NUMERICAL MODELLING OF FLAME ACCELERATION AND TRANSITION TO DETONATION IN HYDROGEN/AIR MIXTURES WITH CONCENTRATION GRADIENT

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ABSTRACT

Hydrogen gas explosions in homogeneous reactive mixtures have been widely studied both experimentally and numerically. However, in practice, combustible mixtures are usually inhomogeneous and subject to both vertical and horizontal concentration gradients. There is still very limited understanding of the hydrogen explosion characteristics in such situations. The present numerical investigation aims to study the effect of mixture concentration gradient on the process of Deflagration to Detonation Transition, and the effect of different hydrogen concentration gradient in the obstructed channel of hydrogen/air mixtures. An obstructed channel with 30% blockage ratio (BR=30), and three different average hydrogen concentrations of 20 %, 30% and 35% have been considered using a specially developed density-based solver within the OpenFOAM toolbox. A high-resolution grid was built with the using adaptive mesh refinement technique providing 10 grid points in half reaction length. The numerical results are in reasonably good agreement with the experimental observations [1]. These studies show that the concentration gradient has a considerable effect on the accelerated flame tip speed and the location of transition to detonation in the obstructed channel. In all the three cases the first localised explosion occurred near the bottom wall where the shock and flame interacted, and the mixture was most lean; and the second localised explosion occurred at the top wall due to the reflection of shock and flame front and later develops to form the leading detonation wave. The increase in the fuel concentration was found to increase the flame acceleration (FA) and having a faster transition to detonation.

1.0 INTRODUCTION

Thomas [2] gave a comprehensive discussion on various forms of DDT and differentiates the terminology between the macroscopic DDT and the microscopic DDT. The large scale macroscopic DDT includes the process from accelerating deflagration up to a propagating detonation. The small scale microscopic DDT governs the actual onset of detonation at the point where the combustion process changes from diffusion controlled to shock heating controlled. In this work, the term DDT is used in the larger definition and includes both acceleration and onset of detonation. Thomas also gives a discussion on the understanding of the weak DDT, where it is not onset by a strong reflected shock wave, however, rather points out the importance of non-isotropic and non-equilibrium turbulence to accelerate a deflagration. Moreover, this will create small hot spots which in turn generate transverse waves and add up to strong pressure waves capable of forming the required shock/reaction complex known as the detonation [2]. Gas explosions inside tubes have been studied for a long time. Most of

these studies were conducted for industrial safety and to describe general mechanisms of flame propagation. So, most of the work has been dedicated to understanding the phenomena related to Flame Acceleration (FA) and DDT in tubes [3].

Industrial pipelines and equipment transport and store a wide range of hazardous materials. The combustible mixtures pose a risk especially when an ignition source is available or when the pressure and temperature exceed the self-ignition limits [3]. In the past, very few studies considered the effect of cloud inhomogeneity on the DDT behaviour.

Thomas et al. [4] and Kuznetsov et al. [5] have carried out experiments on detonation propagation with concentration gradients. They found that the mechanism of detonation initiation in a weaker mixture which propagated in a concentration gradient differs from that in a uniform mixture. In the mixtures with concentration gradients, a secondary shock is observed as the incident shock passes through the interface layer. Also, the reflected shock from the interface can be either a shock or rarefaction depending on the relative acoustic impedances of the reactive and non-reactive gas mixture. Transition to detonation occurred when the reaction wave and the secondary shock attached depending significantly on the sharpness of the concentration gradients. They also stated that smooth concentration gradients tend to assist the transition process, and detonation can propagate through the gradient interface. On the other hand, sharp gradients can separate the shock front and the reaction zone leading to failure of detonation. The possibility of detonation transmission through a mixture gradient interface is also influenced by the property differences of the reactive and less reactive gases [5].

