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# Numerical Studies of Flame Acceleration and Onset of Detonation in Homogenous and Inhomogeneous Mixture

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## Abstracts

Numerical investigations have been conducted for flame acceleration and transition to detonation in a horizontal obstructed channel with 60 percent blockage ratio filled with hydrogen/air mixture. Both homogeneous and inhomogeneous hydrogen/air mixtures have been considered. The later has a vertical concentration gradient. The density-based solver within the OpenFOAM CFD toolbox developed by the present authors [1] is used. High-resolution grids are facilitated by using adaptive mesh refinement technique, which leads to 30 grid points per half-reaction length (HRL) in the finest region near the flame and shock fronts. The forward and backwards jets which represent Richtmyer–Meshkov (RM) instability, were found to impact on the shock front, resulting in the appearance of a secondary triple point on the initial Mach stem on the flame front. Moreover, since both the forward and backwards jet propagates in the shear layer, some small vortices can be found on the surface of the secondary shear layer, which represents the Kelvin-Helmholtz (KH) instability. Additionally, it has been found that the inhomogeneous (non-uniform) mixtures cause higher shock and flame velocities compared to the homogeneous mixtures concentration. Also, for both homogenous and inhomogeneous mixtures with 30% hydrogen concentration, the onset of detonation occurs within the obstructed channel section, but the homogeneous mixtures show slightly faster flame acceleration and earlier onset.

**Keywords:** Flame Acceleration, Detonation, DDT, instability, Numerical, Hydrogen

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## 1. Introduction

Flame acceleration (FA) in obstructed channels have been studied by numerous investigators [e.g. [2], [3]]. Frolov (Frolov, 2012) [4] provided a detailed summary of the acceleration of the Deflagration-to-Detonation Transition (DDT) in gases. DDT in obstructed channels has been studied numerically by Gamezo et al. [5]. Kuznetsov et al. [6] carried out large-scale tests of DDT in an obstructed semi-confined flat layer of stratified hydrogen-air mixture. They also studied the effects of the maximum hydrogen concentration at the top and a vertical concentration gradient on the flame propagation regimes were investigated to derive critical conditions for sonic flame propagation and detonation onset. They found that steeper hydrogen gradients can lead to more reactive mixtures and higher maximum hydrogen concentrations at the top of the layer, which can enable the flame to accelerate to sonic speed. They showed that flame acceleration in mixtures with concentration gradients might be determined by the maximum local hydrogen concentration in semi-confined geometries. Grune et al. [7] conducted large-scale experiments of flame acceleration (FA) and DDT in an obstructed semi-confined flat layer of a hydrogen-air mixture with transverse (vertical) concentration gradients [8]. The authors found that DDT propensity is increased by mixture inhomogeneity for globally lean mixtures, and may be correlated with the maximum local hydrogen concentration within the layer. Vollmer et al. [9] and Boeck et al. [10]–[12] reported that a strong positive effect of concentration gradients could be found on FA, especially in a channel without obstructions. In other words, concentration gradients can result in significantly stronger FA compared to the homogeneous mixtures. Boeck et al. [12] also showed that the FA was stronger in the presence of the gradients. DDT was also observed as reflected shock waves interacting with the deflagration front.

Peraldi et al. [13] showed that for the onset of detonation the tube diameter criteria should be at least equivalent to the detonation cell size. Later, Lindstedt and Michels [14] demonstrated that for a circular pipe, the critical diameter for the onset of detonation is  $D > \lambda/\pi$  (where  $\lambda$  is the detonation cell size). A comprehensive discussion on the critical diameter of a tube for onset of detonation and other characteristics of detonation conditions is described by Ciccarelli et al. [15]. Chao [16] studied the DDT phenomena in a smooth channel, and he stated that due to hot spot generation downstream of the flame front, and local explosion generation will trigger the one set of detonation [17].

Usually, for the onset of detonations a flame speed increases and generally it reaches a supersonic speed [13], [18]–[21]. The procedure of flame acceleration can significantly be affected by obstructions along the flame propagation [13], [19], [20]. In smooth channels/pipes, different physical mechanisms are expected to play a role. Shchelkin [22] and Soloukhin [23] have shown that the flame acceleration and transition to detonation in smooth channels are strongly affected by flame wall interactions and channel/tube wall roughness. They reported that flame acceleration would be promoted by turbulent boundary layer generation downstream of the flame front.

Furthermore, during flame propagation in a smooth tube, the flame shape usually turns into a characteristic “tulip” shape with a leading edge close to the tube walls. Soloukhin [23] also, stated that the local explosion, which lastly results in the onset of detonation, occurs close to the tube wall in the vicinity of flame wall interactions.

Bychkov et al. [24], showed that the mechanism of ultrafast flame acceleration in obstructed channels has another physical nature, which is qualitatively different from the Shelkin explanation. They found that delayed burning between the obstacles creates a powerful jet flow driving the acceleration. The acceleration mechanism is independent of the Reynolds number, with turbulence playing only a supplementary role. They validated their theory by extensive numerical simulations and comparison to previous experiments.

