PHYSICS OF SPONTANEOUS IGNITION OF HIGH-PRESSURE HYDROGEN RELEASE AND TRANSITION TO JET FIRE

Bragin, M.V., Molkov, V.V.
HySAFER Centre, University of Ulster, Shore Road, Newtownabbey, BT37 0QB, UK,
mv.bragin@ulster.ac.uk

ABSTRACT

The main objective of this study is an insight into physical phenomena underlying spontaneous ignition of hydrogen at sudden release from high pressure storage and its transition into the sustained jet fire. This paper describes modelling and large eddy simulation (LES) of spontaneous ignition dynamics in a tube with a rupture disk separating high pressure hydrogen storage and the atmosphere. Numerical experiments carried out by a LES model have provided an insight into the physics of the spontaneous ignition phenomenon. It is demonstrated that a chemical reaction commences in a boundary layer within the tube, and propagates throughout the tube cross-section after that. Simulated by the LES model dynamics of flame formation outside the tube has reproduced experimental observation of combustion by high-speed photography, including vortex induced "flame separation". It is concluded that the model developed can be applied for hydrogen safety engineering, in particular for development of innovative pressure relief devices.

Keywords: spontaneous ignition, high-pressure release, hydrogen, large-eddy simulation, validation

1. INTRODUCTION

The issues of climate change and independence of energy supply stimulate search for alternative energy sources and energy carriers. Hydrogen is an ecologically clean alternative fuel, which can act as a carrier or storage for renewable sources of energy. Safety is the main barrier for the emerging hydrogen economy. Specific hazards associated with hydrogen as an energy carrier has to be first understood and then addressed by engineering design to provide safety of hydrogen technologies at least at the same level as for traditional fossil fuels.

While mass-related energy density of hydrogen is higher compared to other fuels, it is impractical to store hydrogen under normal temperature and pressure. Thus, practical applications, such as hydrogen powered vehicles, require hydrogen to be compressed or liquefied. The requirement of road users to be able to drive at least 450 km on a full tank and the necessity to keep the size of the tank comparable to that of conventional fuel cars bring the maximum pressure of onboard hydrogen storage systems to high values. The pressure of hydrogen in onboard storage reaches 700 bar already and the refuelling stations for such storage operate at even higher pressures. A leak from such high pressure storage can lead to formation of highly underexpanded jet that in turn implies potential fire and explosion hazards and associated risks.

It is well-known that sudden hydrogen release from high-pressure vessel into air can be spontaneously ignited without any apparent ignition sources present, such as spark, hot surface, fire, etc. Many attempts have been made to explain this phenomenon over the last decades starting from pioneering study of Wolanski and Wojcicki in 1972 of the so-called "diffusion ignition mechanism" [1]. Experimental data give critical conditions of the phenomenon, although they are quite scattered and depend on experimental setup. Unfortunately, they can not give a detailed insight into the dynamics of this physical process. For example, exact location of initial ignition spots and progression of chemical reaction within tubing downstream the rupture disk or valve can hardly be identified by experimental means at such high pressures.

Spontaneous ignition of high-pressure hydrogen release is one of the main unresolved problems of hydrogen safety, for which a little fundamental explanation exists. In this study up-to-date experimental data on spontaneous ignition of hydrogen during a high-pressure release and transition into a jet fire is analysed by means of LES technique to provide understanding of underlying physical phenomena. The study aims at validation of the LES model against published experimental data, and its future use for hydrogen safety engineering of emerging technologies and relevant infrastructure.

2. OVERVIEW OF EXPERIMENTAL OBSERVATIONS

Controlled spontaneous ignition of hydrogen releases has been studies recently in laboratory-scale experiments by Mogi et al. [2,3], Dryer et al. [4], Golub et al. [5, 6], and unexpected spontaneous ignition was reported previously in large-scale experiments by Reider et al. [7], Chaineaux et al. [8], Groethe et al. [9]. It is agreed opinion that the probability of hydrogen spontaneous ignition at a sudden release from high-pressure vessel due to equipment failure or activation of a pressure relief device (PRD) is high if mitigation measures are not undertaken. However, no references to spontaneous ignition problem or engineering design to avoid it can be found in codes and standards for piping, storage and use of high-pressure systems handling compressed hydrogen, even the most recent ones. A comprehensive review of postulated mechanisms for spontaneous ignition of high-pressure hydrogen leaks can be found in Astbury and Hawksworth [10]. The authors critically analyzed mechanisms that are most likely responsible for phenomenon of spontaneous ignition.