Ciccarelli et al. [6] found in their experiments that in the fast turbulent flame regime, the shock-flame interaction is the main mechanism of controlling the flame speed; and due to the interaction of reflected shock from obstacles with flame, the interface of burned and unburned gas will be distorted via the baroclinic vorticity generation mechanism. This will trigger the Richtmyer–Meshkov instability (RMI) leading to fine-scale flame wrinkling. They mentioned that formation of a turbulent flame front is because of repeated shock-flame interactions.

Kholkhlov et al. [7] likewise conclude that shock-flame interaction is important to accelerate flames to critical conditions for the onset of detonation. They stated that large-scale RM instability is the primary mechanism increasing the heat release rate during the interaction of a flame with a single shock through macroscopic flame surface area growth.

Mahmoudi et al. [8] have studied the role of hydrodynamic instabilities in the propagation mechanism of detonations through numerical and experimental investigations. Their predictions with relatively low-resolutions were found to be partially in qualitative agreement with the experimental observations. However, although self-sustained propagation of detonation was detected in the experiments, the numerical predictions contained large unreacted pockets as turbulent mixing was only poorly resolved, [6]. Therefore, it can be deduced that without resolving small-scale instabilities, the predicted detonation wave could not be self-sustained and would fail. Moreover, it was also mentioned that in the numerical experiments, numerical diffusion scales are usually larger than the real diffusion scales.

Mazaheri et al. [9], showed that for regular detonation in the hydrogen-air mixture, hydrodynamic instabilities do not play a role in the propagation mechanism of the detonation wave, so there is no need to use a high grid resolution to capture the overall phenomena. Kuznetsov et al. [10] conducted large-scale experiments on FA and DDT in an obstructed semi-confined flat layer of hydrogen–air mixture with transverse concentration gradients. It was suggested that DDT propensity in semi-confined mixtures with concentration gradients might be determined by the maximum local hydrogen concentration for globally lean mixtures. Vollmer et al. [11] and Boeck et al. [12,13] reported a strong effect of concentration gradients on FA and DDT in an entirely closed channel at laboratory-scale. Recent work by Boeck et al. [1] investigated flame acceleration and DDT in a channel with vertically variable hydrogen concentrations. They showed that the flame accelerated faster when it burned in

these gradients. DDT was also observed as reflected shock waves interacted with the deflagration front.

In the present study, high-resolution numerical simulations have been used to elucidate the propagation mechanism of DDT in the inhomogeneous mixture, to examine the effect of different hydrogen/air concentration in the local explosion and transition to detonation.

2.0 Numerical model and its verification

A density-based solver was developed [14] within the frame of open source computational fluid dynamics (CFD) code OpenFOAM toolbox [15]. To evaluate the convective fluxes contribution, Harten–Lax–van Leer–Contact (HLLC) scheme with multidimensional slope limiters ("cellMDLimited" [16]) is used for accurate shock capturing. Compressible Navier–Stokes equations with a flame wrinkling combustion model are solved [17]. For turbulence modelling the Large Eddy Simulation (LES) technique with the one-eddy equation subgrid scale model is adopted. The solver and numerical schemes were initially tested by solving the Sod's shock tube problem [18].

2.1 Experiments considered

DDT phenomena in inhomogeneous hydrogen-air mixture experimentally tested by Boeck et al. [1] is chosen. The experiment was conducted in a horizontal obstructed channel with 30 percent blockage ratio filled with inhomogeneous hydrogen/air mixture. The length of the channel is 5.4 m, the height is 0.06 m, and the width is 0.3 m. The channel is confined with seven flat plate obstacles with a blockage ratio of 60%, and the spacing between the obstacle is S = 0.3 m. The first obstacle is located at $x = 0.25$m from the front plate where a spark ignition located. The last obstacle is placed at $x = 2.05$ m and the rest of the channel is unobstructed. Also, each obstacle has a thickness of 12 mm. The schematic of the computational domain in Figure 1 was set up based on the experimental setup's configuration.

