TRIPLE POINT COLLISION AND HOT SPOT IN DETONATIONS WITH REGULAR STRUCTURE

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Abstract
In the present work, the details of a regular structure detonation are studied using very high-resolution two-dimensional numerical simulations. The evolution of the structure is examined during the collision and reflection processes of a triple point and its associated transverse wave with the wall, at the end of the first half of detonation cell, as well as, at the end of the second portion of the cell cycle. It is found that more than 300 points per half reaction length is required to resolve properly the structure configuration during the collision processes. The detonation structure is found to be a double-Mach configuration, while it changes to a single-Mach configuration shortly before collision of triple points with the walls. During a collision, both in the first and the second half of the detonation cell, three processes occur; i: interaction of rare portion of the transverse wave with the walls at different points ii: simultaneous interaction of strong portion of the transverse wave and the triple point with the walls iii: simultaneous reflection of the transverse wave and the triple point off the wall. During the reflection, the shear layer becomes detached from the front and recedes from it, producing a pocket of unburnt gas. After reflection, the structure is a single-Mach configuration, while it changes to a double-Mach configuration after some times. Shortly before the collision in the second half of the cell, a hot spot creates behind the incident wave at the wall. Hence, in comparison to the first half of the detonation cell, the wall-transverse wave interaction produces lower pressurized region at the end of the cell cycle. This hot spot will burn eventually by turbulent mixing along the detached shear layer due to the existence of small-scale vortices produced by Kelvin-Helmholtz instability.

Introduction
It is well recognized that most self-sustaining detonations have complicated three-dimensional, time-dependent structure [1]. The structure consists of a leading shock, involving a Mach stem and an incident wave. The interior transverse waves move back and forth laterally behind the main front. Triple points exist at the junction of the leading shock front and the transverse waves. The lead shock undergoes cyclic oscillations in space and time [2]. As the detonation propagates forward, the triple points collide with each other or with a solid boundary. Two types of structure, a weak structure and a strong structure, have been observed in experiments [1]. The weak structure is characterized by a single-Mach configuration, with the associated transverse wave being merely a simple shock wave. While, the strong structure is characterized by a double-Mach configuration with a much stronger transverse wave, which is kinked at a second triple point along it [1, 3]. Strehlow and Crooker [4] concluded that in hydrogen/oxygen/argon mixture just after collision of two triple points, the structure appear to be of a weak type. While, after some time the structure became of a strong type. In experiments, it is not clear what happens just after collision of two triple points or collision of a triple point with a wall. Because many wave interactions and fine-scale features are involved in a relatively small region and a very short time

scale in such processes [1, 5]. Besides, a very high spatial resolution and a very short time step should be assigned in numerical investigations to capture properly the physical details of the collision processes. Lefebvre and Oran [6], and Oran et al. [7] using numerical simulation for a low-pressure $H_2/O_2/Ar$ mixture, found that after the triple point collision, the structure changes from a single-Mach configuration to a double-Mach configuration. Sharpe [3] using high resolution numerical simulation of 64 cells per half reaction length with a simple reaction model of detonation wave in $H_2/O_2/Ar$ mixture, found that the structure has a double-Mach-like configuration and there is no change before and after collision of the triple point with the wall. Hu et al. [8] using very high resolution numerical simulation of 220 cells per half reaction length and detailed chemical kinetics in $H_2/O_2/Ar$ mixture, determined that the structure just after the collision shows a regular collision configuration, while it changed quickly to a double-Mach-like configuration.

All the numerical simulation mentioned above, neglect to determine the difference between the collision processes at the end of the first half of a detonation cell with that at the second portion of the cell cycle. Upon collision of triple points at the beginning of a cell, a highly overdriven Mach stem is formed that typically has a velocity of about $1.5V_{CJ}$ (for unstable detonations). It decays subsequently, and before the next collision at the end of the detonation cell, the leading front may decay to about $0.5V_{CJ}$. Thus, the shock strength and the wave velocity at the end of the cell cycle are considerably lower than the wave strength and the wave velocity at the end of the first half of the cell [9]. These differences suggest that the structure configuration at the collision processes of the triple point, at the end of the first half cycle of the detonation cell, differs from that at the end of the second portion of the cell. In the present work, a comprehensive study is performed, via very high-resolution two-dimensional numerical simulations, to determine the details of a regular structure detonation and the type of transverse waves in such detonations during collision processes. The reflection processes of the triple points and the transverse wave with the walls, is then investigated both at the end of the first half of the detonation cell, as well as, at the end of the decaying portion of the cell cycle.