Earlier numerical studies by Liu et al. [11], Bazhenova et al. [12], and Xu et al. [13, 14] were focused on unconfined release from high-pressure storage directly into the atmosphere. While spontaneous ignition was demonstrated by numerical simulations, no experimental proof exists up to date.

Experimental confirmation of spontaneous ignition for releases from a high pressure storage to the atmosphere through a tube was obtained in “controlled laboratory environment” by Mogi et al. [2, 3], Golub et al. [5, 6], Dryer et al. [4], and Pinto et al. [15]. To facilitate spontaneous ignition various extension tubes and attachments were positioned downstream of a burst disk. Figure 1 combines critical conditions for spontaneous ignition obtained by different research groups. The data from Dryer et al. [4] is not shown in Figure 1, because of complicated internal geometry of the fittings used, which lowers the minimum storage pressure sufficient for spontaneous ignition down to 2.04 MPa. Although the data on spontaneous ignition of releases through practical fittings is very useful for hydrogen safety engineering, internal configurations of the fittings leaves a number of uncertainties for formulation of numerical experiments and prevents direct comparison with tests of other groups.

Experimental research on spontaneous ignition of hydrogen releases provides valuable data for the analysis of the phenomenon. Although experimental results published by different research groups agree in general trends, the critical conditions of spontaneous ignition vary substantially due to difference in test arrangements. Sensitivity of spontaneous ignition to different not yet fully understood factors poses a number of issues to be investigated.

Figure 1 shows an essential difference in critical conditions for spontaneous ignition obtained in some recent studies. It can be seen, for example, that for hydrogen storage pressure of 6 MPa in experiments by Pinto et al. [15], the tube length sufficient to provide spontaneous ignition is only 50 mm. At the same storage pressure and practically the same internal diameter, the channel length sufficient to provide spontaneous ignition in Golub et al. experiments [5, 6] is 110 mm, and in Mogi et al. tests [2, 3] the minimum length increases to 200 mm. How can this four times difference in channel length be explained?

First of all, Golub et al. [5, 6] measured the onset of spontaneous ignition by monitoring the shock propagation and location of radiation from chemical reaction inside the tube. Hence, critical conditions for spontaneous ignition in Golub et al. experiments (see Figure 1) represent the distance from the rupture disk to the location, where ignition was captured by the radiation gauge. Transition of ignition into jet fire could not be observed in their experiments due to the setup design.

Mogi et al. judged the occurrence of spontaneous ignition by observing the area near the tube exit. They showed that in some experiments spontaneous ignition did occur, but combustion was blown out by the flow. However, no critical conditions for such releases were reported. Nevertheless, this fact confirms that not all spontaneously ignited releases transit into sustained jet fires. This is a likely reason for the shift of the critical curve in Mogi et al. experiments compared to Golub et al. Another reason for the shift was suggested in [15]. Indeed, in experiments by Mogi et al. the internal surface of the tube between the diaphragm and exit to the atmosphere was washed away by the aqueous Na_2CO_3 solution (1%) in order to allow visualization of the flame via the flame reaction of sodium. This solution could have interfered with boundary layer flow and chemistry of hydrogen combustion and draw away some heat from the process thus the process happened later along the tube for the same initial pressure.

