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# Numerical simulation of detonation failure and re-initiation in bifurcated tubes

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## Abstract

A numerical approach is developed to simulate detonation propagation, attenuation, failure and re-initiation in hydrogen-air mixture. The aim is to study the condition under which detonations may fail or re-initiate in bifurcated tubes which is important for risk assessment in industrial accidents. A code is developed to solve compressible, multidimensional, transient, reactive Navier–Stokes equations. An Implicit Large Eddy Simulation approach is used to model the turbulence. The code is developed and tested to ensure both deflagrations (when detonation fails) and detonations are simulated correctly. The code can correctly predict the flame properties as well as detonation dynamic parameters. The detonation propagation predictions in bifurcated tubes are validated against the experimental work of Wang et al. [1, 2] and found to be in good agreement with experimental observations.

Keywords: Numerical simulations, Deflagration, Detonation, bifurcated tube

## 1- Introduction

Hydrogen industry is growing rapidly [3] and more devices are being built every year which rely on hydrogen as the source of energy. This is mainly because hydrogen is very reactive and only water is produced in hydrogen combustion. However the rapid growth of hydrogen industry has caused a high concern among the experts about the safety of hydrogen production, carriage, storage and consumption facilities.

An accidental release of hydrogen can create a highly reactive mixture with air and the hydrogen ignition energy is very low therefore even a weak ignition is enough to cause severe damage to the surrounding facilities and the people.

Many studies have been carried out in the past to investigate the behaviour of detonation waves in straight tubes [4-6]. Since bends and T-junctions are widely used in the gas pipelines, the present work intends to study propagation, attenuation, failure and re-initiation of hydrogen detonation (a highly destructive and supersonic type of combustion wave) in bifurcated tubes. The information obtained from such studies can be very valuable for risk assessment and management in hydrogen related facilities. The experimental studies of detonation are very costly and very strict health and

safety standards must be followed, hence only a limited number of experiments can be conducted in highly specialised facilities. Therefore reliable numerical studies are ideal alternatives.

Thomas et al. [7] showed that whether detonation fails or sustains through bends depend on the initial pressure, while detonation failed in lower initial pressures it can sustain through the bends in higher initial pressures. Frolov et al. [8] carried out experimental and numerical studies of detonation propagation in shock tubes with U-bends and reported temporary failure of detonation waves due to diffraction in U-bends which was followed by re-initiation of detonation by shock-to-detonation transition (SDT). Kuznetsov et al. [9] studied detonation propagation, decay and re-initiation in non-uniform hydrogen-air mixtures. Ohyagi et al. [10], studied detonation diffraction, failure and re-initiation in backwards facing step. Wang and Guo [1, 2] carried out experimental and numerical studies of detonation propagation in bifurcated tubes filled with different hydrogen concentrations and pressures and demonstrated the re-initiation of detonation by the leading shock reflection in the vertical branch of the tube. Bhattacharjee et al. [11], in an experimental work, studied diffraction and re-initiation of detonation around a cylindrical geometry using a high accuracy (microsecond time resolution) schlieren technique. They observed auto-ignition of detonation by the Mach stem while the transverse wave remained nonreactive. They have also carried out a series of numerical simulations to reproduce their experimental observations. Shepherd and Pintgen [12], studied detonation diffraction experimentally to analyse the effects of detonation cellular instabilities on the diffraction features. They used schlieren photography to obtain qualitative and quantitative measurements. They have reported their observations in different hydrogen oxygen mixture compositions and presence of argon and nitrogen as diluents. Lv and Ihme [13], studied the mechanism of re-initiation and re-ignition of a quenched detonation using a detailed chemistry for hydrogen oxygen mixture and a high resolution Galerkin approach. Different volumes of diluents, were added to analyse the effect of mixture composition and they observed that mixture reactivity plays a crucial role in ignition kernel formation and development. They showed that in more reactive mixtures the ignition occurs behind the reflected shocks and through “Shock Wave Amplification by Coherent Energy Release” or SWACER mechanism [14, 15]. For less reactive mixtures they observed detonation re-initiation through Mach reflection which was mostly driven by flame-shock and shock-shock interactions. Bauwens et al. [16], studied the structure of failed detonation in high activation energy mixtures in a one dimensional numerical simulation and reproduced the formation of hot spots in which detonation re-initiation occurs and showed these hot spots approach the contact surface under the Newtonian limit.

