# Numerical simulations of hydrogen-air detonation wave propagation in a non-uniform semi-confined flat layer

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## Abstract

Detonation propagation in non-uniform combustible gas mixture has largely been overlooked despite being relevant to many accidental scenarios. This particular scenario has recently been investigated experimentally by Rudy et al.(2013) with varying initial hydrogen pressures. The present study aims to use these data to validate our previously developed modelling techniques for flame acceleration and transition from deflagration to detonation. The model is based on the open source computational fluid dynamics (CFD) platform OpenFOAM® and uses the hydrogen-air single-step chemistry and the corresponding transport coefficients developed by the authors and validated against the experimental of Teodorczyk (2008)for fast hydrogen deflagrations and detonations in an obstructed straight channel. Overall six cases tested by Rudy et al. (2013) have been numerically simulated. These cases were conducted with different initial hydrogen pressures at 1300, 1350, 1375, 1400,1475, 1500 and1600mbar but otherwise under the same conditions. The corresponding hydrogen concentration gradient fields were taken into account in the numerical setup. The effects of different hydrogen gradients on the evolution of flame and shock wave are analyzed. Three modes: subcritical, critical and supercritical traveling of the detonation waves were captured by the simulations. In addition, it was found that a series of processes is involved in the critical traveling mode, such as detonation decaying, decoupling, local explosion, transverse detonation travelling, unreacted gas pocket and detonation recovering. The predicted critical initial reservoir pressure is 1400 mbar, and the corresponding maximum hydrogen concentration about 24.4%, which is reasonably consistent with the experimental measurements. The predicted velocities in the range from 3 to 9m for the initial reservoir pressure of 1400mbar and 1500 mbar are also in reasonably good agreement with the measurements, but the detonation layer thickness was under-predicted.

Keywords:*hydrogen safety, flat layer, detonation, non-uniform hydrogen-air mixture*

## 1. Introduction

Although considerable effort has been devoted to the modelling turbulent deflagration and detonation, detonation propagation in non-uniform combustible gas mixture has largely been overlooked despite being relevant to many accidental scenarios. For example, if hydrogen is accidentally leaked into a confined or semi-confined enclosure, a non-uniform hydrogen-air mixture layer will form along the top wall. Accidental ignition of this mixture could result in fast deflagration and transition to detonation. Relatively little is known about the subsequent

propagation of any potential detonation wave in this non-uniform mixture despite their relevance to safety concerns.

Detonation propagation in a semi-confined flat layer filled with non-uniform hydrogen-air mixture with varying initial hydrogen pressures has recently been investigated experimentally by Rudy et al.(2013). It was found that the critical hydrogen concentration is approximately equal to 26% at the top of the layer and 16-17% at the bottom of the layer while the detonation layer height is about 8.5cm.Kuznetsov et al. (1998) conducted related studies on the detonation propagation from a driver mixture of variable length through a concentration gradient of variable width into a less reactive acceptor mixture. They found that the mixture gradient has strong influence on the sustainability of the detonation. More specifically, the sharper the mixture gradient the faster the detonation decay. Ishji and Kojima (2007) experimentally studied detonation in mixtures with concentration gradients normal to the propagation direction. The detonation deflection was found to be induced by the hydrogen concentration effect.

While laboratory experiments are costly and can only be conducted within adequate facilities, it is desirable to conduct numerical experiments with validated predictive tools. The present study is hence aimed at using available experimental data to validate our recently developed models for flame acceleration and transition from deflagration to detonation. The model is based on the open source computational fluid dynamics (CFD) platform OpenFOAM®. It uses the hydrogen-air single-step chemistry and the corresponding transport coefficients developed by the authors. Validation is conducted with the experimental measurements of Teodorczyk (2008)for fast hydrogen deflagrations and detonations in an obstructed straight channel. On such basis, five cases of detonation propagation in a semi-confined flat layer filled with non-uniform hydrogen-air mixture as tested by Rudy et al. (2013) have been numerically simulated. These cases were conducted with different initial hydrogen pressures at 1300, 1350, 1375, 1400, 1475, 1500 and 1600 mbar but under the same conditions otherwise. The effects of different hydrogen gradients on the evolution of flame, shock wave are analyzed. The predicted velocity and detonation layer thickness were also compared with the experimental measurements. Furthermore, the critical hydrogen concentration condition for detonation propagation was established.