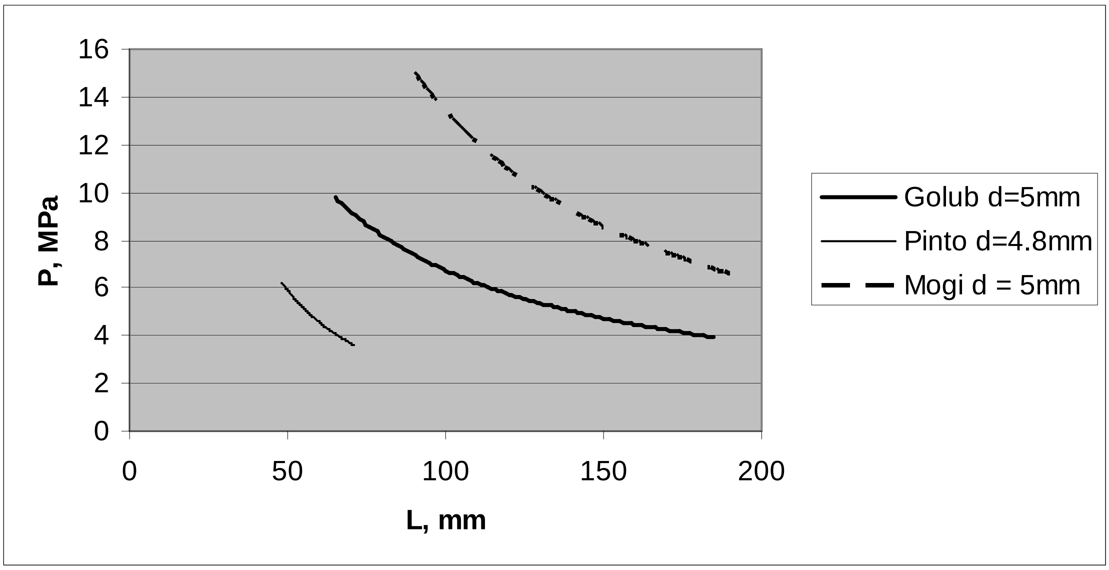

Figure 1. Experimental data for spontaneous ignition of hydrogen releases in tube attachments of 4.8 mm and 5 mm internal diameter.

The main difference in experimental procedure applied by Pinto et al. [15], on the other hand, is compression of hydrogen immediately before the burst disk rupture using a piston combined with the shock tube. Nitrogen gas was injected into the high pressure section of the shock tube upstream of the piston to push it towards hydrogen gas in order to generate high pressure of hydrogen to burst the disk. This compression obviously caused heating of hydrogen in high-pressure chamber and the release was not at the ambient temperature, but somewhat higher. But since, neither the temperature measurements in high-pressure chamber, nor information of the time during which hydrogen was compressed are available, it is difficult to estimate accurately the initial hydrogen temperature. It was shown by Bazhenova et al. [12] that the increase of initial hydrogen temperature stimulates spontaneous ignition to occur earlier and under lower initial pressures. This is the most likely reason for shorter tube required for spontaneous ignition in experiments by Pinto et al. for the chosen pressure compared to experiments by Golub et al. and Mogi et al.

Another important factor for spontaneous ignition could be the way the burst disk rupture happens. In experiments by Golub et al. burst disks were incised in the form of the cross to facilitate sharp “petal” opening, whereas in experiments by Mogi et al., Dryer et al., and possibly others a wider stochastic burst disk rupture pressure distribution was observed. Stochastic nature of an in-house made burst disk rupture produces variations in a structure and strength of the shock wave generated, hydrogen-air mixing [4], even at constant burst pressure, and obviously can affect the repeatability of experimental data. Very good repeatability of experiments is stated by Golub et al. [6] both in the measured pressure behind the generated shock wave, and the minimum initial pressure, which would provide spontaneous ignition at fixed tube length.

Figure 1 shows that the curves are almost parallel to each other, which confirms that for a given setup, the variation of pressure and length affect the spontaneous ignition in a similar way independent on experimental peculiarities. The difference in the minimum pressure required for spontaneous ignition from one experimental setup to another could be explained by different tube attachment/fitting arrangements in addition to factors discussed above. Pinto et al. compared results for smooth and screwed tubes. They found that the same initial pressure causing spontaneous ignition in smooth tube fails to cause ignition in case of screwed tube.

This observation, however, conflicts with the point of view of Dryer et al., who found that experiments with several tubes mated together produced ignition, where single tube (no mating unions) did not for the same initial pressure, the internal diameter and the overall tube length.

These observations underline that the interaction of developing boundary layer with roughness of walls in the tube section downstream of the burst disk can promote as well as delay spontaneous ignition. There is a need to have a “look inside” of the tubes to clarify physics of the spontaneous ignition in order to control it.

Considering the significant scattering of available experimental data and a number of mentioned uncertainties involved, e.g. internal geometry (Dryer et al.), initial hydrogen temperature (Pinto et al.), presence of wetting substance (Mogi et al.), it was decided to compare LES of spontaneous ignition in tubes against experimental data by Golub et al. [6].