Most studies on detonations, including their failure and re-initiation, have been carried out in 2D [1, 2, 7-10] and despite that the computational times have always been high, adding the third dimension to the model would increase the number of grid points and therefore the computational cost drastically. However Houim et al [34] concluded any 3D effect should not qualitatively influence the structure of the predicted waves. Furthermore, Gamezo et al. [35, 36] showed that 2D and 3D simulations of deflagrations, detonations, DDT and the flow instabilities reproduce very similar results which are observed in the experiments. These studies show that even though the reaction front becomes very convoluted in the third dimension, the overall flow structure is dominated by the shock reflections and the Kelvin Helmholtz instability and as a result the global energy release rates and the position of the reaction front and shock waves are very similar in 2D and 3D simulations.

The present work aims to further develop a solver previously developed by the author, to model deflagration to detonation transition [17, 18], and modify it to simulate detonation propagation in bifurcated tubes, the detonation failure due to diffraction and the possibility of detonation re-initiation.

## 2- Numerical model

Detonation waves are supersonic and their extremely high velocity makes the diffusive and viscous effects less significant. Therefore one can simulate detonation waves by solving reactive Euler equations (Navier-Stokes equations simplified for inviscid flow). However the current work intends to study detonation failure and re-initiation meaning that at some stages high velocity deflagration waves with significant contributions from diffusive terms must be simulated. To model this range of combustion regimes e.g. deflagrations and detonations properly, full Navier-Stokes equations must be solved. These equations represent the conservation of mass, momentum and energy:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho U_i)}{\partial x_i} = 0 \quad \text{Mass conservation equation (1)}$$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial(\rho(U_i + V_{k,i})Y_k)}{\partial x_i} + \nabla \cdot (D_i \nabla Y_k) = \omega_k \quad \text{Spices conservation equation (2)}$$

$$\frac{\partial(\rho U_i)}{\partial t} + \frac{\partial(\rho U_i U_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \mu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial U_j}{\partial x_j} \right) \quad \text{Momentum equation (3)}$$

$$\frac{\partial \rho h_0}{\partial t} + \frac{\partial(\rho h_0 U_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( k \frac{\partial T}{\partial x_j} \right) + \frac{\partial p}{\partial t} + \mu \left[ \frac{1}{2} \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right)^2 - \frac{2}{3} (\nabla \cdot \vec{U})^2 \right] + S \quad \text{Energy equation (4)}$$

In the above equations,  $D_i$  and  $S$  represent spices diffusion coefficient and the energy source term.

Taylor et al. [33] have shown that simplified reaction models can produce reasonable results which are in agreement with detailed chemical reaction models. One-step Arrhenius kinetics have previously been widely tested and used to simulate detonations [8, 11, 16, 31, 32] DDT [20, 21, 29, 30], detonation failure and re-initiation [8, 11, 16]. Previous studies show, although one-step Arrhenius kinetics are simplified, if carefully designed and tested, they can reproduce reasonably good predictions of these phenomenon.

Therefore in the present work the Arrhenius equation presented in Eq. 5 is used to predict the reaction rate.

$$\dot{\omega} = 6.85 \times 10^{12} \times \exp\left(-\frac{112971}{RT}\right) \quad (5)$$

The reaction parameters are derived using the method adopted by Wang et al [28].

### 2-1- Turbulence model

Over the past years it is observed that monotone fluid-dynamic algorithms produce results that are in good qualitative and quantitative agreement with experimental results [19]. Monotone fluid-dynamic algorithms do not use explicit turbulence models. Even in some studies which include significant turbulence in sub-grid scales, the monotone fluid-dynamic algorithms have been found to produce reasonably accurate predictions [19-22].