## 2. Numerical modelling

### *2.1 Governing equations*

The reactants are assumed to behave as an idea gas together with the products. The flow is governed by the compressible reactive Navier-Stokes equations as written below:

$$\frac{\partial \rho}{\partial t}+\frac{\partial \rho u_j}{\partial x_j}=0 \tag{1}$$

$$\frac{\partial \rho u_i}{\partial t}+\frac{\partial \rho u_i u_j}{\partial x_j}=-\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right] \tag{2}$$

$$\frac{\partial \rho h_s}{\partial t}+\frac{\partial \rho u_j h_s}{\partial x_j}=\frac{dp}{dt}+\frac{\partial}{\partial x_j}\left(\rho D\frac{\partial h_s}{\partial x_j}\right)+Q \tag{3}$$

$$\frac{\partial \rho Y_k}{\partial t}+\frac{\partial \rho u_j Y_k}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\rho D\frac{\partial Y_k}{\partial x_j}\right)+\omega_k \tag{4}$$

where $\rho$, $u$, $p$, $h_s$ and $Y$ are the density, velocity, pressure, sensible enthalpy and mass fraction of gas mixture, respectively. $\mu$, $D$ denote viscosity and diffusion coefficients. The source term, $\overline{\omega}_k$ is chemical reaction production rate and $Q$ denotes heat release rate per unit volume from a chemical reaction. The turbulence is simulated using standard k-ε model (Launder B. E. and Spalding,1972).

### *2.2 Chemistry model*

For the calculation of the chemical source terms of stoichiometric hydrogen-air combustion, the one step chemistry model developed by Wang et al.(2012) has been adopted. The model basically followed the logic and format of previous models developed by Bane et al. (2010)and Kessler et al.(2010). But the key model parameters as summarized in Table 1 are similar to those proposed by Gamezo et al. (2007) in their hydrogen DDT calculations but differences exist in the reaction order, the pre-exponential factor and the transport coefficients as the oxidizer concentration was taken into account when determining the parameters for the Arrhenius kinetics in the present study.

*Table 1: Model parameters for stoichiometric hydrogen–air mixture*

| Parameter | Values or Expressions | Annotation |
|---|---|---|
| A | $1.13\times1015cm^3/(mol.s)$ | Pre-exponential factor |
| Ea | 46.37RT0 | Activation energy |
| Q | 43.28RT0/M | Chemical heat release |
| Γ | 1.17 | Specific heat ratio |
| $K_0=\mu_0=D_0$ | 7.0×10-5g/(cm.s.K0.7) | Transport coefficient |

### *2.3 Numerical scheme*

The governing equations are discretized using the finite volume method. For time integration, the second-order Crank-Nicholson scheme was employed. The convective terms were integrated by the 2rd MUSCL scheme maintaining the total variation diminishing characteristic. The viscous terms are evaluated with second-order central differencing discretization.

## 3. Numerical validation

For model validation, the flame acceleration and deflagration-to-detonation transition in an obstructed tube with the same geometric dimension and set up as case B in Teodorczyk etal's(2008) experiments was simulated. The tube width was 20mm. All obstacles had the same height of 10mm. A hot burning material with radius of 0.005mm at the center of the left wall was defined to represent the ignition region. Extra energy in the same order of the chemistry-energy was imposed to trigger ignition. Figure 1 presents the pressure profiles at corresponding monitoring locations. The predicted peak pressures are 3.75MPa at 475mm and 5.81MPa at 595 mm from the ignition centre. Both values are within 3% of the experimental measurements of Teodorczy et al. (2008).

