

Mechanisms of Detonation Re-initiation in a Narrow Channel at a Back-Facing Step

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1 Introduction

The propagation of a detonation wave through an area change is an important phenomenon to study related to explosion safety. When the area change is infinite, i.e., the receiver chamber is very large, this represents the fundamental critical tube configuration. In this geometry, for the supercritical case the detonation wave successfully transmits into the receiver channel, and for the subcritical case it fails due to diffraction. The more practical scenario is when the receiver chamber has a finite transverse width that can promote detonation reinitiation due to shock reflection. In the past, this was studied in a series of two axisymmetric tubes using soot foils [1] and 2D rectangular channels using high-speed schlieren [2]. Because of the inherent symmetry of the geometry, the details of the detonation reinitiation can be studied using a simple backward-facing step. When the detonation encounters such a step, the expansion starting from the step corner progressively decouples the detonation wave resulting in a decaying shock and a trailing flame. Detonation initiation occurs when the decaying lead shock reflects from the bottom wall after the step. Historically, in experimental [3,4] and numerical [5,6] studies, detonation initiation was directly linked to the Mach stem (and associated flow structure) that forms at the bottom wall due to irregular shock reflection, independent of the initial detonation cell structure.

The role of the 2D detonation cell structure was highlighted in recent simulations by Floring et al. [7] who proposed that the interaction of transverse waves (or reflected shock from bottom wall) with burned/unburned gas interfaces behind the incident shock leads to detonation initiation. In our previous study in a channel that accommodates several cells across the channel width, we showed the importance of the 3D-interaction between the decoupled shock-flame structure and the bottom wall [8]. Schlieren imaging showed that detonation kernels formed at the bottom wall from the reflection of descending triple-lines (appear as triple-points in side-view schlieren) and the collision of lateral transverse waves that propagate across the bottom wall. In the current study, a channel accommodating a single lateral transverse wave is used to obtain high-quality schlieren images of the interaction of the descending triple-points with the bottom wall and to limit lateral wave collision to the channel side walls.

2 Experimental setup

Experiments were performed in a channel that included a coil-over-plug multi-spark system that ignited the flame at the closed-end of a 76.2 mm diameter tube that was connected to a 76.2 mm square-section

for detonation stabilization (see Fig. 1 and [8] for details). The detonation then enters a narrower 1.2 m long, 12.5 mm wide channel via a “cookie-cutter” paced at the end of the square section. A 25.4 mm bar was placed on the floor to reduce the channel height to 50.8 mm and create a 22 mm back step in the test section with windows integrated into the front and back walls as shown in Fig. 1. Experiments were carried out with stoichiometric $2\text{H}_2 + \text{O}_2 + 2\text{Ar}$ at the initial pressure of 10.5 kPa. Single-pass schlieren was used to visualize the detonation initiation process using a Shimadzu HPV-X2 operated at 2 to 5 million frames per second. Soot foils were used to capture the cell structure evolution both on the side and bottom-walls.

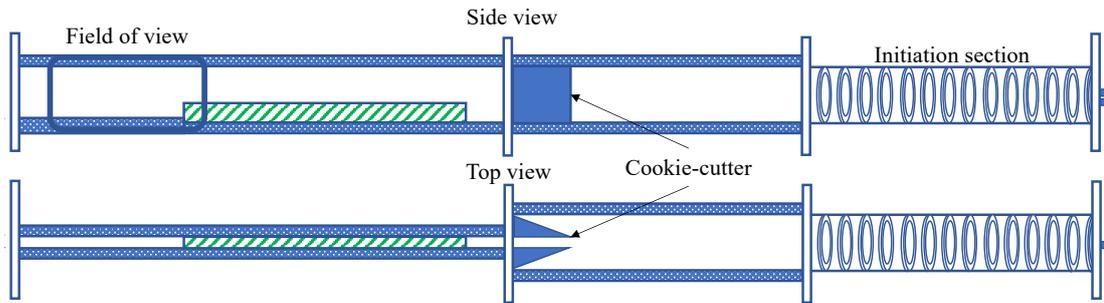


Figure 1: Experimental setup.

3 Results

Two detonation initiation mechanisms were observed in the 12.5 mm wide channel for the chosen step height. The first mechanism, observed in the test results shown in Fig. 2 and Fig. 3, is governed by the lateral and descending transverse waves interacting with each other and the channel bottom wall, similar to the one observed in the wide 76.2 mm wide channel [8]. Superimposed schlieren images for a test carried out at 10.5 kPa showing the detonation decoupling and shock reflection at the bottom wall are shown in Fig. 2. For this test condition there are two detonation cells across the 50.8 mm channel height before the step (located to the right of the field-of-view). Based on this one would expect no more than one lateral wave across the 12.5 mm channel width. The “double front” observed in Fig. 2 is the result of 3D effects associated with an axially shift of the front on either side of the lateral wave. Unlike in the wide channel [8], viscous and heat losses to the channel side walls play a role in the current setup, leading to a slight increase in the cell size and decrease in the detonation velocity to $0.93\text{-}0.95 D_{CJ}$.