There are interesting physical reasons which explain good performance of these methods as described by Oran [19] and Grinstein et al. [22].

Apart from the physical justifications discussed in the literature, the numerical nature of the nonlinear monotone numerical methods exhibits some uniquely valuable properties which can be summarised

in: conservation, and positivity which can be called monotonicity. It means this numerical methods, through their local dissipation, can smoothly connect the large scale, energy carrying, resolved eddies to the smaller unresolved scales, and this is done by the natural dissipation effects which exists in these methods. While using these methods in LES one can trust that the larger scales are resolved with the minimal influence from the numerical errors from the smallest resolved scales [19].

For simulating detonation failure and re-initiation a wide range of time and space scales must be resolved to produce a reliable solution, however, the information about these scales and instabilities involved can be used to make the simulations efficient. As a compromise between computational requirement and accuracy, it is decided to base the present study on monotone fluid-dynamic techniques and Implicit Large Eddy Simulation (ILES), meaning that the sub-grid scale turbulence wouldn't be modelled explicitly; instead the numerical diffusion is used to compensate the sub-grid scale effects.

A solver is developed by the author and based on OpenFOAM CFD toolbox [23] to solve the governing equations, the similar solver was used previously by the author to simulate DDT and reasonable result were achieved [17, 18]. The finite volume method with the explicit Euler scheme for the time derivatives [25] is used. For shock capturing, the Van Leer flux limited method which is a total variation diminishing scheme and a monotone fluid-dynamic scheme is used [26].

### 3- Grid independency test

A set of consistent 2D numerical simulations in a small tube filled with obstacles are carried out to investigate the issue of grid independency and provide recommendation on the desirable grid resolution to achieve grid independent predictions.

The grid dependency tests were carried out for both detonation and deflagration waves but it was found that detonation simulations were less grids-sensitive and grid independency was achieved on a larger grid size compared to the deflagration waves. However since this study includes detonation failure, deflagration waves exist at some stages of the process, therefore it is decided to take “achieving grid independency at the deflagration stage” as the target.

Stoichiometric hydrogen-air mixture is used for the simulations. Six different grid resolution are studied, i.e. 100, 50, 25, 15, 10 and 5 microns.

The domain is a symmetrical tube of 3 cm long and 1 cm wide filled with 5 obstacles. Due to axisymmetric condition, only half of the domain is modelled and the top boundary in Figure 1 is a symmetric boundary. The right boundary is an opening boundary and the rest of the boundaries are set to be wall. A flame is initiated at the left end (closed end) of the domain by using hot burned region of products and the propagation of the flame, flame temperature, velocity and flow pattern are compared for three cases with exactly the same setting only with different grid sizes.