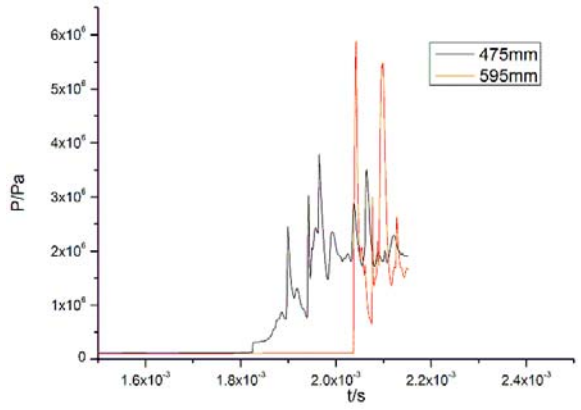
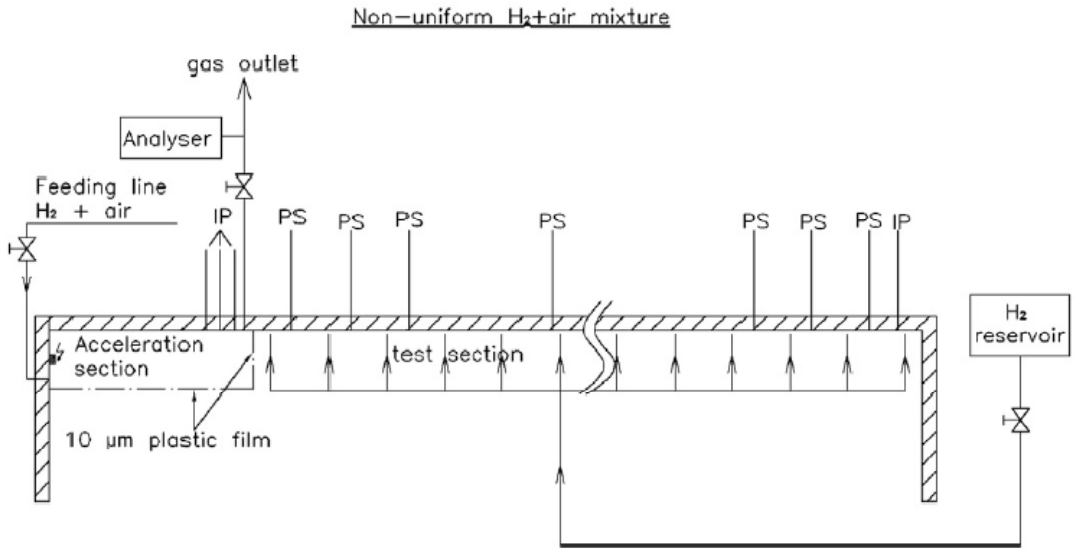


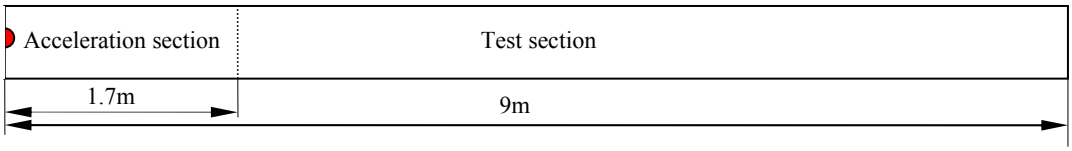

*Figure1. Pressure profiles at two corresponding locations in an obstructed channel.*

## 4. Case setup

Numerical simulations of detonation propagation in non-uniform combustible gas mixture were carried out for a two-dimensional flat layer. The schematic of the computational domain is presented in Figure 2 (b) which mimics the experimental set up shown in Figure 2 (a). This geometry and set up mimics the laboratory tests of Rudy et al.(2013). Overall, the flat layer is 9 m long and 0.2 m wide, consisting of two separate sections. The left section is 1.7 m long and initially filled with stoichiometric hydrogen-air premixed mixture at 1050mbar and 283K for generating a self-sustaining detonation wave. The right hand section is filled with non-uniform hydrogen-air mixture with varying concentration distributions according to the varying reservoir pressure(1300mbar-1600mbar) as shown in Figure 3(Rudy et al. 2013). It should be noted that hydrogen concentration decreases with the increase of the distance away from the top wall. The increase of reservoir pressure will lead to higher hydrogen concentration at the same height. A total of six cases were simulated using uniform grids along the channel centreline and width direction. Eight monitoring points (PT0 to PT7) were set with 1m spacing along the top wall and another eight corresponding monitoring points (PT8 to PT15) were located along the bottom boundary of the flat layer, which was set as non-reflective boundary.