Three different cases have been considered which the reactive mixture includes on average 20%, 30% and 35% hydrogen by volume. The channel is filled with inhomogeneous mixture (average 30 % H_2 in air by volume). The concentration profile is shown in Figure 2, with concentration gradients in the vertical direction.
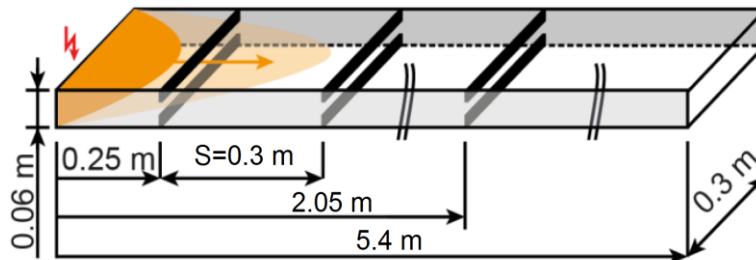

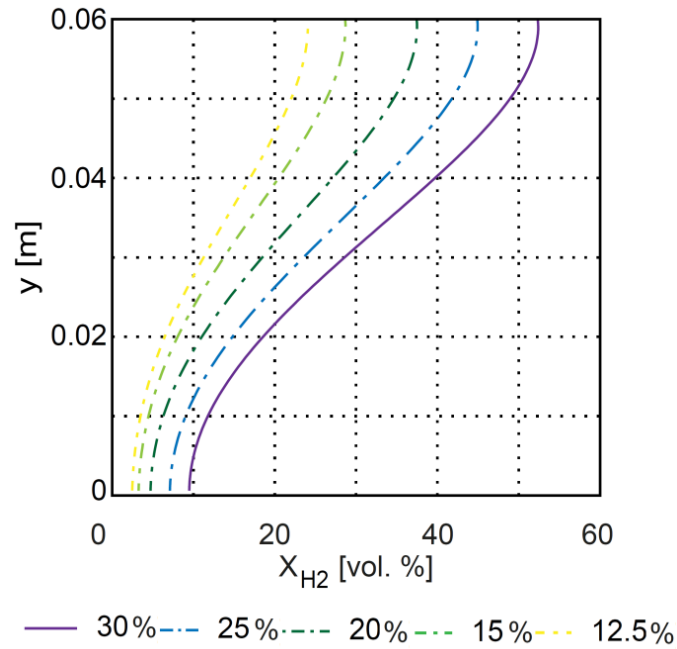Figure 1. Schematic of the computational domain (Reproduced from Boeck et al. [1]).

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Figure 2. The volumetric hydrogen concentration gradients in the experiments (Reproduced from Boeck et al. [1]).

2.2 Numerical setup

Three sets of simulations have been carried out for a blockage ratio BR=30, and average hydrogen concentrations of 20%, 30% and 35%. The computational domain, shown in Figure 1, represents a smooth closed channel with obstacles. The mixture is initially at ambient pressure and temperature. It was ignited by a weak spark in the test. For the numerical simulation, a patch of cells within a radius of 10 mm around the point of ignition (x=0, y=0.03m) was initiated at a temperature of 2200 K and atmospheric pressure. The adaptive mesh refinement capability was used with minimum cell size being 30 μm, giving approximately by average 10 grid points per half reaction length in the finest region near the flame and shock fronts.