Governing Equations

The two-dimensional reactive Euler equations with a single step Arrhenius kinetics model with the assumption of perfect gas are integrated to simulate the structure of gaseous detonation.
The two-dimensional Euler equations are expressed as follows:

$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}=S \qquad (1)$$

where

$$U\equiv\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ \rho E\\ \rho\beta\end{bmatrix}\quad F\equiv\begin{bmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ \rho uE+up\\ \rho u\beta\end{bmatrix}\quad G\equiv\begin{bmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ \rho vE+vp\\ \rho v\beta\end{bmatrix}\quad S\equiv\begin{bmatrix}0\\ 0\\ 0\\ 0\\ \rho W\end{bmatrix} \qquad (1\text{-}2)$$

Here, S is the source term due to combustion. ρ, u, v, and p are density, particle velocity in x and y directions, and pressure, respectively. β is the reaction progress parameter, which varies between 1 (for unburned reactant) and 0 (for product) and E is the total energy per unit mass, which is defined as:

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

where, Q is the heat release per unit mass of the reactant and γ is the ratio of the specific heats. W is the reaction rate, which follows the Arrhenius law as:

$$W = -k\beta \exp(\frac{-E_a}{RT}) \tag{3}$$

Perfect gas law is expressed as follow:

$$p = \rho RT \tag{4}$$

The dependent variables are non-dimensionalized with respect to the unburned mixture properties. Density is non-dimensionalized with respect to ρ_0, and pressure with γp_0. For the velocity, the sound speed of the unburned mixture c_0 is used as the reference. The characteristic length scale used is the length traveled by a fluid particle (in the detonation frame of reference) from the leading shock to the position where β=0.5 in a ZND structure, the so-called half-reaction length (*hrl*).

Numerical issues

In this study, a first order splitting method is utilized to remove the source term from the system of Eqs. (1), [10-12]. The fractional strategy proceeds as follows:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0 \tag{5}$$

Equation (5) represents the two-dimensional inert Euler equations in Cartesian coordinates. The system of equations is discretized with the un-split upwind method of Colella [13]:

$$U_{i,j}^{n+1} = U_{i,j}^{n} + \frac{\Delta t}{\Delta x}[F(U_{i-1/2,j}^{n+1/2}) - F(U_{i+1/2,j}^{n+1/2})] + \frac{\Delta t}{\Delta y}[G(U_{i,j-1/2}^{n+1/2}) - G(U_{i,j+1/2}^{n+1/2})] \tag{6}$$

where

$$U_{i,j}^{n} = \int_{\Delta_{i,j}} U(x, y, t^n)\,dxdy \tag{7}$$

$F(U^{n+1/2}_{i+1/2,j})$ and $G(U^{n+1/2}_{i,j+1/2})$ are the time averaged approximate fluxes at the cell interfaces. The state variable vectors $U^{n+1/2}_{i+1/2,j}$, and $U^{n+1/2}_{i,j+1/2}$ are determined as the solution of the Riemann problem projected in the x and y directions with the left and the right states ($U^{n+1/2}_{i+1/2,j,L}, U^{n+1/2}_{i+1/2,j,R}$) and ($U^{n+1/2}_{i,j+1/2,D}, U^{n+1/2}_{i+1/2,j+1/2,U}$). The solution of Eq. (5) is then used as an initial condition for the systems of ordinary differential equations:

$$\frac{dU}{dt} = S \tag{8}$$

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 fine meshes are used locally at the vicinity of the shock and coarse grids elsewhere. Hence, a simple version of the "adaptive mesh refinement" technique of Berger and Colella [14] is utilized in the present work. The above methods have been extensively used in previous numerical simulations of gaseous detonations (e.g. [11, 15]).

Boundary and initial conditions

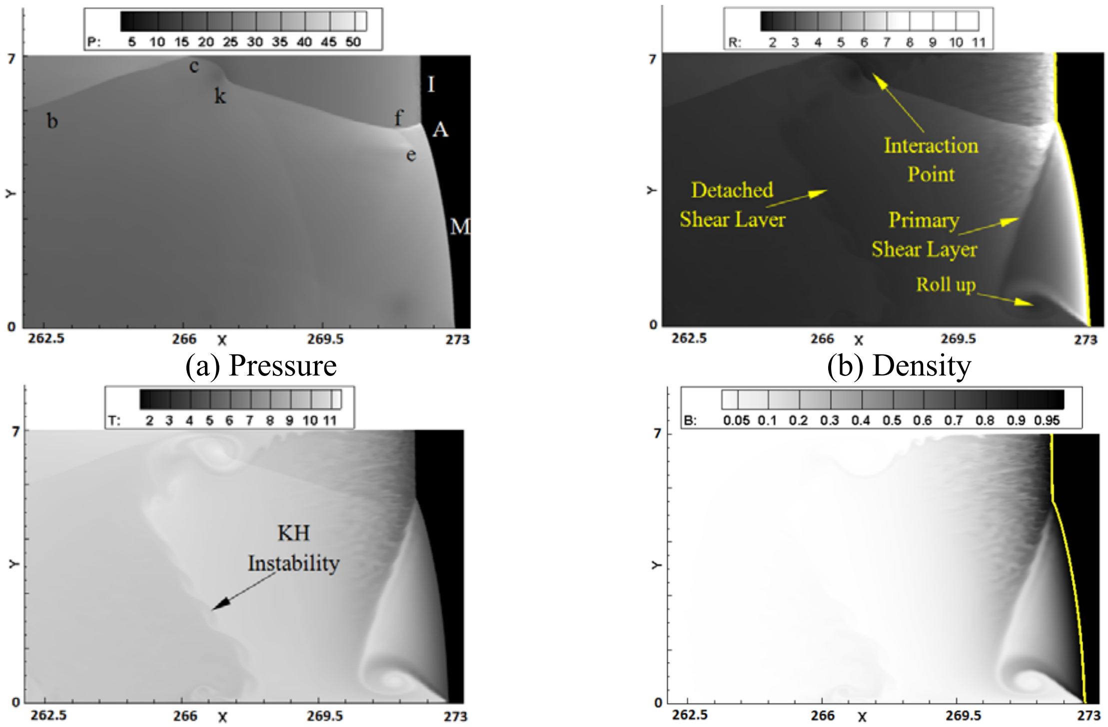
The detonation runs from left to right in the positive x-direction. Since the fluid ahead of the detonation is in its quiescent state, the right-hand boundary condition is irrelevant. The boundary conditions imposed on the lower and the upper sides of the channel are reflecting boundary conditions. To reduce the computational time a non-reflecting boundary condition is imposed on left side of the domain. The detail of the non-reflecting boundary condition and its application to two-dimensional simulation of detonation waves can be found in [16-18]. Comparing the solution of the whole domain with the truncated solution domain, it is found that for mixture with E_a/RT_0=10, Q/RT_0=50 and γ=1.2 the domain length should set to be 20*hrl*, in the present numerical simulations. For the initiation of the 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 between x=5.0 and x=6.0 [3, 11, 15]. The domain width in the y-direction is 7, which is narrow enough to allow very high resolution simulation. The computational domain is chosen such that the detonation propagates for 400*hrl*.