(a) The Experimental set up of Rudy et al. (2013).




**(b)** Schematic of the computational domain.

*Figure 2.Numerical set up of the flat layer simulations.*

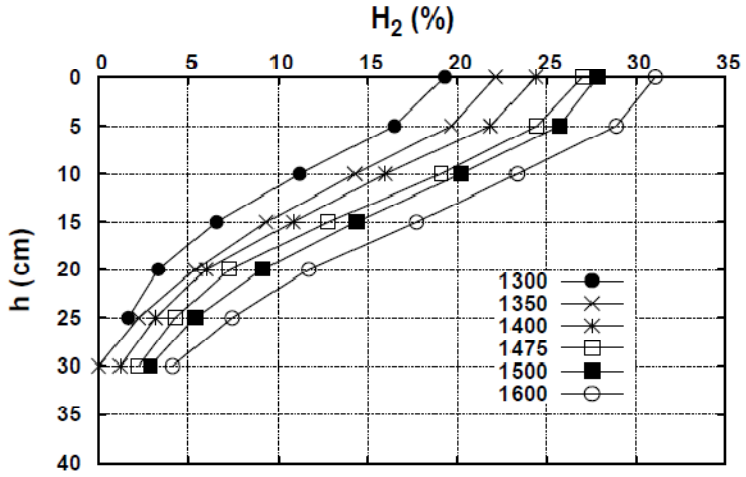



*Figure 3. Hydrogen concentration profile at different initial hydrogen reservoir pressure (reproduced from Rudy et al. (2013).*

## 5. Results and discussion

### *5.1 Grid sensitivity analysis*

In order to obtain converged and acceptable results in numerical simulation,the effect of grid size on the simulation results should be first examined to ensure that the grid size is appropriate. The case at the highest initial reservoir pressure 1600 mbar was taken into account for grid sensitivity analysis since it generates the strongest detonation wave. The determined grid size at this situation can also be extended to the cases at lower initial reservoir pressure. For detonation simulation, if the cellular structure needs to be captured, the grid size needs to be very fine. Sharpe(2001) reported that more than 20 cell per reaction zone length is required to ensure convergence in the simulated phenomena. A large amount of published paper also showed that grid resolutions of 20-64 grids in reaction zone length are used. The current case has a domain of 9m×0.2m and reaction zone length of ~0.2mm. If these guidelines are followed, the grid size needs to be at most 0.01mm and the grid number is at least eighteen billions (900000×20000), which would be computationally too expensive. As a compromise, it was decided to focus on detonation propagation and mean detonation parameters such as detonation pressure, speed and detonation layer thickness, etc. In other words, we are not expecting to resolve the cellular structures.

Three grid sizes of 0.75mm,1mm and 1.25mm were considered. Figure 4 presents the maximum location of the detonation front as a function of time at initial reservoir pressure $p_j$=1600mbar. The grid sizes of 0.75mm and 1mm give similar predictions, while the prediction of the grid size 1.25mm deviates from both curves. Hence, the grid resolution of 1mm was

adopted for the subsequent computations involving overall 1.8M cells. The simulations were run on a 128-processor Linux cluster.

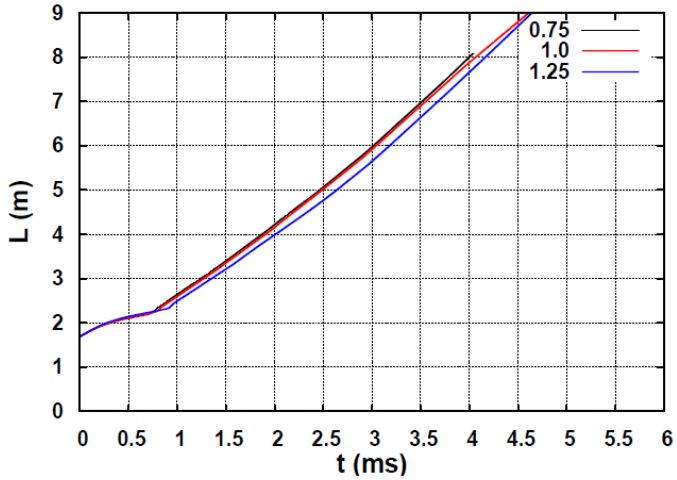


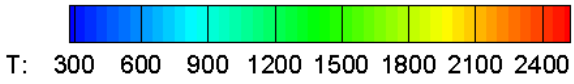

*Figure 4.The maximum location of the detonation frontas a function of time at $p_j$=1600mbar.*