3.0 Results and Discussion

As shown in Figures 3, 5 and 7, the predicted flame position and flame tip speed are in reasonably good agreement with the measurements [1]. In Figure 3, the mixture is lean with 20 percent inhomogeneous hydrogen concentration by average. Based on Figures 3 and 4, it can be found that after the flame interacts with the very first obstacle, (which is located at x=0.25m), due to turbulence generation, the flame velocity increased. After passing all seven obstacles (x=2.05m) the flame tip velocity increased to 1361 m/sec, which is still less than the D_{CJ} detonation speed, which is 1716 m/s for 20% hydrogen. However, in Figure 3, it can be found that after the accelerated flame interacts with a generated shock at x=2.75m of the channel, the lean hydrogen flame transitted to detonation.
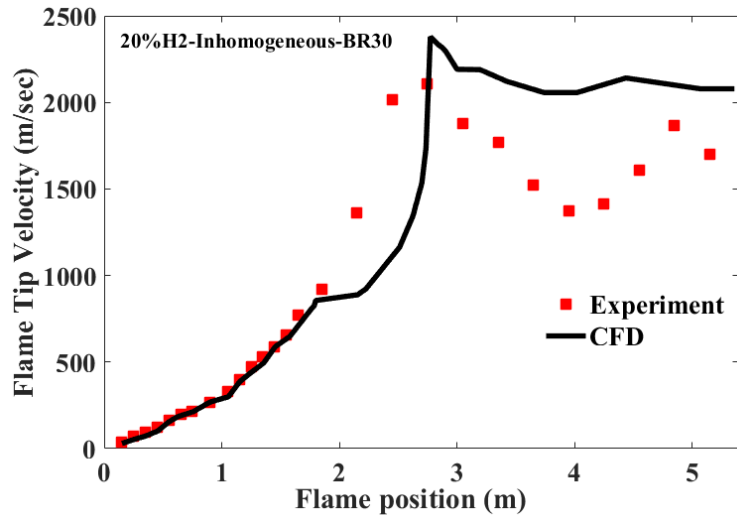
Figure 3. Comparison of the predicted and measured flame tip velocity for 20 % inhomogeneous hydrogen concentration in the 30% BR channel.

Figure 4 shows the onset of detonation in the inhomogeneous 20% hydrogen/air mixture with 30 % blockage ratio.
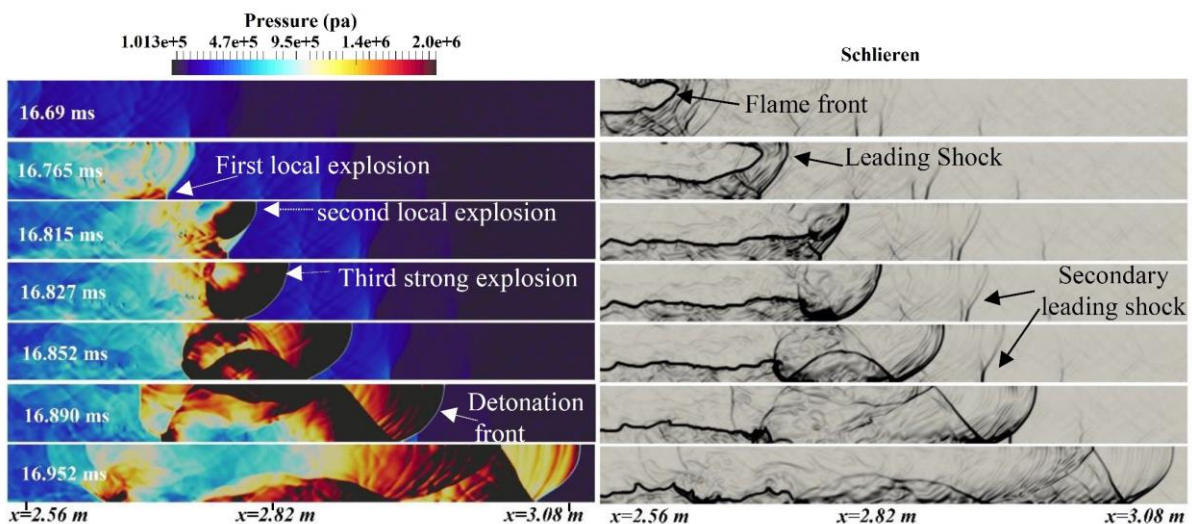

Figure 4. Pressure (left) and numerical Schlieren (right) with the magnitude of density gradient showing the onset of detonation in the inhomogeneous 20% hydrogen-air mixture.