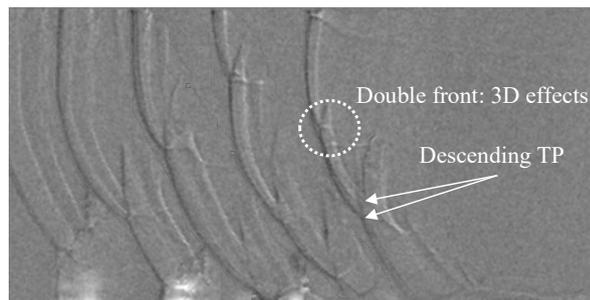


Figure 2: Superimposed schlieren images of decoupled and re-initiating detonation for $2\text{H}_2 + \text{O}_2 + 2\text{Ar}$ at 10.5 kPa between $1.2 \mu\text{s}$ and $49.2 \mu\text{s}$ in increments of $12 \mu\text{s}$. Right-side of field of view corresponds to the back-step.

Two schlieren images from the same test as in Fig. 2, corresponding to $30.2 \mu\text{s}$ and $34.4 \mu\text{s}$, are shown in Fig. 3b and 3c, along with the bottom-wall soot foil imprint shown in Fig. 3d. The schlieren images show the decoupled detonation front with one descending transverse wave and associated triple point at mid channel height, as well as the formation of a Mach stem after the collision of a descending transverse wave with the bottom wall. The light observed after the Mach stem is incandescence from lofted fine

soot particles heated by the combustion products. There is a significant gap between the decoupled shock and flame below the descending triple point.

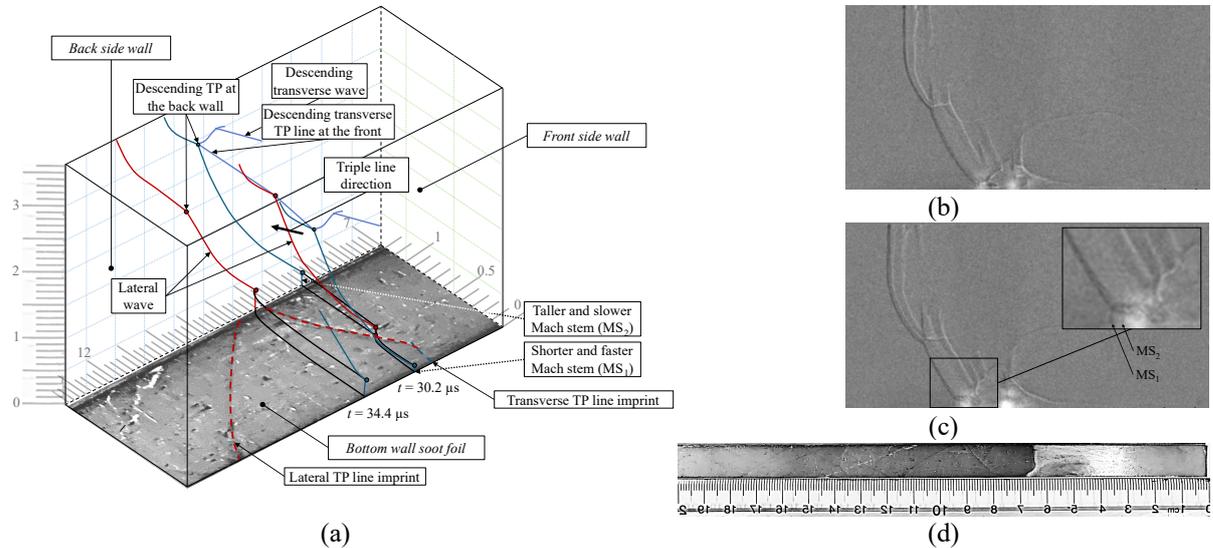


Figure 3: a) Schematic reconstruction of 3D leading shock fronts from schlieren images in Fig. 3b and 3c at two times during the decoupled shock reflection at the bottom wall for the argon diluted hydrogen-oxygen mixture at 10.5 kPa. All lines along the back and front walls are drawn to scale from the schlieren images, the triple point trajectory at the bottom wall replicates the lines observed in the soot foil shown in full in Fig. 3d. The lines across the channel width in Fig. 3a showing the Mach stem and descending triple lines are inferred from the schlieren images. The cm scale is provided along all three axes. Schlieren image at $t = 30.2 \mu\text{s}$ (b) and $34.4 \mu\text{s}$ (c).