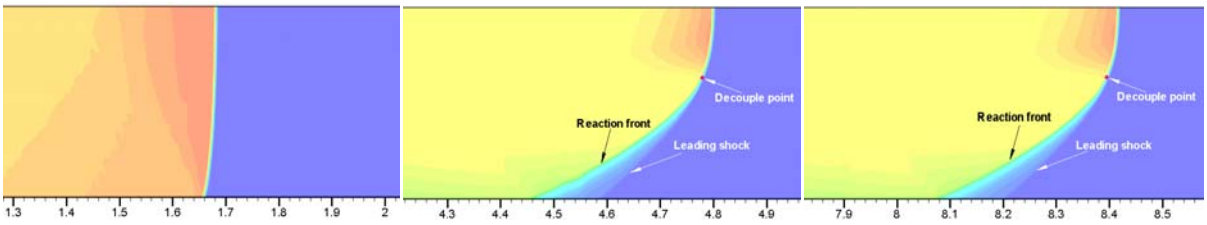
## *5.2 Travelling modes*

The predictions have revealed the existence of three different travelling modes of the detonation wave in the semi-confided flat layer, i.e. supercritical, critical and subcritical travelling.

(a) Supercritical travelling

Figure 5 illustrates the supercritical travelling of detonation in non-uniform hydrogen-air mixture. The detonation wave propagates from left to right at the reservoir pressure of1600mbar. A quasi-steady self-sustaining detonation is formed in the acceleration section filled with stoichiometric hydrogen air mixture as shown in Figure 5(a). Due to the influences of the rarefaction waves from the bottom boundary, the part of the detonation wave front close to it is curved and the temperature at the back of the shock front is slightly lower than that behind the undisturbed detonation wave. As the detonation wave travels in the non-uniform mixture in Figure 5(b), due to the relatively low hydrogen concentration near the bottom boundary and its increase from bottom to top. It is observed that the reaction front is separated from the leading shock. This separation is more evident close to the bottom boundary where the width from the leading shock to the reaction front is about 0.12 m. The separation width decreases from bottom to top. The decoupling point moves from bottom to top until the heat release from the reaction is sufficient to sustain the local leading shock. The un-decoupled detonation wave front above the decoupled point is not planar but curved; and the strength at any point on its surface is different. This behaviour of the detonation wave is continuously kept till it reaches the right end as shown in Figure 5(c).



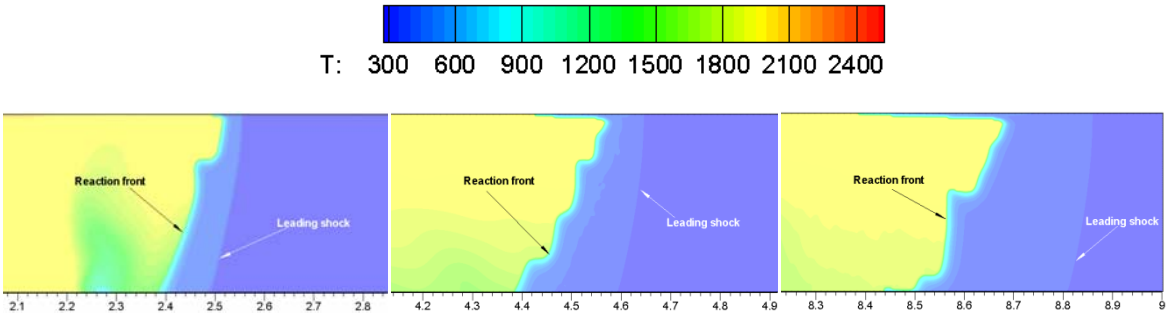



*(a)* *(b)* *(c)*

*Figure 5. Supercritical travelling of detonation in non-uniform hydrogen-air mixture($p_j$=1600mbar).*