Dounia et al. [25], have carried out a study on the influence of kinetic mechanism on DDT modelling. They have shown that in hydrogen-air explosions by using detailed reaction mechanisms, the detonation waves can emerge from a flame brush, unlike what was usually seen in the single-step simulations (Gamezo et al. [5], carried out several DDT simulations with using single-step chemistry). They have illustrated that, especially for the scenarios in which hot spot will trigger deflagration to detonation, using a detailed chemistry mechanism is far more restrictive than single-step chemistry.

Wang et al. [26], have done a study on the effect of chemical kinetics on detonation initiation in methane-air mixture. They showed that using a simplified chemical reaction, such as single-step or two-step, will not reproduce correctly the ignition processes particularly in their tests with methane/air mixtures. The ignition delay times calculated using single-step chemistry, are in orders of magnitude shorter than the ignition delay times calculated using multi-steps (detailed chemistry) models and measured experimentally.

Therefore, for the above-mentioned reasons (predicting local hot spot which can lead to detonation, and precise calculation of ignition delay time), in this study, multi-step chemistry will be used rather than a single step.

## **2. Numerical Model**

The density-based numerical code (VCEFoam) previously developed by the authors is used [1], [8], [27]. The solver is based on the open-source computational fluid dynamic (CFD) toolbox OpenFOAM [28]. The Harten–Lax–van Leer–Contact (HLLC) scheme with multidimensional slope limiters (“cellMDLimited”) is used for accurate shock-capturing. Compressible Navier–Stokes equations with a chemical reaction mechanism [29] are solved and for turbulence modelling the Monotone Integrated Large Eddy Simulation (MILES) technique is adopted. Further details of VCEFoam and its validations can be found in our previous publications[1], [8], [27], [30].

### 3. The Results

#### Predictions of cellular detonation

A two-dimensional test case has been selected to examine the capability of VCEFoam in capturing the cellular detonation structures. The schematic of the rectangular domain is shown in Figure 1. High pressure ( $1000 \times p_0$ ) and temperature perturbation ( $25 \times T_0$ ) were initiated to trigger the detonation waves in the red regions. Where  $p_0 = 6670 \text{ pa}$  and  $T_0 = 298 \text{ K}$ . All four sides of the domain were assumed to have a wall with no-slip boundary conditions.

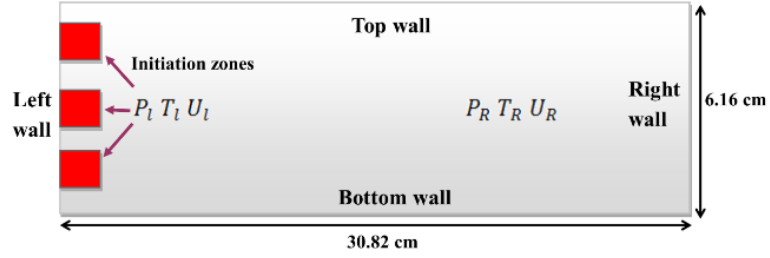


Figure 1. Schematic of the two-dimensional rectangular channel.

As mentioned previously, the mesh resolution has a significant impact in capturing the details of the detonation structure as well as having a direct relation with the induction length. The induction time in the unburned combustible mixture is  $\tau_{i} \approx 119 \mu\text{s}$ , and the induction length is  $L_{i} \approx 1.3 \text{ mm}$ . In this test case, the grid resolution is  $0.065 \text{ mm}$ , providing 20 points in the induction length. The maximum Courant number has been set to 0.15. The Marinov [31] hydrogen/air reaction mechanism is used.

Table 1: H<sub>2</sub>/Air reaction mechanism [31][units: s, mol, cm<sup>3</sup>, cal and K].

Reaction	A	b	Ea
(1) $OH + H_2 \rightleftharpoons H + H_2O$	2.14E+08	1.52	3449.0
(2) $O + OH \rightleftharpoons O_2 + H$	2.02E+14	-0.4	0.0
(3) $O + H_2 \rightleftharpoons OH + H$	5.06E+04	2.67	6290.0
(4) $H + O_2(+M) \rightleftharpoons HO_2(+M)$	4.52E+13	0.0	0.0
low	1.05E+19	-1.257	0.0
(5) $H + O_2(+N_2) \rightleftharpoons HO_2(+N_2)$	4.52E+13	0.0	0.0
low	2.03E+20	-1.59	0.0
(6) $H + O_2(+H_2) \rightleftharpoons HO_2(+H_2)$	4.52E+13	0.0	0.0
low	1.52E+19	-1.133	0.0
(7) $H + O_2(+H_2O) \rightleftharpoons HO_2(+H_2O)$	4.52E+13	0.0	0.0
low	2.10E+23	-2.437	0.0
(8) $OH + HO_2 \rightleftharpoons H_2O + O_2$	2.13E+28	-4.827	3500.0
(8b) $OH + HO_2 \rightleftharpoons H_2O + O_2$	9.10E+14	0.0	10964.0
(9) $H + HO_2 \rightleftharpoons OH + OH$	1.50E+14	0.0	1000.0
(10) $H + HO_2 \rightleftharpoons H_2 + O_2$	8.45E+11	0.65	1241.0
(11) $H + HO_2 \rightleftharpoons O + H_2O$	3.01E+13	0.0	1721.0
(12) $O + HO_2 \rightleftharpoons O_2 + OH$	3.25E+13	0.0	0.0
(13) $OH + OH \rightleftharpoons O + H_2O$	3.57E+04	2.4	-2112.0