In Figure 4, the frame at 16.69 ms shows a weak shock wave generated in front of the hydrogen flame front, then at 16.765 ms, this shock strengthened sufficiently to trigger the first local explosion near the bottom wall, where the mixture is lean. Then at 16.815 ms, the second local explosion happened near to the upper wall due to shock-flame interaction. This is a stronger explosion than the first one. The two local explosions interacted in the middle of the channel and resulted in much stronger explosions. At 16.852 ms, a secondary planer leading shock can be seen to propagate in front of the detonation wave. These predictions are also in line with previous experiments of Thomas et al. [4] and Kuznetsov et al. [5], who found that in conditions with concentration gradients, a secondary shock is observed as the incident shock passes through the interface layer. Subsequently, at 16.890 ms, this secondary shock and detonation wave interacted with each other, and a stronger detonation front was generated in the flame front. Figure 3 also shows that around this location which is at 2.89m, the flame

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tip velocity is at its maximum. At 16.952 ms, the flow became supersonic, and the deflagration completely transited to detonation.
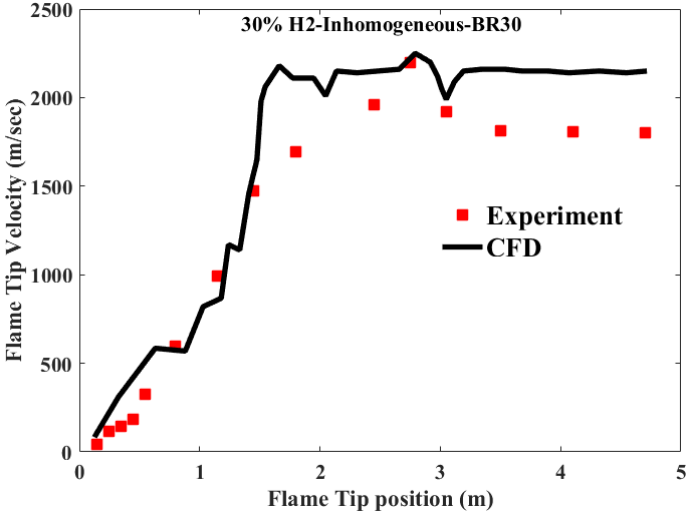

Figure 5. Comparison of the predicted and measured flame tip velocities for 30 % inhomogeneous hydrogen concentration in the 30% BR channel.