(b) Subcritical travelling

Figure 6 presents subcritical travelling of the detonation at the reservoir pressure of 1350mbar. Associated with the lower hydrogen concentration in the semi-confined fat layer, the quasi-steady detonation wave decays rapidly and the resultant temperature behind the wave front also decreases steeply. The heat generated by the chemical reaction cannot sustain the leading shock and therefore its shock front quickly separates from the reaction zone. As shown in Figure 6(a), the reaction front is wrinkled, indicating that turbulence is likely playing an important role. With the decoupled leading shock and reaction front propagating forward in Figures 6(b) and (c), the distance between them increases and the reaction front significantly lags behind the leading shock.



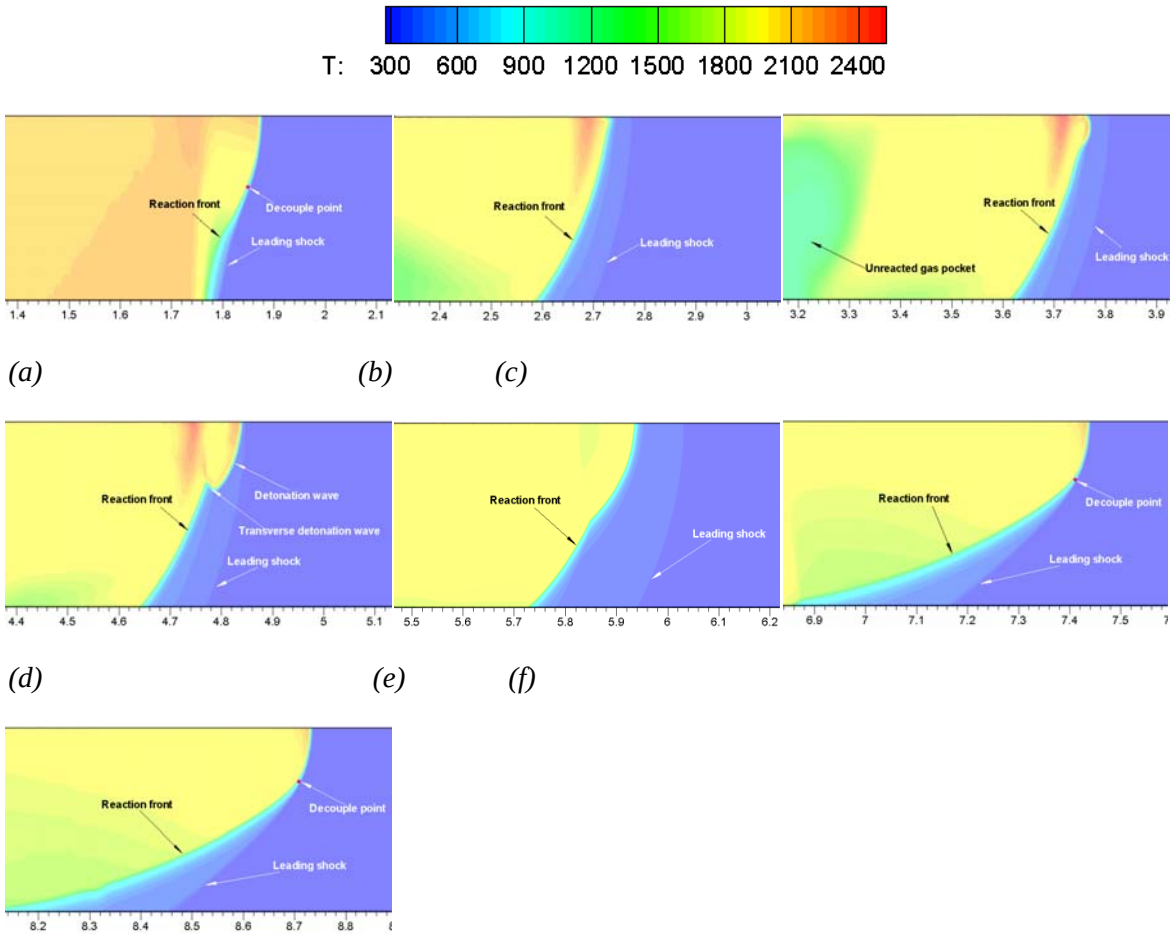

*(a)* *(b)* *(c)*

*Figure 6. Subcritical travelling of detonation in non-uniform hydrogen-air mixture($p_j$=1350mbar).*