(14) $H + H + M \rightleftharpoons H_2 + M$	1.00E+18	-1.0	0.0
(15) $H + H + H_2 \rightleftharpoons H_2 + H_2$	9.20E+16	-0.6	0.0
(16) $H + H + H_2O \rightleftharpoons H_2 + H_2O$	6.00E+19	-1.25	0.0
(17) $H + OH + M \rightleftharpoons H_2O + M$	2.21E+22	-2.0	0.0
(18) $H + O + M \rightleftharpoons OH + M$	4.71E+18	-1.0	0.0
(19) $O + O + M \rightleftharpoons O_2 + M$	1.89E+13	0.0	-1788.0
(20) $HO_2 + HO_2 \rightleftharpoons H_2O_2 + O_2$	4.20E+14	0.0	11982.0
(20a) $HO_2 + HO_2 \rightleftharpoons H_2O_2 + O_2$	1.30E+11	0.0	-1629.0
(21) $OH + OH(+M) \rightleftharpoons H_2O_2(+M)$	1.24E+14	-0.37	0.0
low	3.04E+30	-4.63	2049.0
Troe [0.470 100.0 2000.0 1.0E+15]			
(22) $H_2O_2 + H \rightleftharpoons HO_2 + H_2$	1.98E+06	2.0	2435
(23) $H_2O_2 + H \rightleftharpoons OH + H_2O$	3.07E+13	0.0	4217.0
(24) $H_2O_2 + O \rightleftharpoons OH + HO_2$	9.55E+06	2.0	3970.0
(25) $H_2O_2 + OH \rightleftharpoons H_2O + HO_2$	2.40E+00	4.042	-2162.0

An important factor affecting the detonation cell size is the mixture equivalence ratio, e.g. rich mixture (high reactivity) produces smaller detonation cell size. Therefore, a hydrogen/oxygen mixture diluted with argon was used to capture the cell with lower computational costs. Argon dilution will decrease the mixture reactivity and result in overprediction of the detonation cell size [32]. The stoichiometric hydrogen/oxygen mixture diluted with argon is 2H<sub>2</sub>: O<sub>2</sub>: 7Ar. It is presumed that the diluent Ar substitutes and plays a similar role to N<sub>2</sub> as inert species in the Marinov's reaction mechanism [31].

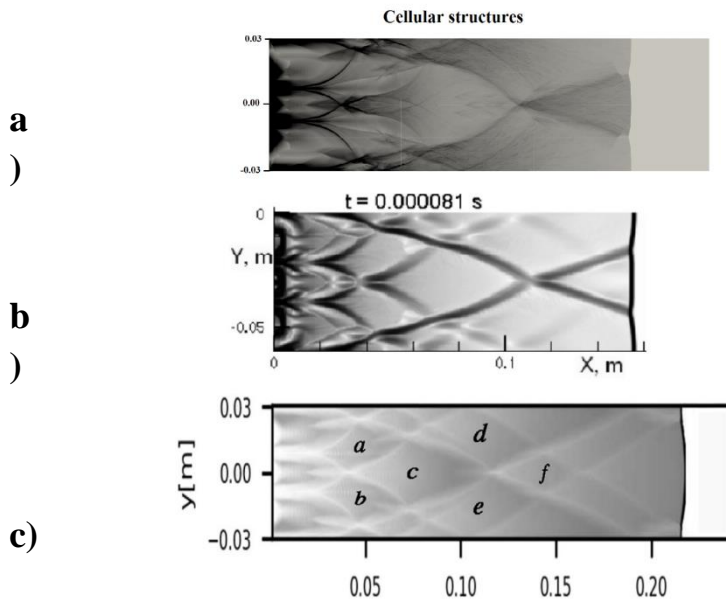


Figure 2. Detonation cellular structure development close to the ignition sources; a) VCEFoam, b) [33], c) [32].

Figure 2 shows the development of the detonation cellular structure close to the ignition sources. In the present work, the cellular structure has been captured by tracing the triple points in the domain. For tracing triple points, the maximum pressure in each time step of the solution has been stored in memory, and as a result, the cellular pattern could have been captured. In Figure 2 other previous CFD works have been included for comparison. It can be seen that the current captured cellular structure is closer to the previous CFD analysis of Kirillov et al. [33] which can be seen in Figure 2-b.

Table 2: Comparison of cellular structure cell size for H2/Air mixtures.