Figure 1 Numerical domain for grid independency studies

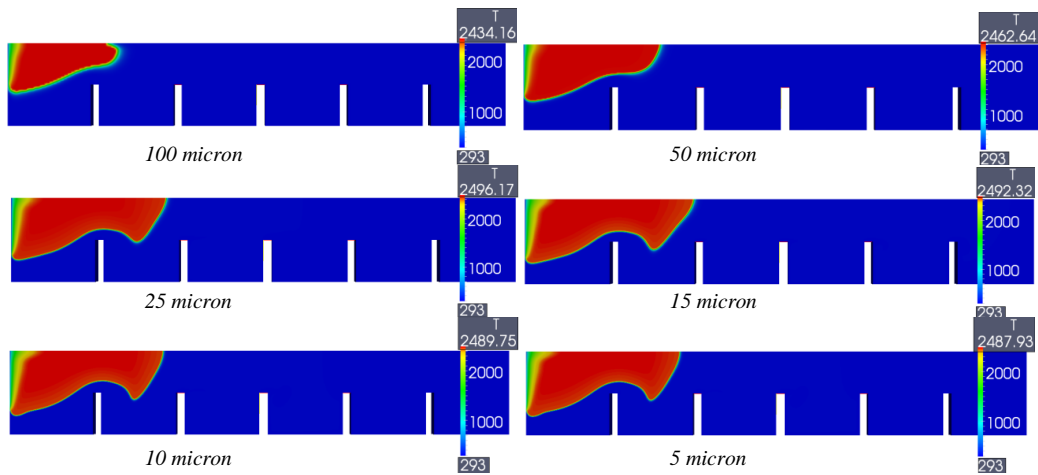


Figure 2 Grid independency studies, grid sizes of 100, 50, 25, 15, 10 and 5 microns

Figure 2 compares the flame propagation at exactly the same time, 2.5 ms after ignition, for different grid resolutions. Comparing the results for grid dependency in Figure 2 reveals that refining the grid size from 100 micron to 50 micron results in a notable change in the flame propagation pattern. Similarly, refining the grid size from 50 to 25 micron makes slight changes in the predicted flame behaviour but the changes are less significant compared to the previous step. Further refining of the grid to 15 micron also results in some slight changes in the shape and location of the flame front. The results for the 10 micron grid are very close to the ones obtained on the 15 micron grid. The location and shape of the flame is in good agreement and the predicted maximum flame temperature is 4 K lower for the 10 micron grid. Further refinement to 5 micron produces a result identical to 10 micron one, no difference can be observed and the predicted flame temperature is less than 1.8 K different, this is equivalent to 0.07% difference in predicted temperature which can be safely considered as zero. Figure 2 clearly shows that refining grid size from 10 to 5 micron does not make any difference in the predictions. The predicted flame and flow behaviour are identical for the grid resolutions smaller than 10 micron. Therefore it is concluded that it is safe to use grid resolutions smaller than 10 micron for the simulations without worrying about the grid dependency of the results.

A further question that might raise here is the issue of resolving the Kolmogorov length scale and extremely fine turbulence length scales.

This question is addressed while explaining the use of monotone fluid-dynamic scheme and ILES. It is reasonable to argue that as long as the energy containing eddies are resolved and the results are grid independent, there is no justification to use finer grid size which could also be computationally unaffordable even by using the biggest available supercomputers. For the case of detonation it is suggested in the literature to have about 20 grid points across the detonation half reaction length [1, 24]. For stoichiometric hydrogen-air mixture the detonation half reaction length is about 0.2 mm therefore the 10 micron grid size puts exactly 20 grid points across the detonation half reaction length as suggested in literature [1, 24].

In the present study, adaptive mesh refinement with one and two levels of refinement is also used for some simulation leading to the minimum grid size of 2.5 to 5 micron which is equivalent to 40 to 80 grid points across the half reaction length and is well above the required grid resolution. In a study on DDT, Oran et al. [20] used 39 grid points across the half reaction length of stoichiometric hydrogen-air mixture which is equivalent of 5.13 micron grid size.

The numerical approach which is developed and validated is then used to simulate detonation diffraction and re-initiation in bifurcated tubes.

## 4- Detonation propagation in a bifurcated tube

Wang et al. [1, 2] carried out a series of experiments to study detonation propagation in bifurcated tubes filled with hydrogen-oxygen mixtures diluted with argon gas. The experiments were performed in a 40mm×40mm square cross section detonation tube [1, 2]. The apparatus used by Wang et al. includes driver sections and very long initial tube for establishing a self-sustained detonation wave, however in the numerical work a very well established and self-sustained detonation wave can be initialised in a very short distance. Since the primary aim of this work is to study the detonation behaviour in the bifurcated section, only the final stage of their experiment is simulated. They used pressure sensors, soot foil and schlieren photography to record their results. They also carried out numerical simulations of detonation propagation using detailed chemistry in low pressures (8 kPa). They found that the detonation wave experiences strong disturbance, failure and re-ignition while passing through the bifurcated tube.