Sharpe [3] reported that resolutions more than 20 cells in the *hrl*, is required to predict properly the detonation structure. Hu et al. [8] using 220 cells in *hrl* in their numerical simulation of regular detonation in $H_2/O_2/Ar$ mixture, commented that a sufficiently high resolution is needed to resolve correctly the detonation structure. Mahmoudi and Mazaheri [15] reported that in regular structure detonations, 100 cells per *hrl* constitutes good solution for the structure of such stable detonations. However, since, the collision and reflection processes, occur in a very small region, therefore, in the present numerical simulation resolution of 500 points in the *hrl* is employed to resolve properly all the fine-scale features arising in such processes.

A scalable parallel reactive Euler code is developed to carry out the two-dimensional computations. The computational domain is divided into different computational zone and spread among six processors. The processors were Intel® Pentium® 4 with clock speed of 3.00 GHz and up to 1GByte of memory. Communication library of message passing interface (MPI) is chosen for parallelizing the code. Typical computation time for resolution of 500 cells per *hrl* and using double precision accuracy, takes about three weeks to allow the detonation to run for 400*hrl*.

Main features of a regular structure

To investigate the regular structure of the detonation, contours of pressure, density, temperature and reaction progress variable are shown in Fig. 1 for a mixture with E_a/RT_0=10, Q/RT_0=50 and γ=1.2. Primary triple point (A), Mach stem (M), incident wave (I) and transverse wave (Ab) are observed in Fig. 1a. Interaction of two segments Af and fc of the transverse wave, creates the reflected shock fe. Such structure has been observed in numerical simulation of Sharpe [3] too. Triple point f along the transverse wave is identical to triple point b in Fig. 1a of Sharpe [3].



(a) Pressure (b) Density

(c) Temperature (d) Reaction progress variable

Figure 1. Detonation structure in the mixture with E_a/RT_0=10, Q/RT_0=50, γ=1.2 and N=500cells/*hrl*.

The above wave configuration resembles that of a double-Mach configuration of a strong transverse wave. As Fig. 1a shows, before the interaction of the triple point with the wall, the extended portion of the transverse wave collides with the wall at point c, which produces reflected wave bc back into the main flow. The primary shear layer is clearly visible in Fig. 1b, emanating from the triple point and ending with a rollup structure close to the lower boundary.

The detached shear layer shown in Fig. 1b is a shear layer, which has been isolated after collision of the triple point with lower wall at previous cell cycle. The interaction of the transverse wave with the roll-up structure associated with the detached shear layer caused the formation of kink k on the transverse wave in Fig. 1a. Besides, little evidence of turbulence is observed along the detached shear layer in Fig. 1c, which gives rise to the appearance of small-scale vortices. The vortices are produced by Kelvin-Helmholtz instability mechanism. Figure 1d displays the contour of reaction progress variable. It is observed that, no un-reacted gas pocket exists behind the front, indicating that the shock front ignites almost all the gases that have passed through it. Figure 2 shows the maximum pressure history of the detonation wave, in which a regular cellular structure with a sole track of the triple point (A) is seen in this figure. The straight trajectory of the triple point indicates a weak type of the triple point in such detonations [1].