Reference	$\alpha$ (Cell length) (m)	$\lambda$ (Cell height) (m)	$c^{ar}$ (aspect ratio) $\lambda/\alpha$	Reaction kinetic
Marcantoni et al. [32]	0.074	0.032	0.43	Marinov [31]
Kirillov et al. [33]	0.078	0.033	0.42	Marinov [31]
Eckett [34]	0.054	0.03	0.55	8species/24reactions [35]
Oran et al. [36]	0.055	0.03	0.54	8species/24reactions [35]
Lefebvre & Oran [37]	0.077	0.03	0.42	Two steps model [37]
Lefebvre et al. (Experimental) [38]	0.17	0.09	0.52	smoke foil
VCEFoam (present work)	0.785	0.033	0.0420	Marinov [31]

Table 2 shows a comparison of cellular structure cell size for H2/Air mixtures. In this table, the detonation cell length ( $\alpha$ ), Cell height ( $\lambda$ , also called cell size), and the cell dimension aspect ratio ( $c^{ar} = \lambda/\alpha$ ), have been provided for different numerical and experimental observations. It can be seen that the predicted cell size ( $\lambda$ ) of the present work (VCEFoam) are in acceptable agreements with results of Kirillov et al. [33], Marcantoni et al. [32] and Lefebvre & Oran [37]. Note that the numerical setup (boundary and initial conditions) in the present work, is similar to the numerical work done by Kirillov et al. [33] and Marcantoni et al. [32].

The experimental data presented by Lefebvre [38] shows a significant difference in cell size, compared to all the other numerical studies; however, the presented aspect ratio of the experimental observation is close to those given in Refs. [34], [36]. One of the possible reasons would be the case that in the experimental observation, due to having a strong ignition source, the first detonation cell was not clear in the shadowgraphs; therefore, the neighbour cell downstream of the tube has been presented. Hence, for further investigation, the same test case has been modelled with tube length extended to 0.5 m.

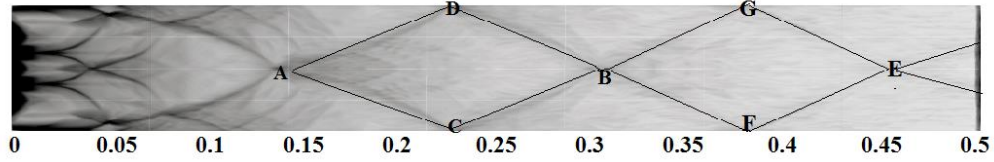


Figure 3. Cellular structure in the extended channel.

The numerical schlieren of the maximum pressure which indicates the cellular structure for the extended channel (to 0.5 m), is presented in Figure 3. In the initial stage, the cellular structure is similar to a shorter channel. However, in the middle of the domain towards downstream two much bigger cell has been (ACBD, and CFEG). These developed cells have a length of  $\alpha_{ACBD} = 0.165m$  and  $\alpha_{CFEG} = 0.15m$  these are very close to the value presented in the experimental observation ( $\alpha_{Experiment} = 0.17m$ ).

Next, a qualitative comparison of the predicted detonation cell ACBD will be compared with other numerical works as well as an experimental observation.

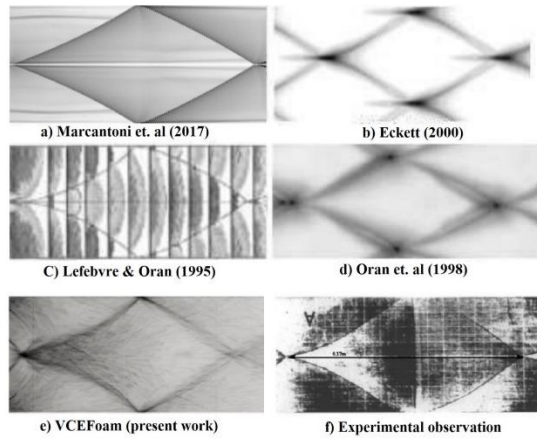


Figure 4. Comparison of Detonation cellular structure.

Figure 4 shows a comparison of detonation cellular structure in hydrogen/air mixture of various other CFD and experimental works. It can be seen that the current captured detonation cell (Figure 4-e), is in good agreement with other past similar works. The captured detonation cell in this study is more similar to the experimental observation as well as the work done by Lefebvre and Oran [38], (Figure 4-c-f).

Figure 5 shows the density distribution of the cellular structure formation process. The evolution of triple points can also be seen in these snapshots. Figure 5 ( $t=0.688 \mu s$ ) shows the three ignition areas which act as detonation initiations. Also, in the density snapshot, some small-scale features have been captured, such as forward and backward jets in the detonation fronts which indicates the Richtmyer Meshkov (RM) instability.



Figure 6 shows the numerical schlieren of the maximum pressure distribution of the cellular structure formation process. Also, the evolution of triple points can be seen in these snapshots. It can be seen that the first three perturbations have generated some triple points in the detonation front. Moreover, as a result of a secondary shock collision with the detonation front, a new triple point has been produced (23  $\mu\text{s}$ ). The trajectory of the triple points has produced some fish-cell sketches which represent cellular structure. The evaluation of triple points and how they produce a cellular structure can be found by comparing the numerical schlieren of maximum pressure and the density contours at the same time. At  $t=0.688 \mu\text{s}$ , three ignition areas which act as detonation initiations can be found. At 8  $\mu\text{s}$ , three semi-circular detonation fronts propagate downstream and also, as a result of interacting these detonation waves, two critical points (triple points) have been generated on the detonation front. Later, some shock waves reflect from both top and bottom walls before interacting with the other transverse and reflected shocks (at  $t=23 \mu\text{s}$ ). This interaction of the reflected shock and detonation front will produce an additional triple point. From 29.5  $\mu\text{s}$  onwards it can be seen that the two triple points are moving from top and bottom towards the middle of the domain. At 74.40  $\mu\text{s}$  it can be found that the two triple points meet each other in the middle of the domain, and as a result, another strongly localised detonation occurs. At 90.50  $\mu\text{s}$  it can be seen that two triple points are diverging from the middle and moving towards the top and bottom. Eventually, by tracking these triple points, the trajectory of these points will show “fish-cell” sketches which represent detonation cellular structure.