(c) Critical travelling

Figure 7 presents subcritical travelling of the detonation wave in non-uniform hydrogen-air mixture. The critical reservoir pressure for the detonation to reach the right end is found to be 1400 mbar in our numerical simulations. This is slightly higher than the 1375 mbar suggested by the experiments of Rudy et al.(2013). More complicated phenomena is observed here. In Figure 7(a), the detonation wave just transmits from the premixed uniform mixture to the right hand section with non-uniform hydrogen concentration. The decoupling point is about 2/3 of the width. Below it, the separation between the leading shock and the reaction front is beginning to occur. In Figure 7(b), the reaction front has completely been decoupled from the leading shock, which is marked as the first complete separation. With the wave continues to propagate towards the right end, a local forwardly projecting region can be found near the top wall in Figure 7(c), representing local explosion. An unburnt gas pocket is seen in the downstream region. Further on as shown in Figure 7(d), the local explosion travels forward and overtakes the part of leading shock close to the top wall. Simultaneously it transversely propagates downward within the mixture compressed by the leading shock. This transverse

part can be approximately regarded as transverse detonation wave and would be overdriven. However, this explosion or newly formed detonation wave fails to create a detonation wave emerging on the surface of the leading shock, and therefore the separation is still maintained. But it can be looked as the second complete separation because the existence of local re-coupling and decoupling in the small region. As the wave travels around 7.45 m away from the left end, a stable detonation structure similar to that shown in Figure 4 is observed. This is maintained until the detonation wave reaches the right end as shown in Figures 7(f) and (g). Generally, in this critical condition, the detonation wave undergoes decaying, decoupling, local explosion and re-coupling, etc.




*(a)* *(b)* *(c)*

*(d)* *(e)* *(f)*

(g)

*Figure 7. Critical travellingof detonation in non-uniform hydrogen-air mixture($p_j$=1400mbar).*

### *5.3 Detonation layer thickness*

Figure 8 presents the predicted and measured detonation layer thickness for different initial hydrogen reservoir pressure. The predicted values are evidently smaller than those from the measurements(Rudy et al., 2013). If the different critical conditions between the simulation and measurement are taken into account, it is found that the predicted detonation layer thickness at 1400 mbar is close to the measured values at 1375mbar. In another word, at the critical condition, the predicted values are reasonably consistent with the measured values. Simultaneously, the predicted values at 1500 mbar are in reasonably good agreement with the measured measurements at 1400 mbar.

The above discrepancy between numerical and experimental results should be attributed to the initial pressure in flat layer. In the experiments of Rudy et al. (2013), the non-uniform hydrogen-air mixtures were generated by injecting pure hydrogen under initial pressure (1600-1350 mbar) through 75 injection points placed near the top of the test section while the initial ambient pressure in the semi-confined flat layer is 1050 mbar. This indicates that a pressure gradient should exist in the flat layer, but unfortunately the pressure distribution was not measured. Therefore, an initial pressure with uniform value of 1050 mbar was set in the numerical model. In addition, the bottom boundary should also be extended to avoid the boundary effect in the numerical simulations. But a non-reflective boundary is set there instead due to lack of information about hydrogen concentration distribution in the extended region.

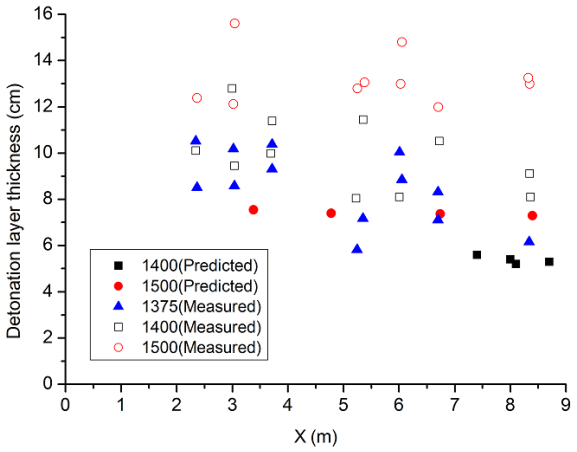



*Figure 8.Predicted and measured detonation layer thickness for different initial $H_2$ reservoirpressure.*