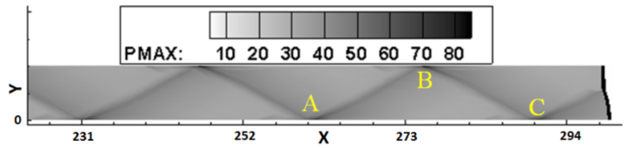
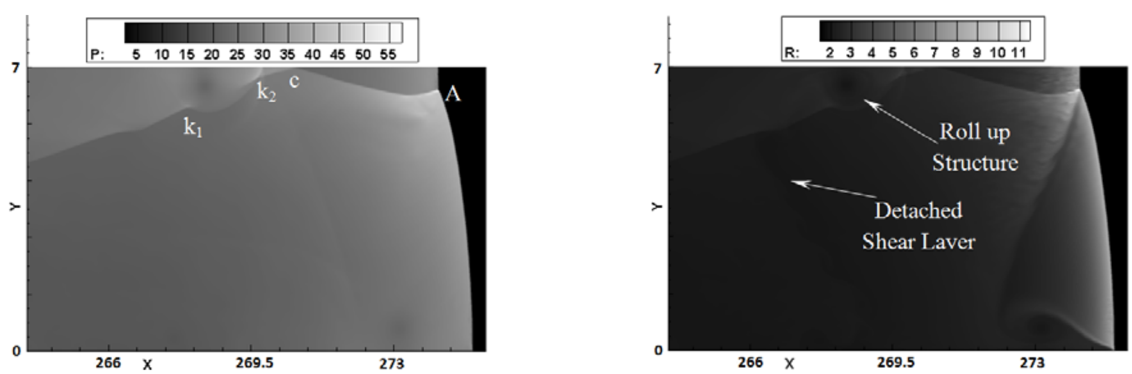


Figure 2. Numerical smodek foil based on maximum pressure history in mixture with E_a/RT_0=10, Q/RT_0=50, γ=1.2 and N=500cell/hrl.

The region between A and B is referred to as a first half of a detonation cell, where the Mach stem sweeps the channel width. The region between the B and C is called the second half of the detonation cell, where the gases are processed by the weak incident wave. In the following sections, in order to investigate the growth and evolution of hydrodynamic instabilities, the structure of detonation will be presented between sections A and C (Fig. 2) through a complete cell cycle.

Collision with the wall, at the end of the first half of the detonation cell

In this section, the collision and reflection processes of the transverse wave and its associated triple point with the wall at the end of the first half of the detonation cell (i.e. collision with upper wall at point B, Fig. 2) is investigated. Figures 3a to 3h show the contours of density and pressure of the structure. Figure 3a displays that shortly before collision, the extended section of the transverse wave interact with the wall at point c. Since, the rear section of the transverse wave is a weak wave, hence its interaction with the wall does not create high-pressurized region at upper boundary. The kink points, k_1 and k_2 are appeared due to interaction of the transverse wave with the rollup structure along the detached shear layer .Comparison of Fig. 3a with Fig. 1a shows that, as the triple point moves toward the wall, the shock wave fe vanishes and it is not present in Fig. 3a. Hence, the double Mach configuration in Fig. 1a becomes a single Mach configuration in Fig. 3a. As the triple point propagates more, the transverse wave reflects off the wall at point c and interacts with it, at a new point c_1. The structure of detonation at the time of collision of triple point A with the upper boundary is shown in Figs. 3c and 3d. The transverse wave interacts with the wall at point c_2, which is closer than point c_1 to triple point A. Moreover, as Fig. 3c shows, a part of transverse wave and the triple point interact with the wall, simultaneously.



(a) (b)