3. SPONTANEOUS IGNITION IN TUBES

3.1 Experimental data

The experimental data used for the LES model validation are those published by Golub et al. [6]. The experimental setup includes a high-pressure chamber filled with hydrogen to required pressure, and a low-pressure chamber with air at atmospheric conditions connected by a tube of 5 mm internal diameter. The chambers were separated by a copper burst disk of 0.1-0.2 mm thickness, depending on designed rupture pressure, installed at entrance from the high-pressure chamber to the tube. When the pressure in the high-pressure chamber exceeds the critical value, the burst disk ruptures and shock wave propagates through the low-pressure chamber (tube). Critical pressure of hydrogen in high-pressure chamber varied in the range 2.0-13.2 MPa, while a length of the tube varied between 65 and 185 mm. In each experiment the bust disk completely opens in a controlled manner with its petals fully pressed to tube walls. A pair of a pressure transducer and a light sensor was installed at different distance from the diaphragm to detect shock wave propagation and radiation from spontaneous ignition. It should be noted, that in each of the experiments only one pair of sensors was present. The distance from the burst disk to sensors pair was changed from one test to another at the same conditions to identify the location of spontaneous ignition.

From a series of experiments the test with initial hydrogen pressure of 9.73 MPa and 65 mm extension tube was chosen in order to keep simulation time to minimum. From the experimental data it is known the spontaneous ignition occurred before 33 mm from the burst disk. Experimentally observed pressure behind the shock wave was in the range 2.69-3.40 MPa, and the delay between the shock wave front and the chemical reaction front (spontaneous ignition) at 33 mm from the burst disk was in the range 18-24 μs.

3.2 The LES Model

The LES technique is the most promising computational fluid dynamics (CFD) approach to solve scientific and engineering problems, including those related to hydrogen safety. Different LES models were developed previously and successfully applied to model deflagrations [17], detonations [18], non-reacting underexpanded jets [19], and jet fires [20]. The set of main governing equations can be found elsewhere [17]. In current work the RNG model was employed for subgrid-scale modelling of turbulence. The reaction rate that appears in species transport equation was modelled using eddy-dissipation-concept model by Magnussen [21]. It incorporates detailed Arrhenius chemical kinetics in turbulent flames. In this study the detailed 21-step chemical reaction mechanism of hydrogen combustion in air employing 37 elementary reactions by Gutheil et al. is applied [22]. Where the mesh is too coarse to resolve the laminar sub-layer, the near-wall treatment of the flow is carried acording to the law-of-the-wall, where κ – von Karman constant and E = 9.793.

$$\frac{\bar{u}}{u_\tau} = \frac{1}{\kappa} \ln E\left(\frac{\rho u_\tau y}{\mu}\right)$$

3.3 Geometry, mesh and boundary conditions of simulation domain

The geometry of high-pressure chamber in experiments [6] was simplified and substituted with a single cylinder in order to reduce overall number of cells in a computational domain. The simulated high-pressure chamber was 140 mm long and 20 mm diameter cylinder, the simulated low-pressure chamber was 145 mm long and 5 mm diameter cylinder.

The grid was created using GAMBIT tool of commercial CFD package FLUENT. A slice of the meshed computational domain along the axis is presented in Figure 2. In order to exclude the effect of mesh irregularities on combustion in reacting flow, the low-pressure chamber was meshed with an unstructured hexahedral grid with uniform CV size of about 200 μm both along the tube and a similar characteristic CV size in the cross-section (see Figure 3). The high-pressure chamber was meshed with the smallest CV size of about 250 μm clustered near the entrance to the simulated tube/low-pressure chamber and rapidly increasing away from it reaching the maximum cell width of 10 mm. The total number of control volumes was equal to 430,976.

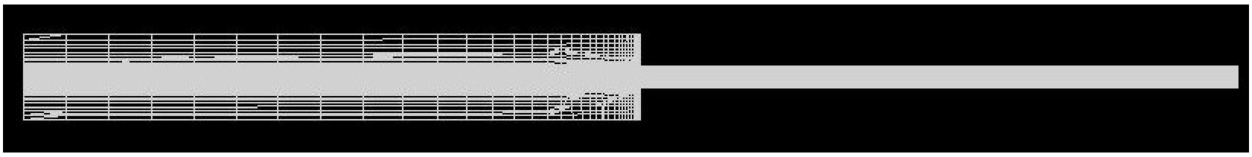

Figure 2. The meshed computational domain of high- and low-pressure chambers.