Figure 3a shows a 3D schematic reconstruction of the leading shock front from the schlieren images in Fig. 3b and 3c during the detonation initiation process. An image of the soot foil located at the bottom wall (see Fig. 3d) is also incorporated into the schematic in Fig. 3a. The leading shock front, depicted in Fig. 3a, consists of the incident shock with transverse waves descending to the bottom wall as well as a single lateral wave propagating across the channel width, the triple point trajectory on the bottom wall soot foil is highlighted by the red dotted line. Note, in the $30.2 \mu\text{s}$ image (Fig. 3b) the lateral wave is located roughly at mid-channel width, whereas at $34.4 \mu\text{s}$ image (Fig. 3c) it collides with the side wall so the 3D effect is less prominent because there is no interruption of the front.

The re-initiation of detonation begins with the 2nd descending transverse wave hitting the bottom wall at $t = 28.8 \mu\text{s}$ (not shown in Fig. 3). As soon as the transverse wave interacts with the bottom wall, bright light from soot incandescence appears in the schlieren image, and slightly later, two vertical lines, instead of one corresponding to a single Mach stem, are observed (see MS₁ and MS₂ in Fig. 3c). As the colimated schlieren light passes through gas with non-uniform density, it diffracts, forming a schlieren (or shadowgraph) image. The largest diffraction of light is expected as it goes through the shock front, where the refraction index also changes the most. This supports the idea that two Mach stems from shock reflection appear in schlieren images, pointing to the role of 3D in re-initiation of detonation. The axial positions of these Mach stems are measured at the bottom wall and plotted on the $x(t)$ diagram in the reference frame moving at the Chapman-Jouguet velocity (D_{CJ}) in Figure 4. The transition to such a frame of reference allows us to identify if waves are moving at a velocity larger or smaller than D_{CJ} while smoothing out the perturbations. Initially there is only a single Mach stem that travels at roughly 1320 m/s. After the descending transverse wave hits the bottom wall at $x - D_{CJ}t = -0.35$ (see Fig. 4a) MS₁ is produced and propagates at roughly D_{CJ} (constant $x - D_{CJ}t$ in Fig. 4) pulling away from the original Mach stem (now called MS₂) that propagates at ~ 1690 m/s. Based on schlieren, the distance between the Mach stems is the largest when the lateral wave propagating along the channel bottom reaches the back wall of the channel. This is also supported by the bottom soot foil (Fig. 3d), where the triple point trajectory of the Mach stem reaches the edge of the soot foil at the location of 9.2 cm. After

that collision with the side wall, another bright spot appears in the schlieren image, and MS₂ accelerates eventually catching up to MS₁. The merged fronts propagate downstream at ~2000 m/s (1.02 D_{CJ}) along the bottom wall (see Fig. 2 and Fig. 4).

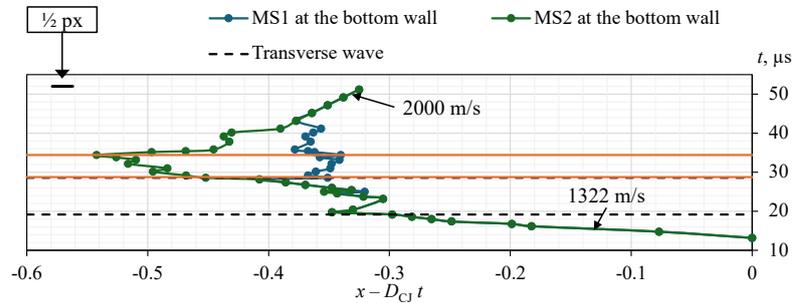


Figure 4: The $x(t)$ diagram of the Mach stems at the front (MS1) and the back (MS2) walls of the channel. Positions x are taken at the bottom wall. The position $x - D_{CJ}t$ on the x -axis is in the reference frame moving at D_{CJ} (negative slope means the Mach stem propagates slower than D_{CJ}). The orange lines denote the time of appearance of the bright spots in schlieren images in Fig. 3b and c, the black dashed lines denote the time when a descending transverse wave interacts with the bottom wall. The black line at the top left corner of the graph shows the error in the coordinates measurement, which is half of the pixel. The indicated velocities correspond to the fixed-reference frame velocity of the denoted line segment.