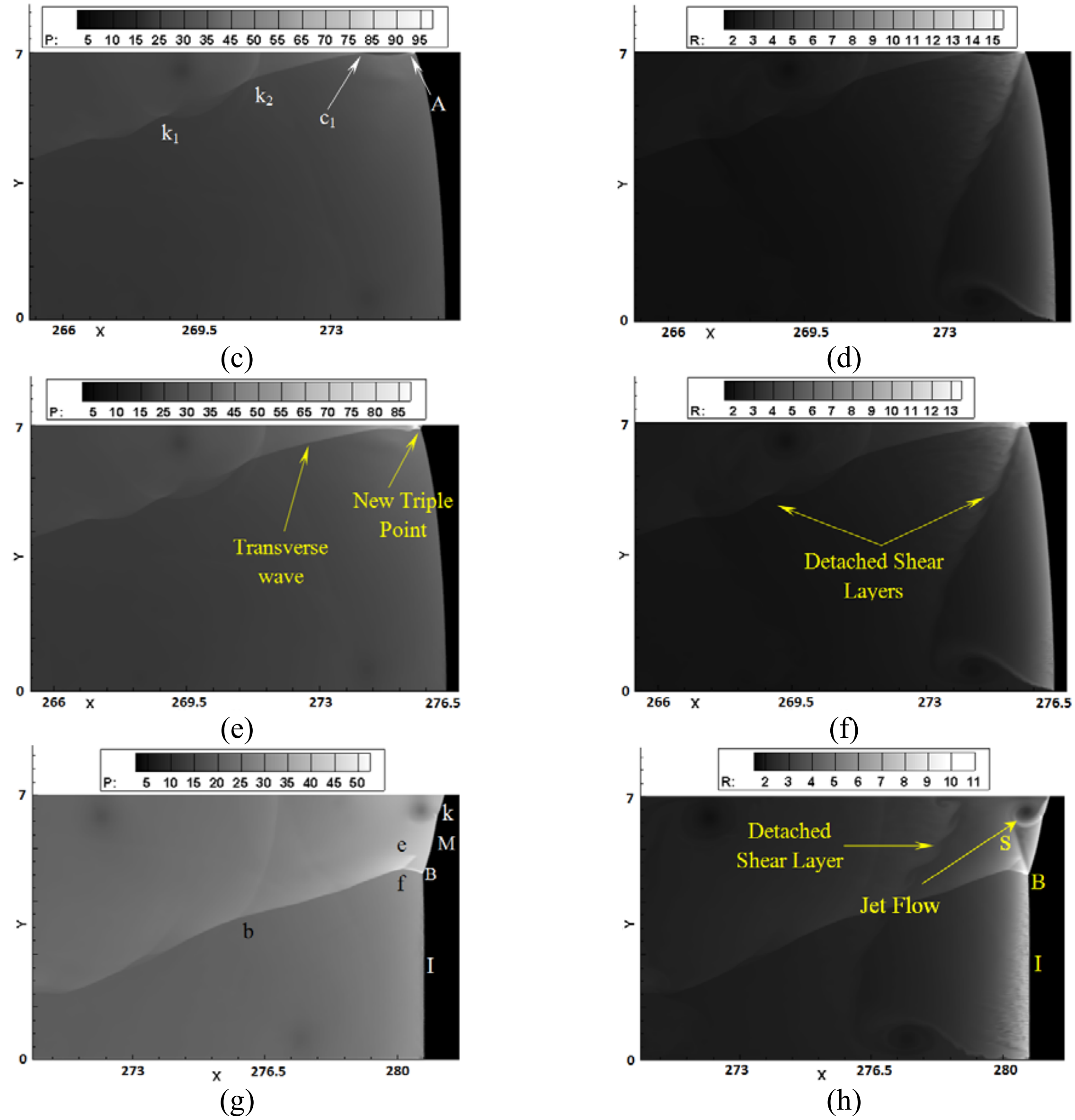
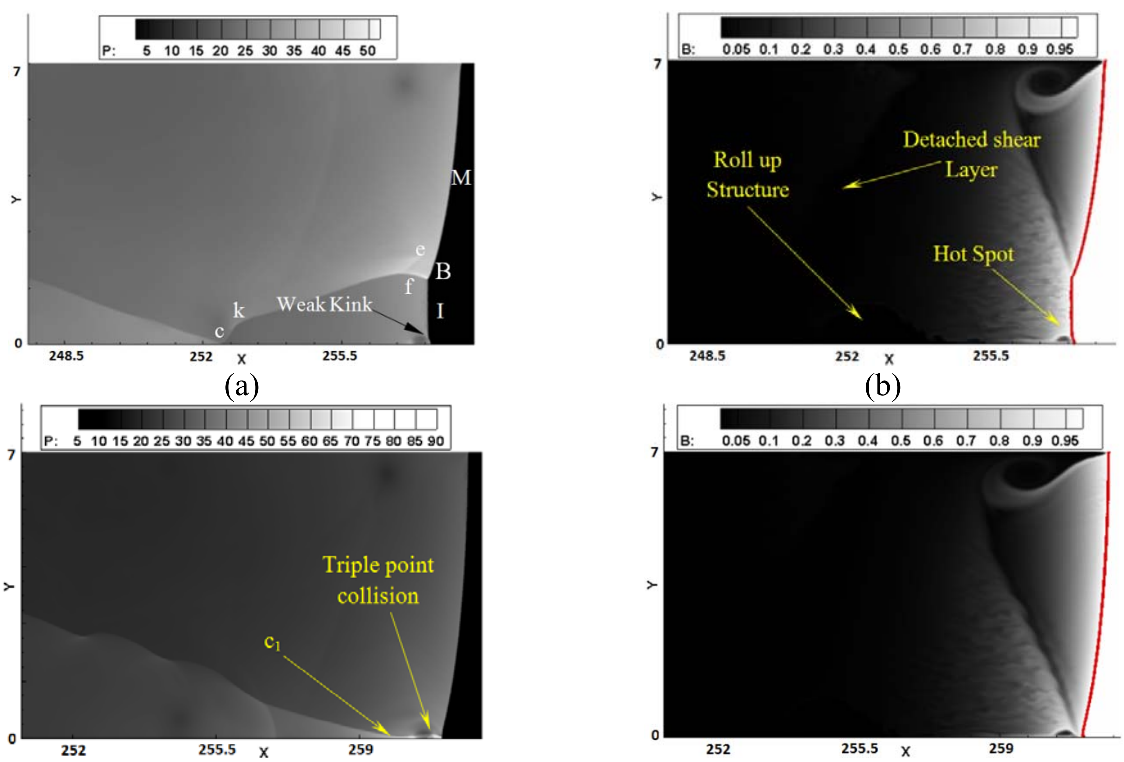


Figure 3. Detonation structure during the collision of triple point with the wall at the end of the first half of the detonation cell in a mixture with E_a/RT_0=10, Q/RT_0=50, γ=1.2 and N=500cells/*hrl*. Left figures: Pressure contour; Right figures: Density contour.