The 2-D simulations in the present work are carried out using parallel processing on 32 processors.

Figure 3 shows the numerical results for the detonation wave and the triple points before entering the bifurcated section. The experimental results of Radulescu [27], for detonation propagation in a straight tube with the same mixture condition, are included for qualitative comparison of the predicted multi-headed wave front before arriving at the bifurcated section. As the detonation wave moves onward (from left to right) the trajectories of the triple points sweep over the domain and leave the cellular pattern behind. This is recorded in simulations by tracing the maximum pressure points (triple points) and recording the history of their location over the domain as the simulations go on.

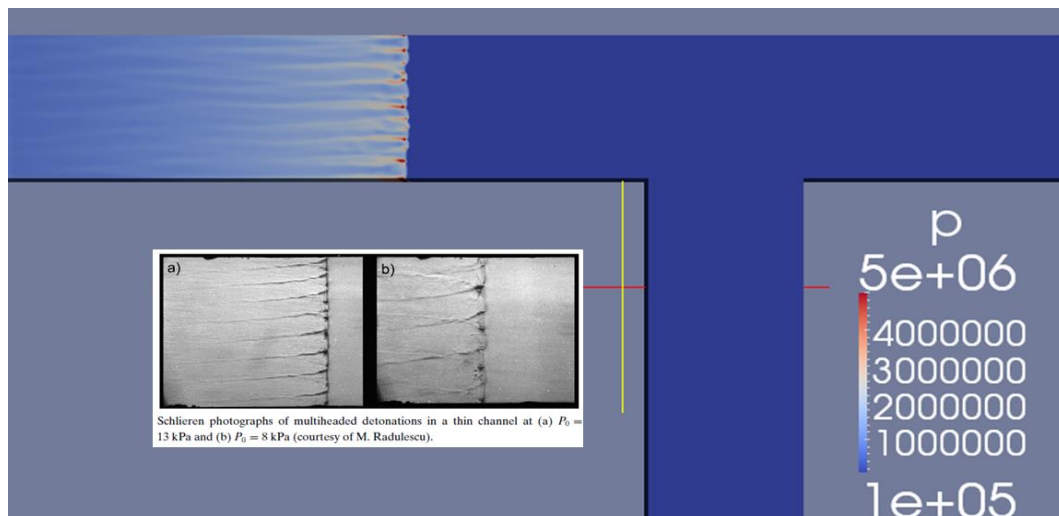


Figure 3 Pressure field for detonation propagation in bifurcated tube from present work (top image) schlieren photography of detonation front by Radulescu, (bottom left image) [27]

When the detonation wave reaches the bifurcated section the leading wave diffracts from the bifurcated corner. Consequently the leading shock wave and the combustion region decouple due to the detonation wave diffraction. The bottom part of the wave experiences the diffraction first, therefore the maximum flame shock decoupling happens at the areas around the diffraction corner, the top areas of the wave see the effect of the diffraction much later and are least affected by the bifurcated section. This process is illustrated in Figure 4, where the top 3 images show the experimental data by Wang et al. [1] and bottom images show the temperature field obtained in the present work. In Figure 4, red and yellow areas show the burned regions and the light green areas are the preheated regions due to shock passage. At the bifurcated section the shock-heated region is separated from the reacted region and moves ahead of the flame front, this represents the shock flame

decoupling and detonation failure due to wave diffraction. The disappearance of the detonation cellular pattern in bifurcated section, as shown in Figure 5, confirms the detonation failure at this region.