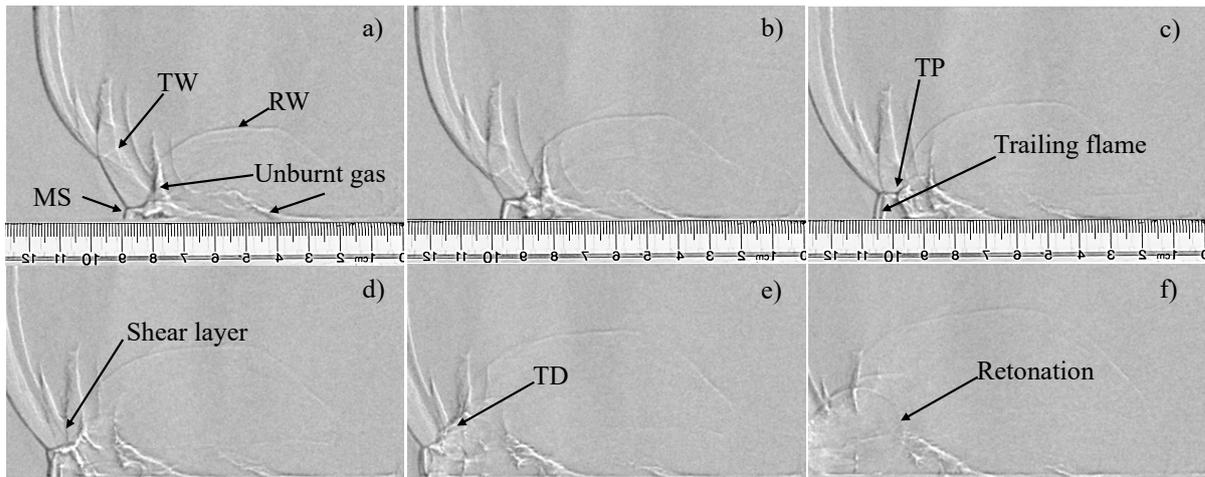


Figure 5. Series of schlieren images of decoupled and re-initiating detonation for the argon diluted hydrogen-oxygen mixture at 10.5 kPa with 5 μ s between the frames.

If detonation does not re-initiate through interaction of the first two descending transverse waves with the bottom wall (when the Mach stem from shock reflection is still short), another mechanism is responsible for detonation re-initiation. Figure 5 shows a series of schlieren images with 5 μ s between each at the same 10.5 kPa initial pressure. The step is located at the right edge of the field-of-view. In Fig. 5a, a Mach stem (MS) is travelling at a velocity slightly below CJ velocity, previously amplified by interaction of a transverse wave with the bottom wall. With time the Mach stem induced reaction decouples forming a trailing flame, see Fig. 5c – 5d. Meanwhile, the reflected wave (RW in Fig. 5a) propagates upwards through shocked-unreacted gas as well as burnt gas affecting the shock profile due to the temperature and molecular weight dependence of the local sound speed. Before the descending transverse wave (labeled as TW in Fig. 5a) collides with the rising reflected wave in Fig. 5c there is a shock-induced laminar reaction zone behind the Mach stem and reflected wave that has two segments separated by a triple point (see TP in Fig. 5c). When the descending transverse wave interacts with the reflected wave RW (Fig. 5c – 5d), the reaction zone becomes closely coupled with the reflected wave leading to the formation of a transverse detonation wave (TD in e) propagating in the compressed gas

between the decoupled shock and flame. This interaction occurs in the vicinity of the shear layer (Fig. 5d) between tongues of unburnt gas associated with the decoupled detonation wave. In Fig. 5e the well-defined structures below the reflected shock disappear and the transverse detonation wave is fully formed. The presence of the retonation wave (Fig. 5f) points to an explosion, initiated as the reflected wave interacted with the descending shear layer. In contrast to the previous test where transverse detonation formed after interaction of a transverse wave with the bottom wall, the transverse detonation forms above the bottom wall in this case. Floring et al. [7] carried out 2D simulations looking at similar interactions and postulated different mechanisms for detonation initiation, included shock focusing (associated with the tongues of unburnt gas), induction time gradient driven amplification, and Kelvin-Helmholtz interface instability driven reaction.

Many experiments were conducted with the $2\text{H}_2 + \text{O}_2 + 2\text{Ar}$ mixture at initial pressures of 10 kPa, 10.5 kPa, 11 kPa. The incident detonation structure varied stochastically, represented in Table 1 by the number of descending triple points at each pressure (e.g., 4 to 5).