The maximum pressure in the structure corresponding to the triple point at upper wall is about p≈98, in contrast to the maximum pressure of the structure at earlier time, Fig. 3a that is about p≈57. Such high-pressurized region at upper boundary, results in ignition of partly burned gases at shear layer close to the upper wall [3]. Consequently, the shear layer detaches from the front. Figures 3e and 3f show that after collision, the transverse wave and the triple point, reflect off the wall simultaneously, and propagate downward. Subsequent to the collision, a new triple point B forms, and propagates downward (Figs. 3g and 3h). A jet flow is formed upon collision of triple point with the wall, by Richtmyer-Meshkov instability involving the baroclinic vorticity production mechanism (see Fig. 3h). Such feature has also seen in previous numerical simulations (e.g. [3, 15, 19-20]).The upper portion of the new triple point is a Mach stem (M), whereas the lower part is an incident wave (I). A new shear layer (S) is formed, which emanates from the new triple point B and rolls up near the upper wall. The interaction of the jet flow with the Mach stem, originates the kink k in the Mach stem. The appearance of such kink point has been also observed previously in numerical simulation of gaseous detonations (e.g., [3, 15, 19]). In addition, a shock wave fe is now formed in Fig. 3g, implying that the structure is like a double-Mach strong-type configuration. The strong transverse shock structures shown here were also observed by Sharpe [3]. The present results manifest that, the structure evolves from a double-Mach to a single-Mach configuration, before collision. Upon collision, the structure depicts a single-Mach configuration. However, after some times the structure changes to a double-Mach-like configuration, with a secondary triple point on the transverse wave.

Collision with lower wall at the end of the detonation cell cycle

The structure of stable detonation during the collision process of the triple point with the wall (i.e. collision with lower wall at point A, Fig. 2) in the second half of detonation cell is investigated in this section. Shown in Figs. 4a to 4j are the contours of pressure and reaction progress variable. Figure 4a displays that before collision with the lower wall the secondary triple point f is observed on the transverse wave, and hence the structure is like a double-Mach configuration. The interaction of the extended section of the transverse wave with the wall at point c and the kink k along the transverse wave are clearly seen in Fig. 4a. Figure 4b shows that a "hot spot" is created behind the incident wave (I) near the lower boundary. Such hot spot contains hot (i.e. $T\approx11.52$) and partly burned gases, with reaction progress variable about $\beta\approx0.21$, in comparison to $T\approx0.83$ and $\beta\approx1.0$ for cold and unreacted materials. The interaction of this hot spot with the incident wave (I) causes a weak kink at the incident wave near the lower boundary. Such hot spot is not apparent in the first half of the detonation cell (Figs. 3).