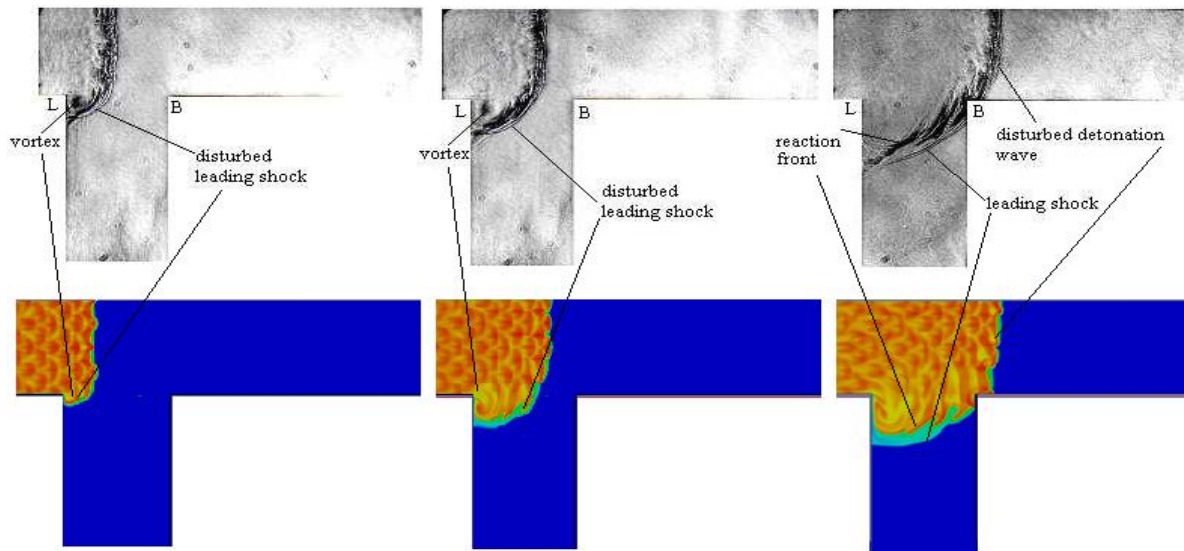


Figure 4 Detonation diffraction through bifurcated section (the current results compared with Wang et al. [1])

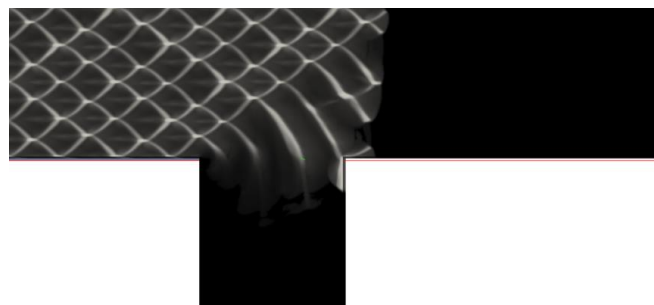


Figure 5 Detonation cellular pattern vanishing at the bifurcated section.

When the wave front reaches the opposite corner of the bifurcated section, the wave hits the tube wall and reflects back forming a high pressure region around the tube corner. The reflected shock from the right corner of the vertical tube causes rapid increase in pressure, temperature, chemical reaction and consequently leads to detonation re-initiation. This phenomenon is simulated in the present work and compared with the experimental and numerical results of Wang et al. in Figure 6. The detonation passing through the horizontal tube only experiences minor disturbance which are not strong enough to extinct the detonation but in the vertical tube the temporary detonation failure due to diffraction persists for some times until the re-initiated detonation grows again. The re-initiation is due to the collision of the reflected shock from the right wall and the decoupled shock, this collision results in strong shock heating and formation of a self-sustained detonation propagating in the rest of the tube.