### *5.4 Travelling speed*

Figure 9 presents the predicted and measured velocities for different initial hydrogen reservoir pressure.In general, the predicted leading shock velocities are lower than the measurements of Rudy et al. (2013). At the reservoir pressure of 1500 mbar, in the range from 3m to 9m, the leading shock velocities are under-predicted by about 12.5%. At the reservoir pressure of 1400 mbar, due to the occurrence of complete decoupling between the leading shock and the reaction front in the simulation, as shown in Figure 7, the predicted values are evidently lower from 2 m to 7 m. In the subsequent process, due to detonation emergence, the leading shock velocities significantly increase and are only under-estimated by about 13%. As the reservoir pressure falls to 1350 mbar, the difference is significant between the predicted and measured values. It is hence decided to examine the leading shock velocities at the initial stage when the detonation wave transmits from the uniform mixture to the non-uniform mixture. The measured values are about 2500m/s for the reservoir pressure of 1400 mbar and 1500 mbar, and 2000m/s for 1350 mbar. These velocities are significantly higher than the Chapman and Jouguet (CJ) detonation velocity of about 1972 m/s at 1050 mbar or 1980m/s at 1500mbar. Moreover, in the present cases, the detonation wave along the top wall travels from the stoichiometric mixture to a lean mixture. It is unlikely that detonation wave would accelerate. This casts some doubt on the measured leading shock velocities.

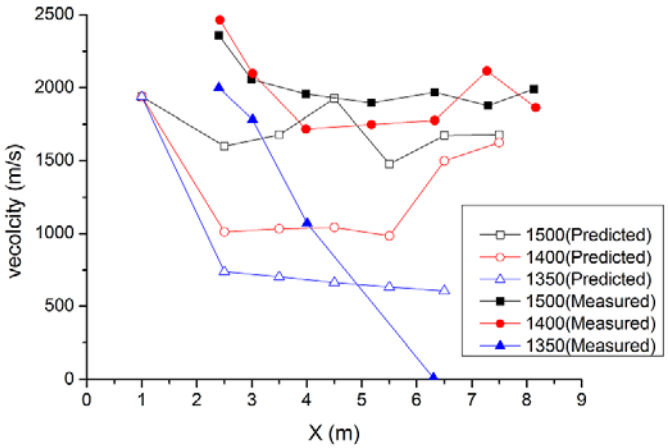



*Figure 9.Predicted and measured velocities for different initial $H_2$ reservoir pressure.*

## 6. Conclusions

Hydrogen-air detonation wave propagation in a non-uniform semi-confined flat layer has been numerically investigated. Overall six cases tested by Rudy et al. (2013) have been numerically simulated using the recently developed hydrogen-air single-step chemistry by the authors. These cases were conducted with different initial hydrogen pressures at 1300, 1350, 1375, 1400,1475, 1500 and1600mbar but otherwise the same conditions. The corresponding hydrogen concentration gradient fields were taken into account in the numerical setup. The effects of different hydrogen gradients on the evolution of flame and shock wave are analyzed, indicating three travelling modes of detonation wave propagation through the layer, i.e. subcritical, critical and supercritical traveling. A series of physical processes is involved in critical traveling mode, such as detonation decaying, decoupling, local explosion, transverse detonation travelling, unreacted gas pocket and detonation re-emerging, etc. The predicted critical initial reservoir pressure of 1400 mbar and the corresponding maximum hydrogen concentration of 24.4% are both reasonably consistent with the measurements. The predicted velocities in the range from 3m to 9m for the initial reservoir pressure of 1400mbar and 1500 mbar are also in reasonably good agreement with the measurements. However, the detonation layer thickness is under-predicted. This discrepancy might be caused by some uncertainty in the experiment which led to much higher leading shock velocities than the CJ detonation speed. It might also be partially caused by the boundary effect as non-reflective boundary is set at the bottom of the flat layer. Strictly speaking the domain should be extended well into the lower part of the channel.

## Acknowledgements

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