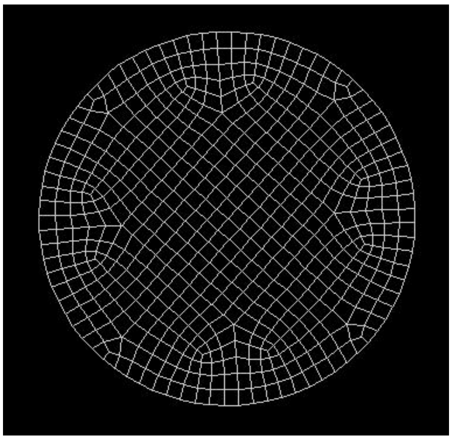

Figure 3. The cross-section of the low-pressure chamber.

Non-slip impermeable adiabatic boundary conditions were used on all of the walls. The shock tube was modelled as "closed" to exclude potential effects of numerical boundary conditions on the process. This assumption is applicable as the low-pressure chamber is long enough to simulate the process of ignition without getting the reflection of the shock wave from the closed end.

Initial conditions for high-pressure chamber were P_0 = 96 atm, T_0 = 300 K and the mole fraction of hydrogen equal to 1. Low pressure chamber was filled with air (0.23 mass fraction of O_2 and 0.77 of N_2) at P_0 = 1 atm and T_0 = 300 K. Non-physical values were encountered due to numerical instabilities if the imaginary rupture disk, i.e. the boundary separating gases, was placed exactly at the border between high- and low-pressure chambers. Therefore, in order to avoid instabilities during simulation of strong discontinuity in pressure accompanied by strong discontinuity in area, the simulated "burst disk" was moved one tube diameter (5 mm) downstream, i.e. high-pressure hydrogen was also initially present in the first 5mm of the tube. Imaginary rupture disk was removed instantly and shock wave was allowed to propagate.

The problem was simulated using general-purpose CFD package FLUENT 6.3.26, which realises control-volume based finite-difference method. The solver used explicit linearisation of the governing equations with explicit method for solution of linear equation set A third order MUSCL scheme with AUSM flux splitting was applied for flow discretisation. The four step Runge-Kutta algorithm was employed for advancement of solution in time. The time step was determined from Courant-Friedrichs-Lewy condition, where the CFL number was equal to 0.5 to ensure stability.

3.4 Results of numerical experiments

The dynamics of spontaneous ignition during the first 56 μs since the burst disk rupture is presented in Figure 4 for temperature (left) and hydrogen mole fraction (right). At the initial moment *t*=0 the "burst disk" boundary separating high-pressure hydrogen and atmospheric air, located at *x*=0, is instantaneously removed and a shock wave propagates into air heating it up due to compression. The shock wave is followed by a contact surface separating cold hydrogen and heated air. The thickness of heated air layer between the shock front and the contact surface increases with time. The shock wave propagates along the tube as a plane wave without any curvature. The shape of the contact surface changes from plane to slightly convex due to non-slip conditions at the tube walls. The highest temperature is observed in the boundary layer due to velocity decrease. Owing to diffusion of gases and heat through the contact surface, the spontaneous ignition occurs when critical conditions are reached. The chemical reaction propagates in the direction from the wall to the tube axis as the contact surface propagates downstream. After 45 μs from the start of the process at distance 20 mm from the "burst disk" location, the combustion occupies the whole cross-section area of the tube. Initiation of the chemical reactions in the boundary layer accelerates propagation of the reaction front along the wall compared to the axial part leading to change of the convex shape of the contact surface in the most of the tube cross-section to a slightly concave form.

