig. 5d is larger than that in Fig. 5b. Consequently, the size of the unreacted pocket decreases. The new jet flows near the sidewalls grow significantly and extract the partly burned gases of the primary shear layer into their rolling zone and enhance the burning rate of the unburnt materials.

# Hydrodynamic instability in detonation with regular structure

To elucidate the possible role of hydrodynamic instabilities in the propagation mechanism of detonations with regular structure, the computations are repeated for a mixture with activation energy  $E_a/RT_0=10$ . The channel width is chosen in such a fashion that 1.5 cells are formed across the channel. Figure 6 represents the contours of reaction progress variable, illustrating the evolution of Richtmyer-Meshkov instability. Figure 6a shows the structure shortly after collision of two triple points A1 and A2, when the triple point A3 is just reflected off the upper wall. After collision of A3 with the upper wall, a triangular-shaped unreacted gas pocket (TUGP1) is isolated from the front, which contains the partly burned gases ( $\beta=0.46$ ) that have passed through the incident wave at the previous cell cycle. However, the forward jet, which is produced at previous cell cycle, eats the unburned materials inside this pocket. Due to collision of A1 and A2, another triangular-like unreacted gas pocket, (TUGP2) isolates from the shock front. A pair of forward and backward facing jets creates upon collision of A1 and A2. These new jets facilitate the ignition of the TUGP2 via turbulent mixing.



**Figure 6**. Reaction progress variable of detonation structure in a mixture with  $E_a/RT_0=10$ ,  $Q/RT_0=50$  and  $\gamma=1.2$  and N=320cell/hrl.

Figure 6b illustrates the detonation structure at a position where A1 reflected off the lower boundary and A2 is close to collide with A3. The new jets grow significantly. The size of TUGP1 and TUGP2 is also, decreased noticeably. It is seen that the forward jet becomes larger compared to that at earlier time, Fig. 6a. Furthermore, a distinct keystone-like unburnt region, bounded by the incident wave and the two shear layers correspond to the triple posits A2 and A3, is observed in Fig. 6b. The existence of such distinct feature in detonation with regular structure, is in excellent agreement with the experimental observation of stable detonations performed by Austin et al. [14]. This keystone-shaped region, contains the unreacted gases ( $\beta$ =0.92) that have passed through the incident wave at earlier time. This region should not be confused with the unburned gas pockets that became isolated from the main detonation front after the collision of two triple points or a triple point with the wall (i.e. TUGP1 and TUGP2 in Fig. 6a). Figure 6c shows that due to interaction of triple points A2 and A3, a new pair of forward and backward jets is created. When triple point A1 moves toward A2, the forward jet that was produced due to collision of A1 and A2 becomes isolated from the shock front, which is labeled by "detached forward jet" in Fig. 6c. This indicates that before the collision of two triple points, the jet flow detached from the main shock. Shown in Fig. 6d is produced at position where the triple points A1 and A2 collides with each other. The new keystone unburnt pocket is also observed in this figure. The results show that as the detonation propagates more, the size of the detached jet reduces dramatically. However, it persists to remain about one third of the cell length behind the front.

# The role of transverse waves

One of the key questions in detonation theory is the role of the transverse waves in propagation mechanism of detonation waves. Radulescu et al. [4], using numerical simulations, commented that the transverse waves do not have a profound role in ignition mechanism of unstable detonations. They reported that the prime role of these waves is enhancing the large vortical structures during the interaction of these waves with the shear layers by the mechanism of RMI [4]. Generally speaking, two points of view have been expressed regarding the role of transverse waves in detonation propagation (e.g. Pintgen et al. [15]):

- 1. The transverse waves are simply manifestations of instability and do not play an essential role in the propagation mechanism.
- 2. Transverse waves are essential to detonation propagation. The transverse waves and interactions of transverse waves provide high-temperature regions that serve as reaction centers.

The present results explore the role of transverse waves and hydrodynamic instabilities in detonations with both laminar and turbulent reaction zone structure. The following deductions are achieved during this study:

- i- In regular structure detonations, main portion of the reaction, takes place behind the lead shock, thus the transverse wave and the hydrodynamic instabilities do not play substantial role in propagation mechanism of such stable detonations (first point of view).
- ii- In irregular structure detonations, most portions of the gases cannot be ignited via shock compression, hence, large unreacted pocket is formed behind the lead shock. The transverse waves are of strong type with a secondary triple point along them, however, these waves are not strong enough to ignite the unburnt pockets and no noticeable reaction takes place behind the transverse waves. Radulescu et al. [4] pointed out that the transverse shocks role is to enhance the burning rates of the unreacted pockets by the baroclinic vorticity generation mechanism during the interaction of these shocks with the shear layers. While the present numerical experiments explore that the transverse waves do not play a role in producing the vortices during the interaction of these shocks with the shear layers. As such interaction results in randomization of these waves and producing a system of shocklets. Therefore, the first conclusion is that the transverse waves, directly, have

no essential role in propagation mechanism of detonations with irregular structure. This behavior is close to the first point of view as mentioned above. However, the collision of triple points corresponding to these transverse shocks produces high-pressure region, results in formation of large vortical structure by the baroclinic vorticity production mechanism via RMI, which promote the burning rate of the unreacted pockets. Hence, indirectly, the transverse waves have substantial role in the propagation mechanism of unstable detonations. This behavior is close to the second point of view as mentioned above.

# Conclusions

A comprehensive study is performed in the present work to determine the evolution of the hydrodynamic instabilities in detonations structure via two-dimensional high-resolution numerical simulation. The role of hydrodynamic instabilities and transverse waves in consumption mechanism of unreacted gas pockets is then studied in both low and high activation energy mixtures. Results obtained for both mixtures show that a pair of forward and rare facing jets are formed upon the collision of two triple points. The interaction of the backward jet with the unreacted gas pocket causes randomization of these pockets. As the structure evolves, the Richtmyer-Meshkov instability grows dramatically and the size of the both forward and backward jets increase progressively. However, the forward jet grows faster than the backward jet. The backward jet is consumed after short time as it moves into the hot products behind the shock. The forward jet, however, drags the unburned materials into its circulation zone and produces large vortices. As the surface of the jet becomes distorted, the secondary instability, (i.e. KHI) develops. However, in initial growth process of the RMI, as more hot and burned gases entrained into the jet flow, the small-scale vortices generated by KHI are consumed inside the circulation zone by these hot materials. In regular case, a distinct keystone-like feature of unreacted materials is observed behind the incident wave close to the collision location of two triple points.

It is found that the transverse waves have indirectly a key role in the mechanism by which the unstable detonations propagate. The collision of two triple points, correspond to the transverse waves in detonations with irregular structure, produces large vortices that contribute significantly in the burning processes of the unreacted gas pockets. However, in the regular case, it is observed that the main shock consumes almost all the gases that have passed through it and hence, the transverse waves and the hydrodynamic instabilities have no profound role in propagation mechanism of such stable detonations.

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