In Figure 5, the flame velocity rises continuously in the obstructed part of the channel (around the 7th obstacle, $x \leqslant 2.05$ m) due to flame interaction with the obstacles, resulting in combustion-induced expansion and turbulence generation. Figure 6 shows, the transition of accelerated hydrogen flame to detonation in the inhomogeneous 30% hydrogen/air mixture with 30 % blockage ratio.
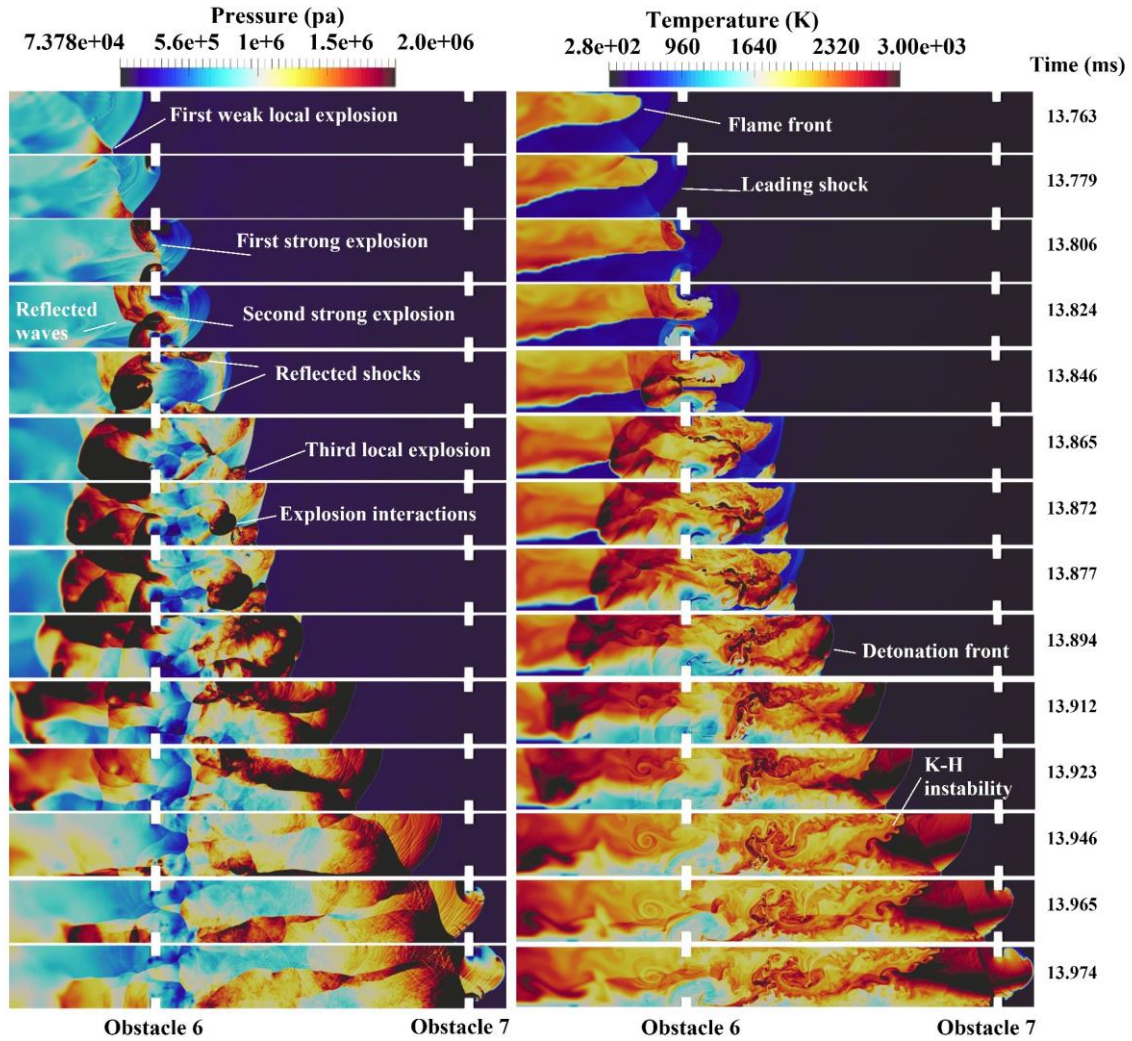
Figure 6. Pressure (left) and Temperature fields for DDT in the inhomogeneous 30% hydrogen-air mixture.