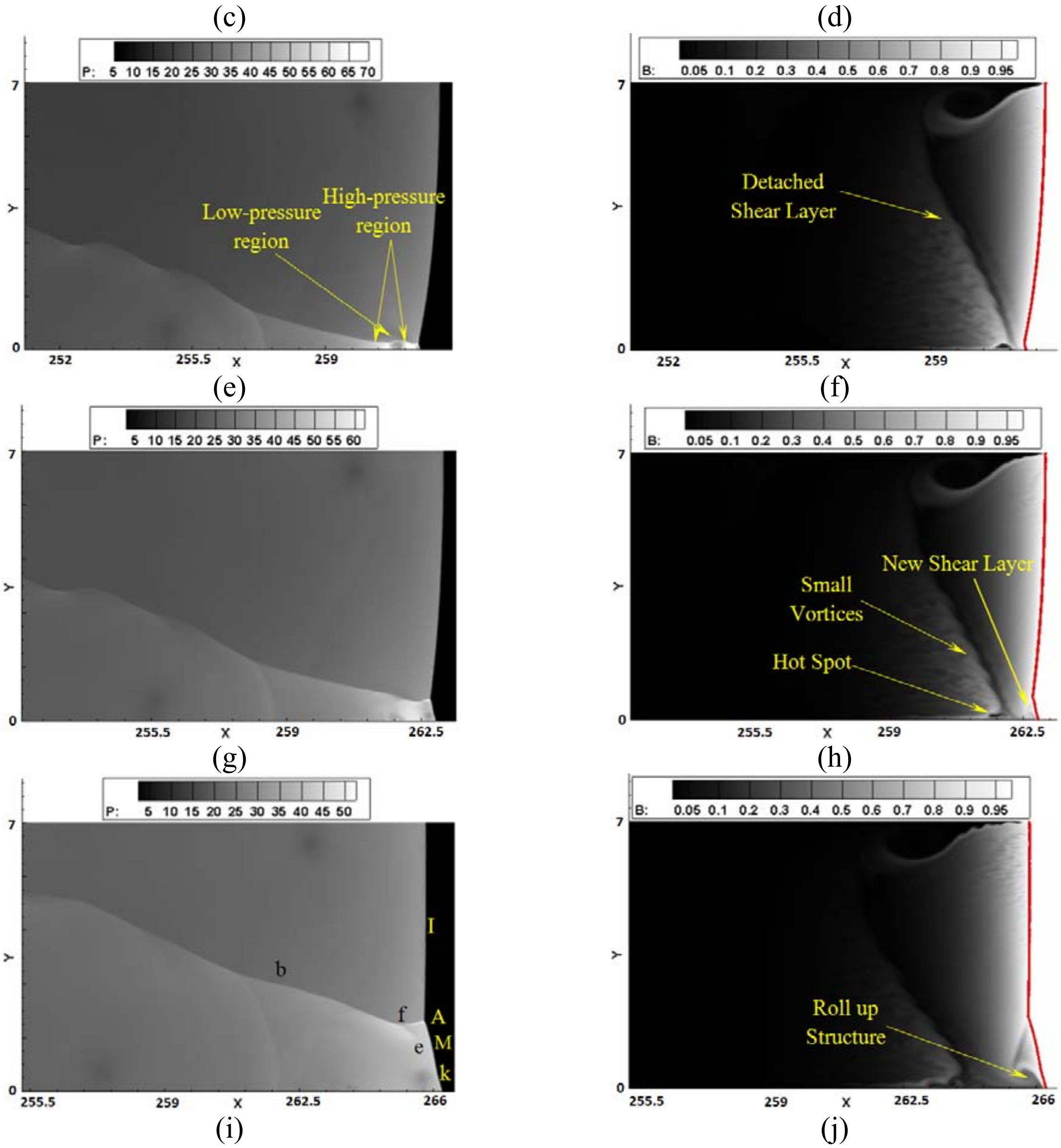


Figure 4. Detonation structure during the collision of the triple point with the wall, at the end of the second half of the detonation cell in a mixture with E_a/RT_0=10, Q/RT_0=50, γ=1.2 and N=500cells/*hrl*. Left figures: Pressure contour; Right figures: Reaction progress variable. Solid line indicates the shock position.

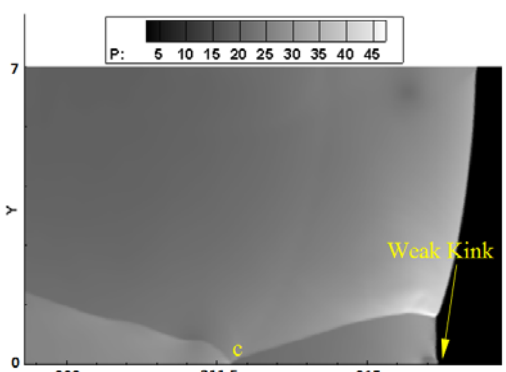
The question is "why the hot spot is created, *just* at the end of the cell cycle and is not observed in the first half of the cell cycle?" This is due to the fact that in the first half-cell, the strong Mach stem propagates in the channel and consume all the gases that have passed through the leading front. Thus, no noticeable unburnt gases remain behind the front to create any hot spot.

Figures 4c and 4d show that the triple point B collides with the bottom boundary. By this time, the transverse wave collides with the wall at a new point, c_1. Besides, the shear layer is about to detached from the main front. Despite the high-pressurized region that emerges at the bottom boundary, the hot spot still present behind the front and even its morphology remains unchanged, Fig. 4d. Figure 4e shows that the pressure at the position of the hot spot (p≈55) is lower than the pressure of the neighboring regions (p≈70). This implies that the interaction of transverse wave with the wall takes on a simpler structure and produces lower pressurized region at the wall in comparison to the neighboring regions. In other word, the hot spot breaks the transverse waves into two parts, and each part interacts with the wall and creates a high-pressurized region. Figure 4f shows that the shear layer becomes detached and recedes the front. Figure 4g shows the triple point and the transverse wave reflect off the wall simultaneously, subsequently a new single-Mach configuration is formed which travels upward. Figure 4h depicts that the shape of the hot spot is changed and its size is smaller than that in Fig. 4f. It is observed that collision of the triple point and its associated transverse wave with lower wall cannot cause the consumption of the hot spot. While, the small-scale vortices along the detached shear layer (produced via Kelvin-Helmholtz instability) facilitate the consumption of this hot spot through turbulent mixing of neighboring burned gases and unburned gases inside the hot spot. Figure 4i and 4j represents that a new double-Mach configuration is now formed where the second triple point and shock fe are appeared in the structure. Moreover, Fig. 4j illustrates that the hot spot is vanished. Hence, similar to the collision process in the first half of the cell, the structure evolves from a single-Mach configuration to a double-Mach configuration after collision in the second half of the detonation cell. The collision processes with the walls, in both first and second half of the detonation cell is summarized as follows:

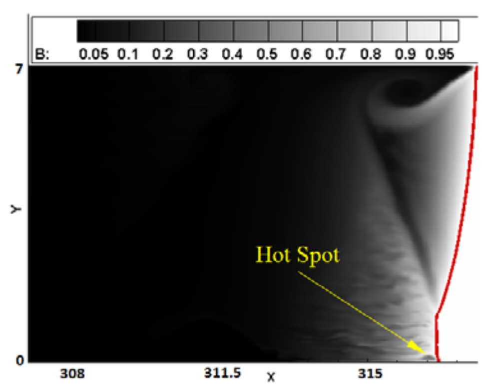
i. Interaction of the extended transverse wave with the wall at different points.
ii. Simultaneous collision of the strong portion of the transverse wave and triple point, with the wall.
iii. Simultaneous reflection of the transverse wave and the triple point off the wall, which gives rise to the appearance of the new double-Mach configuration.
iv. A hot spot forms at lower boundary, shortly before the collision of triple point with the wall in the second half of the cell cycle.

Resolution study

To determine the effect of grid-resolution on the capturing of small-scale structures, mainly hot spots, the computations are repeated for resolution of 300 and 200cells per *hrl.* The results are shown in Figs. 5 and 6, respectively. Comparison of Figs. 5a and 5b with Fig. 4a and 4b shows that the weak kink, the hot spot and the shock fe are present in the structure for resolution of 300 cells per *hrl*.



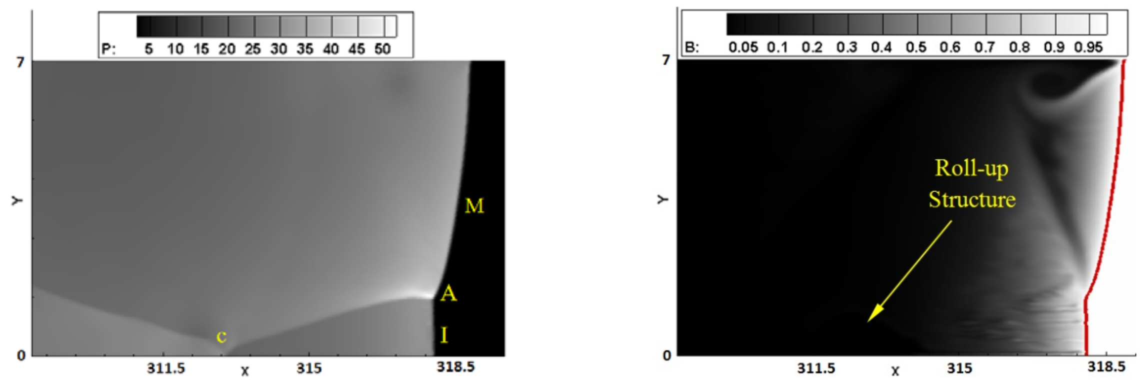
(a) Pressure



(b) Reaction progress variable

Figure 5. Detonation structure before the collision of triple point in a mixture with E_a/RT_0=10, Q/RT_0=50, γ=1.2 and N=300cells/*hrl*.

Figures 6a and 6b show that as the resolution decreases to 200 points per *hrl*, neither the hot spot nor the shock fe cannot be captured. The hot spot, which is formed behind the incident wave, before the collision of a triple point with the wall at the end of the detonation cell, has not been observed in previous numerical simulations (e.g. Sharpe [3] and Hu et al. [8]) due to the low grid-resolution. It seems that insufficient grid-resolution augments the artificial diffusion and hence, leads to the loss of some fine features. Therefore, a sufficiently high resolution is needed to resolve properly the structure configuration and its evolution behavior during the collision and reflection processes.



(a) Pressure (b) Reaction progress variable

Figure 6. Detonation structure before the collision of triple point in a mixture with E_a/RT_0=10, Q/RT_0=50, γ=1.2 and N=200cells/*hrl*.

Conclusions

In this paper, high-resolution two-dimensional numerical simulations have been performed to determine the detonation structure and the collision processes of a triple point with the wall, for a detonation with regular structure. It is observed that the shock front compresses almost all the gases passing through it and no noticeable unreacted gas is formed behind the main shock. Thus, it is concluded that the classical shock ignition mechanism still preserved the propagation mechanism of regular structure detonations and the transverse waves and the hydrodynamic instabilities have no significant role in propagation mechanism of such stable detonations. During the collision with the walls, in both first half-cell and second half-cell, shortly before and after the collision, the structure is more like a single-Mach configuration. However, the structure changes to a double-Mach configuration as the triple point recedes from the wall. Shortly before the collision with the wall, at the end of the second half of the detonation cell cycle, a hot spot forms behind the incident wave. The small-scale vortices along the detached shear layer enhance the ignition of this hot spot. The results of grid study reveal that at least 300 cells per *hrl* are required to resolve properly the structure during the collision and reflection processes.

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