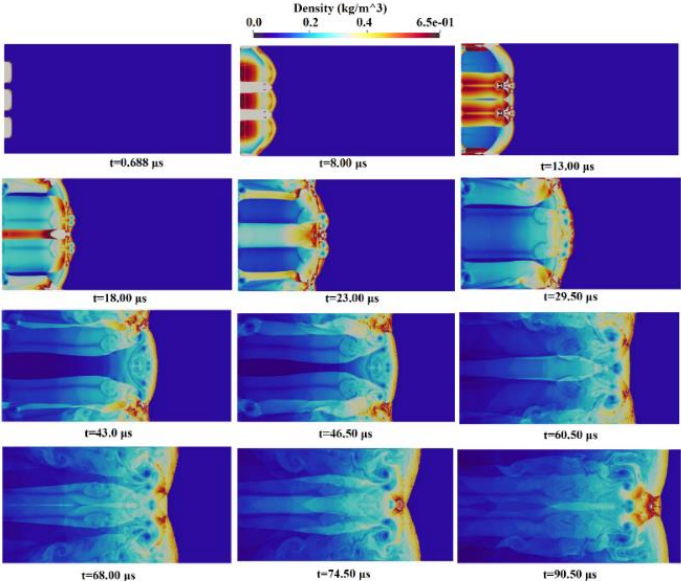


Figure 5. Density distribution: Cellular structure formation process: Evolution of triple points.

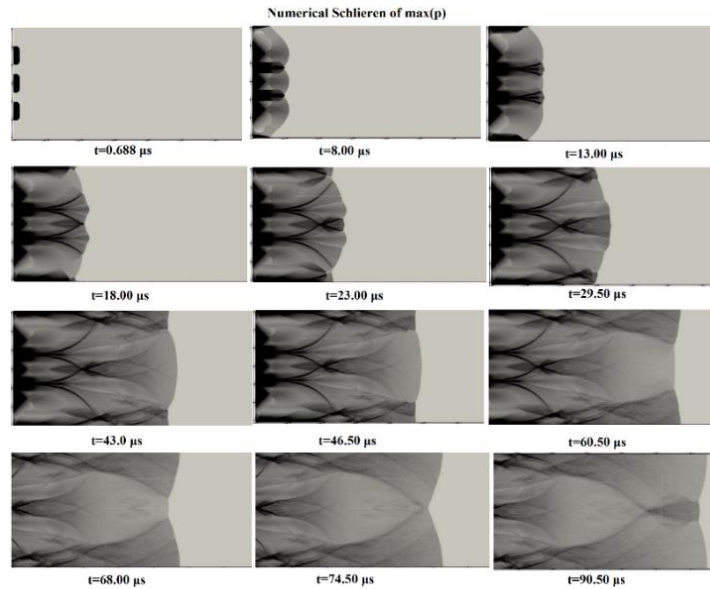


Figure 6. Numerical schlieren of maximum pressure distribution: Cellular structure formation process: Evolution of triple points.

Figure 6 shows the Numerical schlieren of the maximum pressure distribution of the cellular structure formation process. Also, the evolution of triple points It can be seen in this snapshots. It can be seen that the first three perturbation has generated some triple points in the detonation front. Also, it can be found that as a result of a secondary shock collision with detonation front, a new triple point has been produced (23  $\mu$ s). The trajectory of the triple points has produced some fish-cell sketch which represents cellular structure. The evaluation of triple points and how they produce a cellular structure can be found by comparing the numerical schlieren of maximum pressure and the density contours at the same time. At  $t=0.688 \mu$ s, can be found that there are three ignition areas which act as detonation initiations. At 8  $\mu$ s it can be seen that three semi-circular detonation front propagates toward downstream and also, as result of interacting these detonation waves, two critical points (triple points) have been generated on the detonation front. In later time, some shock wave reflects from both top and bottom walls, and then they will interact with the other transverse and reflected shock (at  $t=23 \mu$ s). This interaction of the reflected shock and detonation front will produce an additional triple point. From 29.5  $\mu$ s onwards it can be seen that the two triple points are moving from top and bottom towards the middle of the domain. At 74.40  $\mu$ s it can be found that the two triple points meet each other in the middle of the domain, and as results, another strongly localised detonation has occurred and at 90.50  $\mu$ s can be seen that two triple points are diverging from the middle and moving towards top and bottom. Eventually, by tracking these triple points, the trajectory of these points will show a “fish-cell” sketches which represent cellular detonation structure.