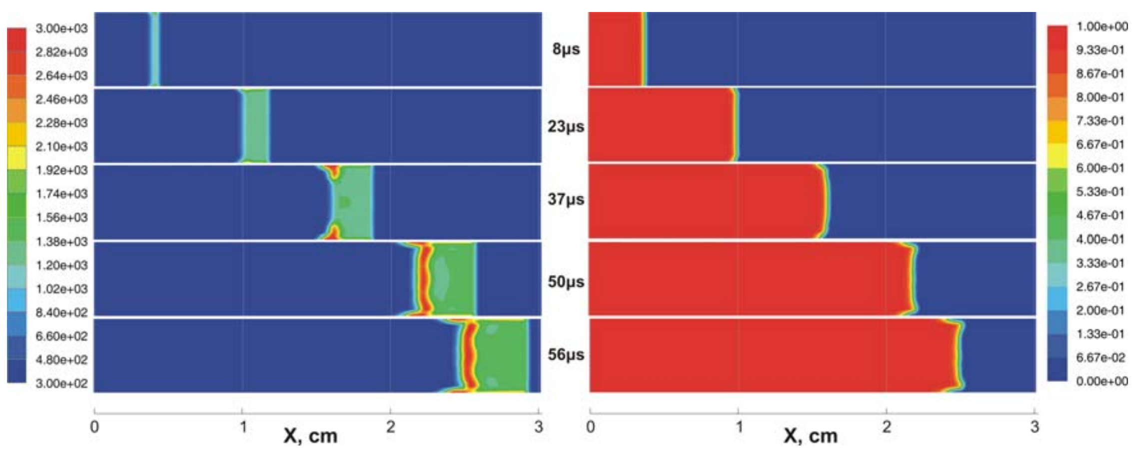

Figure 4. Dynamics of spontaneous ignition: temperature (left) and hydrogen mole fraction (right).

In numerical simulations the reaction front is established throughout the pipe cross-section at distance 20 mm from the burst disk at time 45 μs after the instantaneous rupture. In the experiment by Golub et al. [6] the light sensor was located 33 mm from the burst disk. However, the time of the shock arrival was not reported. In LES the leading shock reached the light sensor location of 33 mm at 58 μs, and the reaction front followed the shock with a delay 7-10 μs. In the experiment the sensor started to register light 18-24 μs after the shock arrival. The deviation in delay of the flame front arrival after the shock could be partially explained by the delayed opening of real diaphragm, which was not accounted for in the simulation. Additionally, the real burst-disk rupture facilitates turbulent mixing downstream. The process of diaphragm opening should be simulated in future studies to improve the predicting capability of the model reported in this study. Another factor, which could explain the deviation, is the absence of heat transfer from the reaction zone to walls in the model. The effect of CV size on the simulation results should be investigated further as well, since a quite course grid with 200 μm mesh was applied in this study.

4. TRANSITION OF SPONTANEOUS IGNITION INTO A JET FIRE

4.1 Experimental data and numerical details

Sequence of photographs was obtained by Mogi et al [2, 3] using high-speed digital colour video camera. Initial pressure of hydrogen in chosen for numerical simulations experiment was 14.5 MPa and the tube length was 185mm. The tube wall thickness was 4 mm. This sequence of snapshots shows combustion of hydrogen-air mixture spontaneously ignited inside of the tube and then emerging outside and stabilizing in the vicinity of the tube exit. The authors [2, 3] observed that, once the emerged from the tube flame is stabilized near the nozzle, it acts as a pilot flame and ignites/sustains the jet fire later on. Therefore, the numerical observation of flame "stabilization" near the tube exit may be taken as an indication of transition from the spontaneous ignition to the sustained jet fire.

In this series of simulations we have shifted the focus from the resolution of spontaneous ignition towards the transition from ignition within the tube to combustion outside the tube in the atmosphere. Therefore, it was decided to sacrifice resolution in the channel further in order to reduce CPU time to practically reasonable. The characteristic size of control volumes was twice rougher than in simulations described in section 3 and was on the order of 400 μm. The larger cell size attached to the wall makes the boundary layer "wider" and thus, due to reducing the heat dissipation from the ignition spot, facilitates faster ignition.

The area in the immediate vicinity of the tube exit in the atmosphere was coarsely meshed initially with cells clustered around the anticipated underexpanded jet shock structure. Immediately before the leading shock wave and spontaneously ignited mixture reach the end of the tube, the grid outside was adapted for the first time. As the process evolved and the jet increased in size, second adaptation was performed at 220 μs from the burst disk rupture and the corresponding mesh is shown in Figure 5. The number of control volumes increased due to the grid refinement from 261,640 to 478,528 during the simulation.

Since temperatures of hydrogen and surrounding air were not reported in the experimental paper, they were taken as 300 K in simulations. Atmospheric pressure of hydrogen was taken as 101,325 Pa. Air was taken to consist of 23% of oxygen and 77% nitrogen by volume. At time t = 0 the imaginary rupture disk was instantaneously removed to commence the discontinuity decay. Non-slip impermeable adiabatic boundary conditions were used on all walls. Non-reflecting "far field" boundary conditions were set in the downstream and radial directions.