Based on figure 5, and figure 6, can be found that after the flame passed the 6th obstacle, the flame speed reached around 2100, which is the Chapman-Jouguet (CJ) detonation velocity of stoichiometric hydrogen-air mixture. After the flame and detonation wave passed the last obstacle which is located in x=2.05 m, the flame speed reached to maximum of around the 2200 m/s before decreasing slowly. The detonation speed of homogenous mixture of hydrogen-air in atmospheric condition and stoichiometric range is around 1480-2150 m/s while in the present study the predicted flame speed of 1450 to 2250 m/s in the present non-homogenous mixture just covers a slightly wider range. It is also noted that the first local explosion occurred near the bottom wall, where the mixture is most lean with the volumetric hydrogen concentration being around 10% and the local speed of sound is around 361m/s [14]. Also, after the flame transited to detonation, two shear layers have generated in the burned gas, and small-scale vortices which indicate Kelvin Helmholtz instability (K-H instability), was generated in these shear layers.
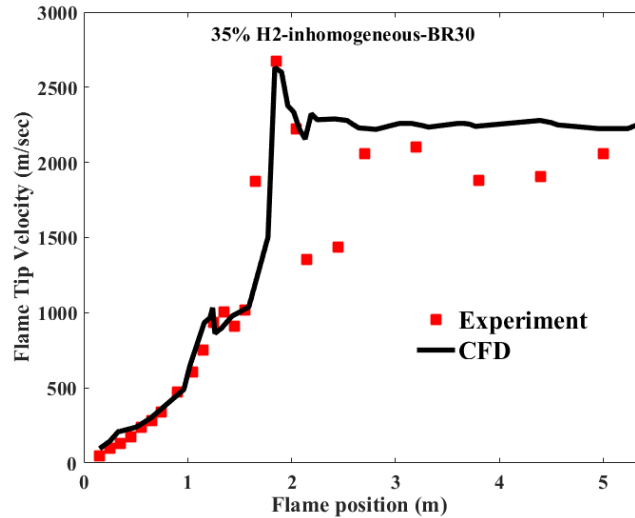
Figure 7. Comparison of the predicted and measured flame tip velocities for 35 % inhomogeneous hydrogen concentration in the 30% BR channel.

Figure 7 shows that relatively good agreement has been achieved between the predicted and measured flame tip velocities for the inhomogeneous mixture with average 35% hydrogen concentration by volume. Comparing the results in Figure 7 with those in Figures 5 and 3, it can be seen that the maximum flame tip velocity is much higher in the 35% concentration case than the 30% and 20% cases. Also, the maximum flame speed in the 30% hydrogen concentration was higher than in the 20 % case, which indicated that within the tested range of between 20% to 35% average hydrogen concentrations by volume, increasing the average hydrogen concentration would lead to increases in the maximum flame tip velocity.
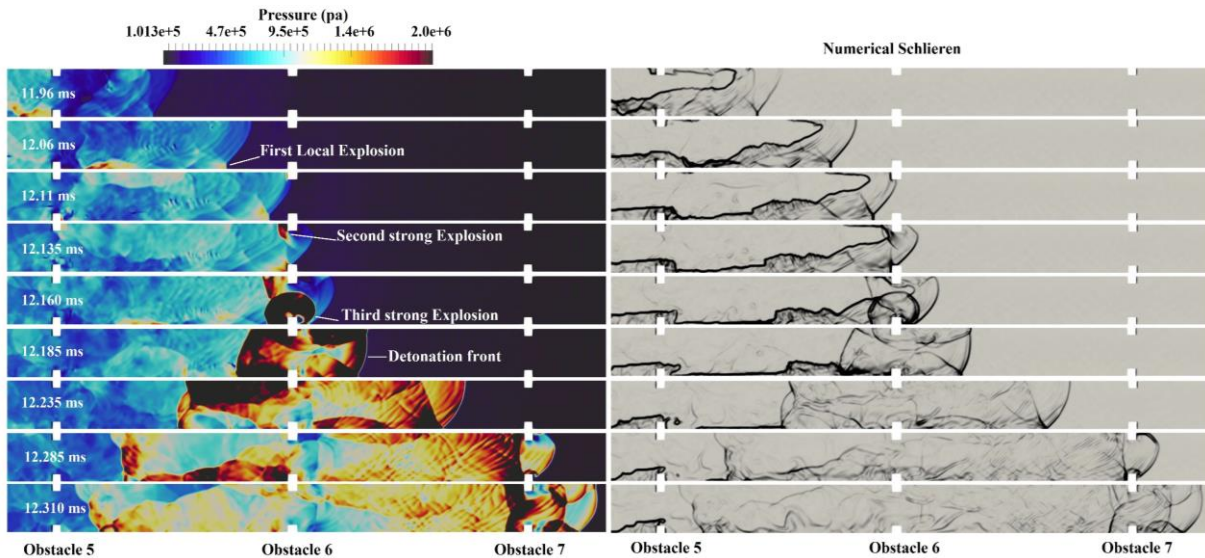

Figure 8. Pressure (left) and numerical schlieren (right, magnitude of density gradient) fields of onset of detonation in the inhomogeneous 35% hydrogen-air mixture.