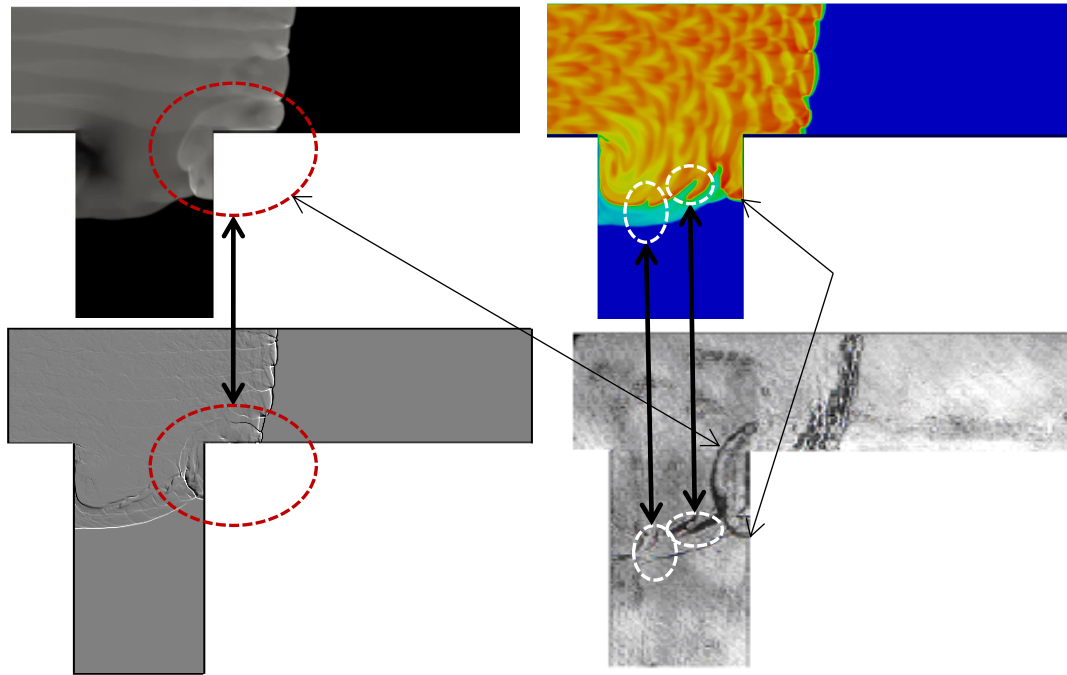


Figure 6 The present work results for the detonation propagation, diffraction, failure, reflection and detonation re-ignition in a bifurcated tube compared with Wang et al. experimental and numerical results [1].

Figure 7 shows the numerically recorded detonation cellular pattern in the present work compared with the soot-foil detonation cell recordings of Wang et al. [1]. It shows that the detonation wave moving in the horizontal direction never failed but experienced some strong disturbance which is recognisable through the irregularity of detonation cells at the areas around and after the vertical tube. However, in the vertical tube the cellular pattern has completely vanished and does not re-appear for some time which confirms the detonation failure in the vertical tube. When the reflected shock from the right corner catches up with the decoupled shock wave in the vertical tube, a self-sustained detonation is formed which propagates in the rest of the vertical tube. This is illustrated in Figure 8 which shows the experimental result of Wang et al. [1] (left image) compared with the present numerical results for the pressure (right image) which represents a good agreement in predictions.