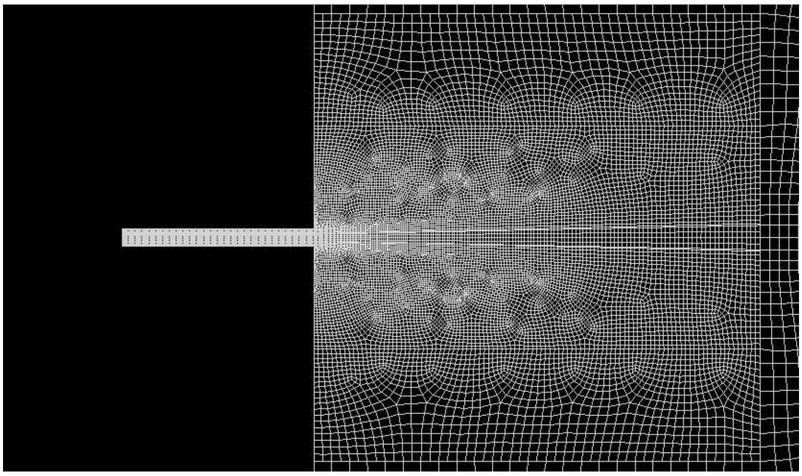

Figure 5. The grid with two levels of refinement in the vicinity of the tube exit.

4.2 Results of numerical experiment

Dynamics of temperature, velocity, hydrogen and hydroxyl mole fractions are shown in Figure 6. The field of view in all numerical snapshots is kept constant, where the channel length shown corresponds to 66.5 mm, and the outside area has 148 mm long and 130 mm wide. All snapshots represent 2D cross-section along the tube axis. The maximum and minimum values in each series were fixed in order to lock the relation between colours and corresponding parameters in all frames. Minimum and maximum values in each set of frames were fixed to 0–2400 K for temperature, 0–3000 m/s for velocity, 0–1 for hydrogen mole fraction, and 0.001–0.01 for hydroxyl mole fraction. If values fall out of these limits, they are coloured according to the colour of limits – red for values above the upper limit and blue for values below the lower limit.

The dynamics of spontaneous ignition in the tube was similar to the one described in section 3 and hence is not shown here. The resulting flame front assumes “>”-shape and its tip gets behind the shock wave by about 7 mm by the end of the tube. The flame front width is about 3 mm near the tube axis, while near the wall it extends as long as 35 mm. Combustion is more pronounced near walls, having wider regions with high temperature. The first frame in time series corresponds to the time 131.5 μs from the burst disk rupture. For ease of interpretation of the transition process the reference time was set to 0 μs (see Figure 6).

As the shock wave emerges from the tube exit it diffracts and transforms from a plane to a hemispherical form. The shock propagates outwards and quickly loses the strength. It is followed by the flame front pushed by the expanding hydrogen. Once hydrogen leaves the tube, hemispherical expansion starts and the flame front is forced to follow expansion. The formation of Mach disk commences shortly after (28 μs frame) and the expansion of hydrogen is held back increasing the separation distance between the leading shock and the contact surface. Sudden deceleration of hydrogen stimulates turbulent mixing.

In parallel to the Mach disk formation, the outer annular flow at the disk’s periphery forms. Owing to viscous forces this supersonic annular flow generates a big vortex, which turns the flow back towards the tube exit. The formation of vortex breaks the combusting gas (48 μs) into two parts – downstream and upstream (see comparison with experimental snapshots below).