#### 4. Quantitative comparison

The experiments of Boeck et al. [12] involving inhomogeneous (non-uniform) and homogeneous (uniform) DDT phenomena of hydrogen-air mixtures were chosen for quantitative validation in the present study. The experiments were conducted in a horizontal obstructed channel with 60% blockage ratios as well as a smooth channel without obstruction. The channel was 60 mm high, 5.4 mm long and 300 mm wide, respectively. The concentration gradients are in the vertical direction. Concentration gradients were generated by gas injection through the channel top plate, formation of a hydrogen layer near the channel ceiling, and subsequent diffusion. The gradients were oriented vertically, thus perpendicular to the main direction of flame propagation. Therefore, in the case with the inhomogeneous mixture, the bottom of channel will have lean mixture, and top of the channel will contain rich mixture. In the present study, the average volumetric hydrogen concentration is 30% which is close to the stoichiometric value for hydrogen/air mixture. Two sets of data were used:

1. A homogenous mixture of 30 % H<sub>2</sub> (BR60).

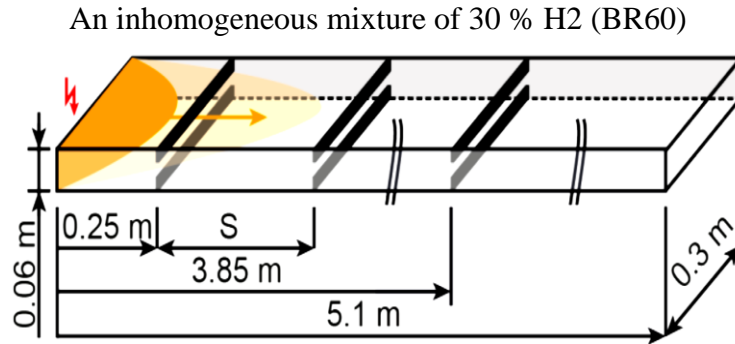


Figure 7. Schematic of the computational domain (Reproduced from [12]).

Figure 7 shows the computational domain which represents a smooth closed channel with obstacles. The mixture was initially in ambient pressure and temperature. In order to initiate ignition, a patch of cells within a radius of 10 mm around the point of ignition ( $x=0$ ,  $y=0.03\text{m}$ ) was set with a temperature of 2300 K and atmospheric pressure. The half-reaction length of hydrogen changes by equivalence ratio. Moreover, the minimum length is belonging to the stoichiometric value. Therefore, using an adaptive mesh refinement method provided the minimum cell size of 10  $\mu\text{m}$ , giving approximately by average minimum 30 grid points per half-reaction length (HRL) in the finest region near the flame and shock fronts.

In the mechanism developed by Bychkov et al. [24], due to delays in burning between the obstacles, in the free part of the channel, flow changes direction to the axial one, accumulates into a strong jet and pushes the leading flame tip forward. Flame sweeps extremely fast along the free channel part leaving behind new pockets of the fresh fuel mixture. This produces positive feedback between the flame and the flow and leads to strong exponential acceleration of the flam tip.

In the current study, the considered experiment done by Lorenz et al. [12] similar to the DDT study by Ciccarelli [15], the obstacles are installed with rather large spacing, which led to strong pulsations of the flame velocity, however, the theoretical model developed by Bychkov et al. [2008], is laminar, and it does not reproduce pulsations.

As shown in Figure 8, the predicted flame position and flame tip speed are in reasonably good agreement with the measurements [12] for the 30 percent hydrogen concentration. For both the homogeneous and inhomogeneous mixtures, the flame velocity rises continuously in the obstructed part of the channel due to flame interaction with the obstacles, resulting in combustion-induced expansion and turbulence generation. Moreover, it can be seen that in the 30 % hydrogen concentration, the homogeneous and inhomogeneous mixture of hydrogen/air, is almost having the same trend of flame acceleration and transition to detonation.

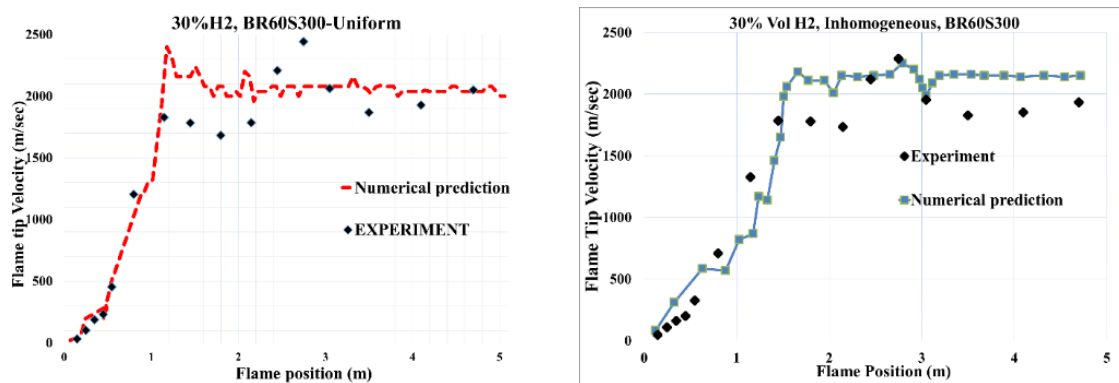


Figure 8. Comparison of between the predicted and measured the flame tip speed in the 30% hydrogen concentration; left: homogenous mixture of hydrogen/air; right: Inhomogeneous mixture of hydrogen/air.