Figure 8 shows the onset of detonation in the inhomogeneous 20% hydrogen/air mixture located around obstacle 5 and 6. On the right hand side, it can be found that at 11.96 ms a planer shock is moving downstream of the flame front. Then due to an interaction of the leading shock and hot spots, the first local explosion happened near to the bottom wall at 12.06 ms. However, this explosion was not strong enough to trigger detonation. At this stage, the overpressure was about 15 bar, which is in the CJ detonation pressure ratio limits (CJ detonation pressure ratio for the stoichiometric hydrogen-

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air mixture is 14.1 bar). This phenomenon is known as incident CJ detonation, but still, the flame has not transited to detonation as it is still not coupled with the shock wave. Then at 12.135 ms, combining the information on both the right- and left- hand sides in Figure 8, it can be seen that the second strong explosion happens due to shock and flame front interaction next to obstacle 6 in the upper wall. Then, at 12.160 ms this explosion wave generated a third strong explosion near the bottom wall. Subsequently, the transition to detonation occurred at 12.185 ms. From the detonation structure at 12.235 ms, it can be found that the gas compressed by the shock wave is free of disturbances and all the chemical energy released in the reaction zone goes to support the detonation. The process eventually reached steady state, and the shock wave propagated at nearly the C-J velocity. However, at 12.285 ms, while the detonation front interacted the obstacle, the flame tip velocity decreased as well as the overpressure. This is thought to be due to the existence of turbulence behind the shock wave which influenced the interaction between the shock wave and the reaction zone. Although turbulence can accelerate the flame front and assist the onset of detonation (e.g. Figure 8 at 12.185 ms), here at 12.285 ms, it increased losses of energy and quenched the flame by mixing the burned and cold unburned gases; thus, decreasing the amount of chemical energy available to support the detonation. Then, at 12.310 ms, the two reflected shock wave from upper and lower wall interacted downstream of the flame front and generated a steady detonation wave, which propagated along the channel.

Figure 8 also illustrated that in the case of 35% hydrogen concentration, the transition of hydrogen flame to detonation happens earlier than the other cases with less average hydrogen concentration. Hence it can be concluded that by increasing the average hydrogen concentration from 20% to 35%, the flame will transit to detonation faster and in less distance to the ignition point. It is interesting that in these cases, the first local explosion happens near the bottom wall as CJ incident detonation.

5.0 CONCLUSIONS

Numerical studies have been conducted to investigate DDT of an inhomogeneous mixture of hydrogen-air in an obstructed channel with 30% blockage ratio (BR=30) for three different average hydrogen concentration, i.e. 20%, 30% and 35% by volume. A density-based solver developed in-house within the OpenFOAM CFD toolbox is used. A high-resolution grid with using adaptive mesh refinement technique provided ten grid point in half reaction length. The predicted flame position and flame tip velocities are in reasonably good agreement with the measurements of Boeck et al. [1] for all three cases. In all the three cases the first localised explosion occurred near the bottom wall where the shock and flame interacted, and the mixture was most lean. Moreover, then the second localised explosion occurred at the top wall due to the reflection of shock and flame front. This second local explosion further developed to form the leading detonation wave. It can be concluded that the concentration gradient has a considerable effect on the accelerated flame tip speed and the location of transition to detonation in the obstructed channel. Also, the increase in the fuel concentration was found to increase the FA and faster transition to detonation.

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