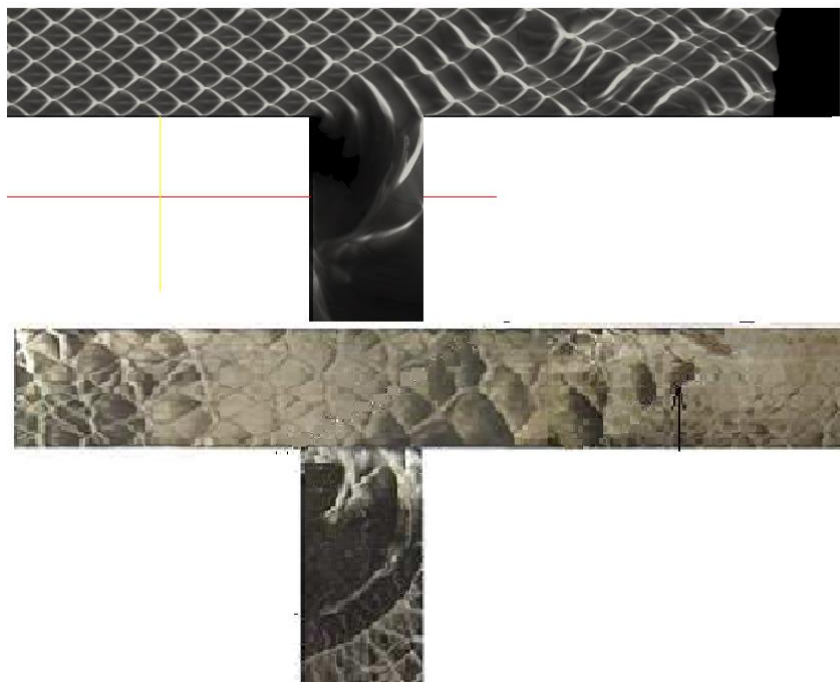


Figure 7 The numerically recorded detonation cellular pattern in the present work compared with the soot-foil detonation cell recordings of Wang et al. [1].

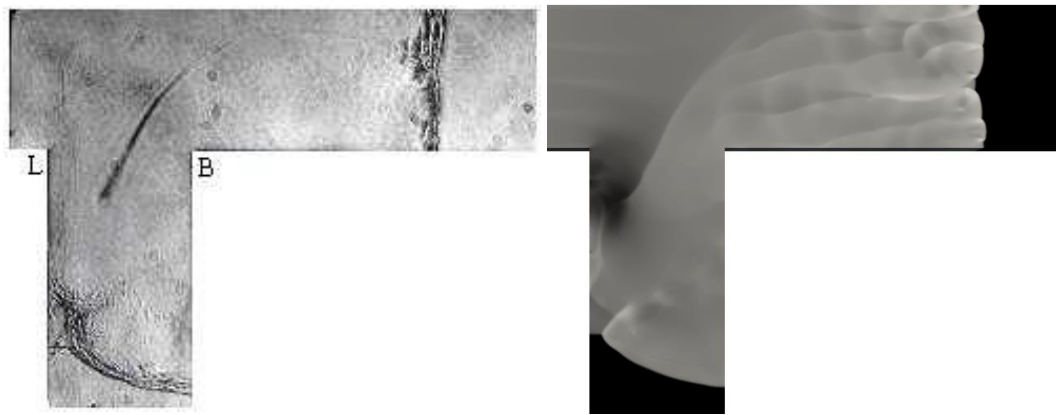


Figure 8 The experimental result of Wang et al. [1] (left image) compared to numerical results of present work for the pressure field (right image).

## 5- Conclusion

A newly developed ILES based solver is used to carry out numerical simulations of detonation propagation, diffraction, failure and re-initiation. The aim is to study the condition under which detonations may fail or re-initiate in bifurcated tubes. It is also intended to validate the new solver and to utilise it for simulating detonation structure and behaviour while passing through bifurcated channels.

. The grid independency studies are carried out and suggested that a grid size of below 10 micron is acceptable; however in some cases by incorporating adaptive mesh refinement a grid size of 2.5 micron was used which corresponds to 80 grid points across half reaction length. The numerical approach was then used to simulate detonation propagation inside bifurcated tubes. The numerical results for detonation right before and after entering to the bifurcated section are in good agreement with the experimental results of Wang et al. [1]. The results shows that the detonation sustains and propagates in the straight section of the tube with some temporary disturbances due to the diffraction at the bottom part, therefore the presence of the bifurcated section could not effectively interrupt the propagation of the detonation in the straight section and secondary measures such as detonation arresters are essential for quenching a detonation wave. However the numerical results show that the detonation wave in the bifurcated section re-initiates only because of the reflected shocks from the opposite bifurcated corner, meaning that some minor tweaking and use of shock absorbent materials within a small region at the bifurcated section could significantly reduce the chance of detonation re-initiation in that section. The presented results for the detonation cellular pattern are a good measure for identifying the regions where detonation is failed or re-initiated. The obtained results demonstrate the capability of this numerical approach in predicting the behaviour of real accidental explosions.

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