Figure 9, shows the predicted temperature contour around the last obstacle ( $x=2.05$  m), where the flame has been fully detonated. At the time 8.0587ms the planner flame ahead with a leading shock interacts to the obstacle and as a result, two reflected shock waves generated in the flame front. Then these reflected shock waves interact in the middle of the channel which leads to a strong shock focusing. In 8.0660 ms can be found that a shear layer has been generated in the reflected detonation wave as a result of the strong shock focusing in the middle of the obstacle. In 8.0702 ms, mushroom shape Jets have generated in the shear layer, which illustrates the existing of Richtmyer- Meshkov (RM) instability. Moreover, the forward jet and backwards jets which are a mushroom form flow, represent the RM instability on the interface between the burned and unburned gas. The forward jets were found to impact on the shock front causing the appearance of a secondary triple point on the initial Mach stem on the flame front. Also, in 8.0828 ms, can see that the leading detonated flame interacts to the upper and lower walls and as a result secondary reflected shock

wave interacts the downstream of the flame. These shock-flame interacting cause a secondary shear layer in the flame with some small vortices which represent the existing of Kelvin-Helmholtz (KH) instability.

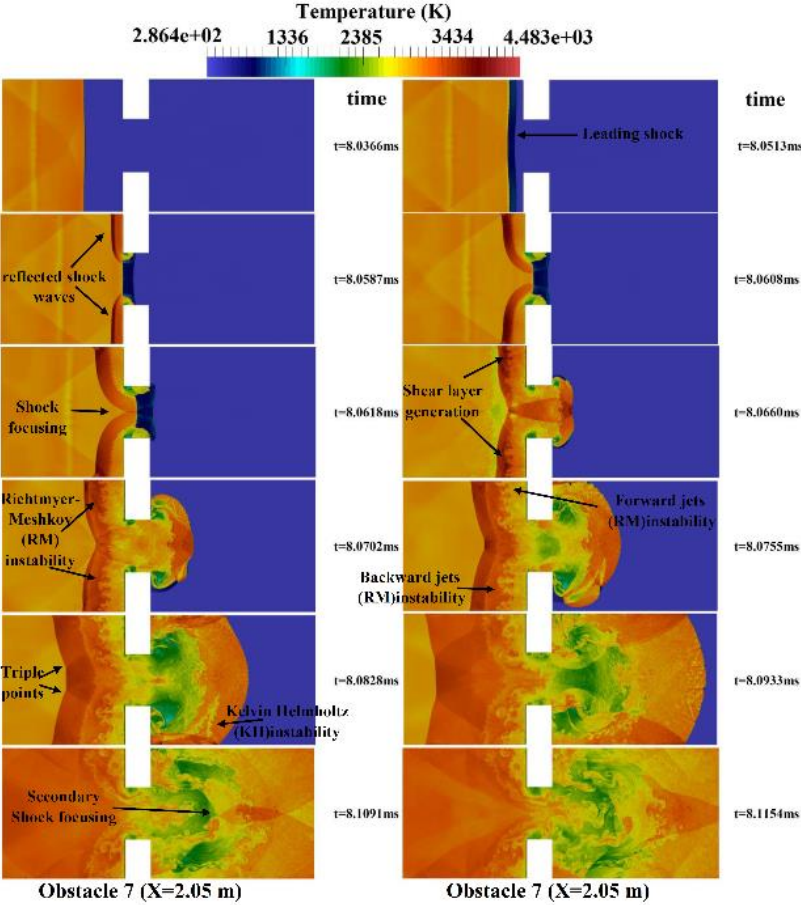


Figure 9: predicted temperature contour in the uniform mixture of 30% hydrogen concentration.

Figure 10 shows the pressure and temperature fields produced from the predictions for the case with 30% inhomogeneous mixture of hydrogen/air. In the experiments [12], DDT was initiated by precursor shock reflection at the upstream faces of an obstacle, leading to local explosions behind the reflected shock wave and the onset of detonation either directly from the local explosions or secondary hot-spots downstream of the obstacle. In the homogeneous mixture onset of detonation has got a regular detonation front, while in the inhomogeneous mixture the detonation structure is irregular.