Table 1. Number of tests where 4 or 5 descending TPs were observed for each initial pressure.

p_0 , number of descending TP	10 kPa, 4 TP	10 kPa, 5 TP	10.5 kPa, 4 TP	10.5 kPa, 5 TP	11 kPa, 4 TP	11 kPa, 5 TP
Number of tests	10	6	9	6	8	5

The chart in Fig. 6 summarizes the re-initiation mechanisms observed under different initial conditions, including the initial pressure (p_0) and the number of descending triple points. The results indicate that re-initiation mechanisms vary across tests, ranging from re-initiation driven by lateral and transverse wave interactions (red columns, Mode 1 in Fig. 6) to re-initiation triggered by the interaction of a descending transverse wave with the reflected wave (blue columns, Mode 2 in Fig. 6). These mechanisms are not mutually exclusive; in some cases, it is unclear whether detonation would have re-initiated without the presence of the other mechanism (yellow columns in Fig. 6).

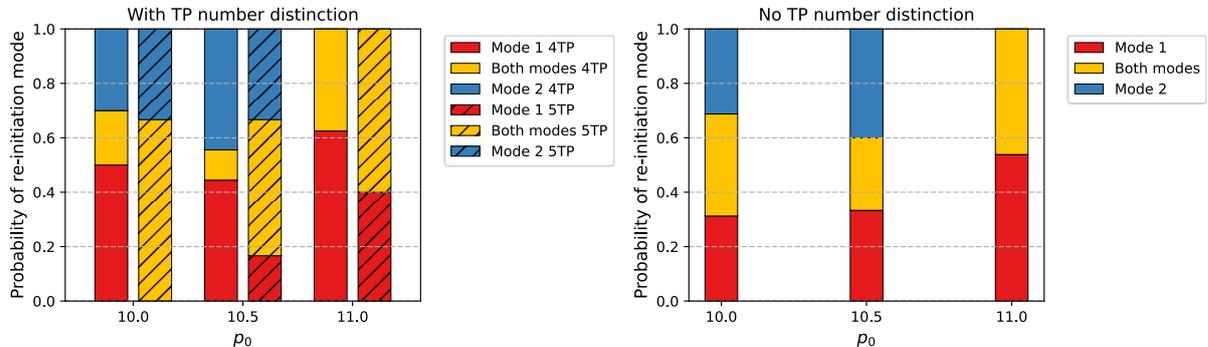


Figure 6: The summary of experimental results for $2\text{H}_2 + \text{O}_2 + 2\text{Ar}$ mixture. “Mode 1” refers to re-initiation via interaction of descending transverse waves with the bottom wall, “Mode 2” denotes detonation re-initiation via interaction of a transverse wave with the reflected wave above the bottom wall. “Both modes” denotes re-initiation through both mechanisms simultaneously. Striped bars in the left image denote the data where 5 triple points descend to the bottom wall.

While Figure 6 mostly demonstrates once again the stochastic nature of detonation, some other conclusions can also be drawn. The probability of detonation re-initiation via the first mode is higher if there are four triple points descending to the bottom wall. In addition, at a higher initial pressure, the probability of both mechanisms being responsible for detonation re-initiation also decreases. At $p_0 > 12$ kPa, there are at least two lateral waves propagating across the channel width (thus the waves can interact not just with the walls), and the detonation mostly re-initiates via Mode 1. It should be noted that the detonation always re-initiated via Mode 1 in a wide channel with similar geometry and mixture [8]. This

is attributed to a larger number of collisions of lateral and transverse waves at the bottom wall. In addition, there are fewer losses to the channel walls in the wide channel, which also makes the temperature higher at the collisions of lateral and transverse waves promoting detonation re-initiation via this mechanism.

4 Conclusion

This study reveals that slight variations in initial conditions significantly alter the dominant mechanism of detonation re-initiation in a narrow channel with a backward-facing step. Re-initiation occurs either through the interaction of transverse waves with the bottom wall (as observed in wide channel experiments), or via the interaction away from the bottom wall of a descending transverse wave, and/or the Mach reflected wave, and a burned/unburned gas interface. Although the detailed detonation initiation mechanism in the current channel has not been conclusively identified, we are confident that it involves the interaction of compression waves (descending transverse and/or reflected wave) with a burned/unburned gas interface behind the Mach stem triple point, like that observed in recent 2D numerical simulations with a 4-step chemistry model [7]. This implies that if you suppress lateral transverse wave collisions, by using a narrow channel like in this experiment, detonation initiation in this geometry approaches a two-dimensional phenomenon. Conversely, when predicting the true nature of detonation initiation one must use wide channels, accommodating multiple lateral transverse waves, and 3D numerical simulations

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