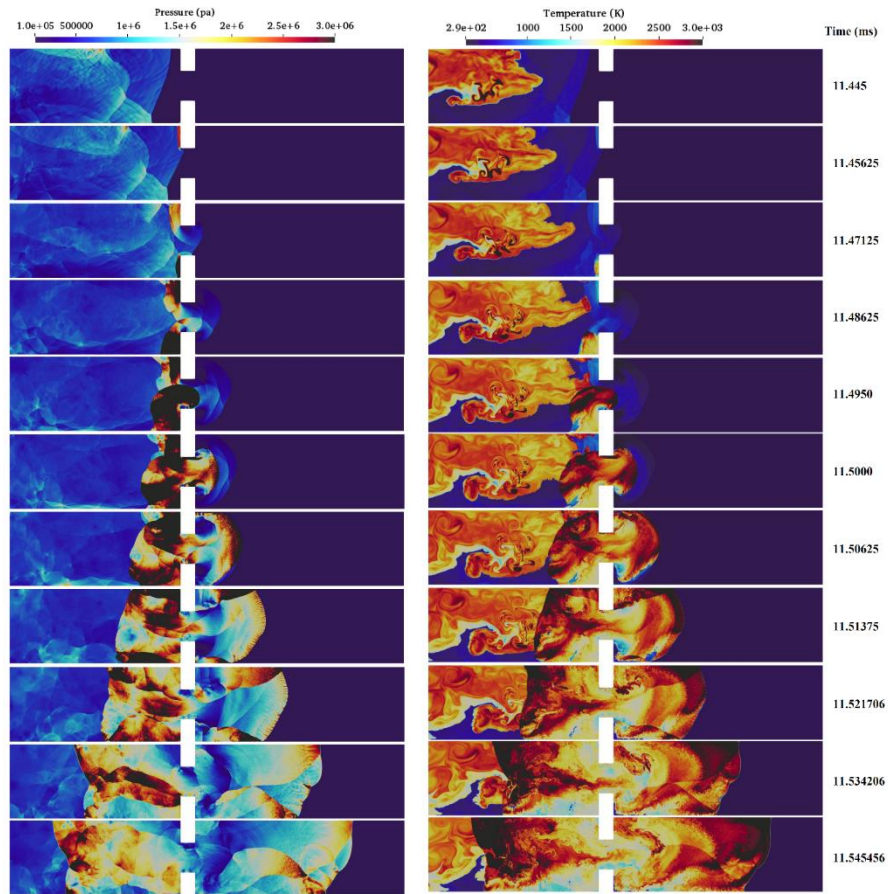


Figure 10: The predicted pressure (left) and temperature fields for the inhomogeneous with 30% hydrogen concentration. The obstacle in the field of view (FOV) is located at  $x=1.45$  m.

Figure 11 shows the onset of detonation in both homogeneous and inhomogeneous mixture of 30% hydrogen/air. Based on figure 6, can be found that in the homogeneous mixture the detonation front is regular however in the inhomogeneous case, the detonation front is irregular, and even the location of triple points is different in these two mixtures. These can be due to having a difference in induction time for the inhomogeneous mixture, rather than the homogeneous case which everywhere the induction times are equal everywhere in the channel.

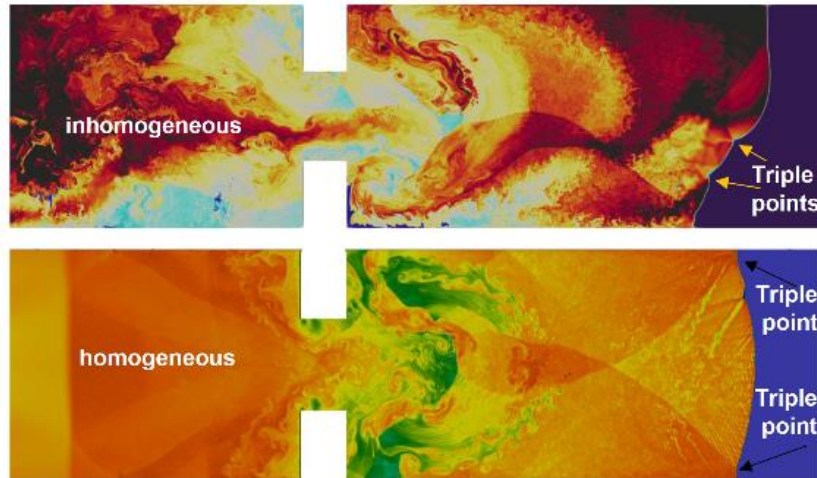


Figure 11. Temperature fields for comparison of onset of detonation, between the inhomogeneous and homogeneous mixture of 30% hydrogen-air.

## 5. Conclusion

A Numerical model has been developed for flame acceleration and transition to detonation in a horizontal obstructed channel filled with hydrogen/air mixture. DDT test case has been modelled to study the comparison between pressure-based and density-based solution methods. The density-based solver within the OpenFOAM CFD toolbox developed by the present authors [1], [27] is used. The numerical code has been verified by using a detonation test case, and the cellular detonation structure has been captured in agreement with experimental observations. In the detonation initiation test case the capability of the current numerical code in capturing the detonation cellular structure has been examined. A small test case has been modelled with using three high ignition point to produce detonation initiation. The CFD results have been compared against both quantitatively and qualitatively with the other previous works as well as an experimental observation. For detonation initiation cases, it would be recommended to use at least 20 cells per induction length. After detonation verification, two medium-scale DDT case, filled with 30% hydrogen-air mixture (homogenous and inhomogeneous mixture) have been modelled in an obstructed channel. In the DDT cases, high-resolution grids are facilitated by using adaptive mesh refinement technique, which leads to 30 grid points per half-reaction length (HRL) in the finest region near the flame and shock fronts. Overall, the predicted flame tip velocities, overpressures, and locations of detonation onset are in reasonably good agreement with the measurements. For both uniform and non-uniform mixtures with 30% hydrogen concentration, the onset of detonation occurs within the obstructed channel section, but the homogeneous mixtures show slightly faster flame acceleration and earlier onset. The captured detonation cell size was in good agreement with the other CFD works and the experimental observations. Furthermore, it has been found that the

non-uniform mixtures cause higher shock and flame velocities compared to the uniform mixtures concentration.

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