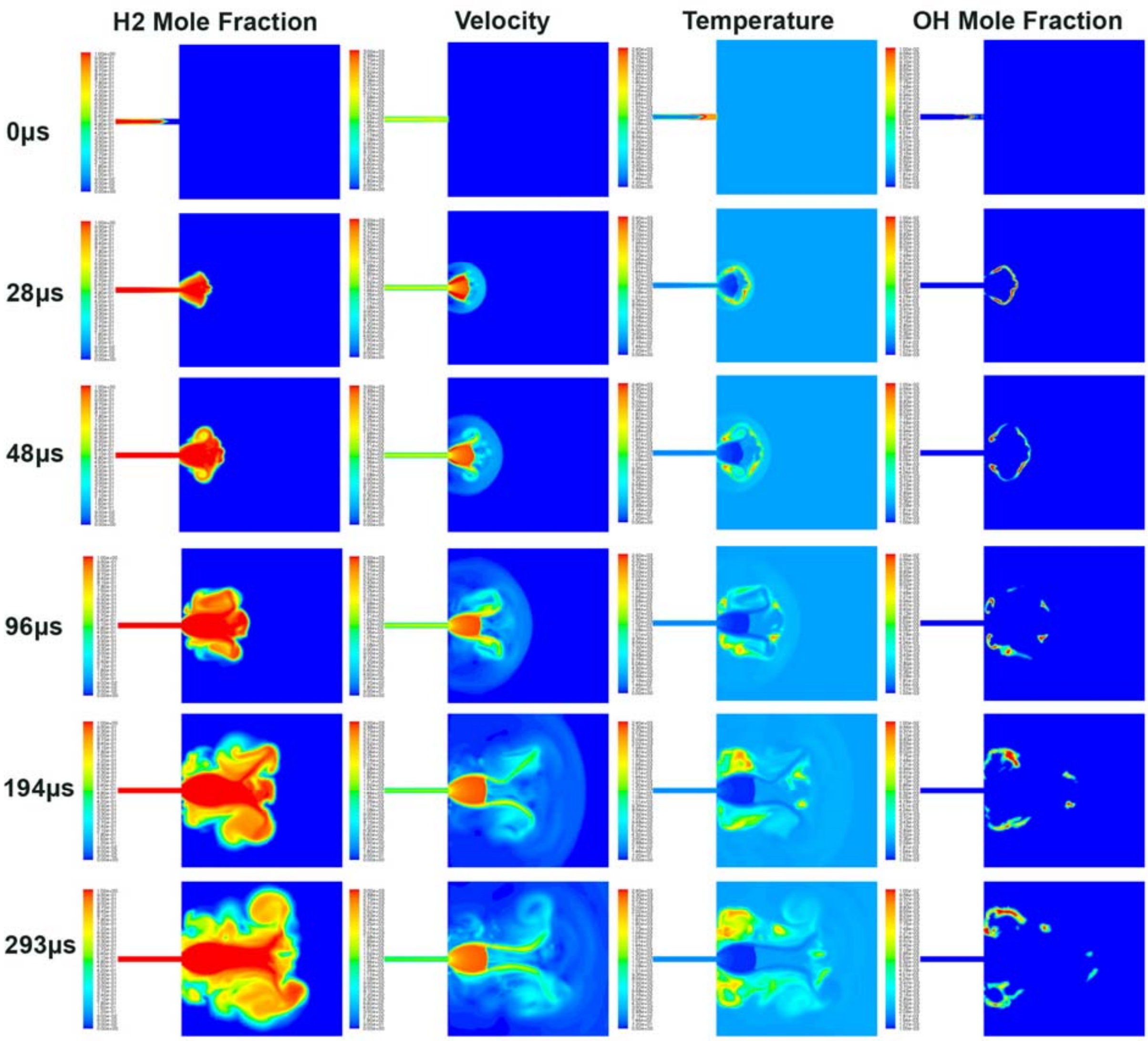

Figure 6. Dynamics of the velocity, temperature and mole fractions of hydrogen and hydroxyl in 2D slice along the tube axis.

Meanwhile, the shock barrel is not yet stabilized. Upstream combustion region is pushed back by the vortex tip (96 μs), while downstream combustion region in the vicinity of jet axis is forced out. As the vortex straightens, the supply of hydrogen to the recirculation area dies out and reduction of flow velocity allows necessary induction time for intensification of combustion. It can be seen, that combustion affects the gas dynamic evolution of the jet and results in non-axisymmetrical to some extent flow beyond the Mach disk (194 μs).

Shock barrel is stabilized around 200 μs. The annular vortex increases in size widening distance from the axis where hydrogen is present. By the time of the last frame in Figure 6 (293 μs) the downstream combustion is fully ceased, while the upstream combustion in the recirculation zone is sustained.

4.3 Comparison between the LES model predictions and experimental data

Unlike 2D slices of reacting flow parameters obtained by means of CFD, experimental snapshots give a side-view on the 3D combusting jet. Therefore, it is impossible to see the jet to the level of details the numerical experiments can produce, including profiles of all the parameters of interest.

Experimental data on flame size [3] was critically analysed. The uncertainty in published snapshots lies in the scale of frames presented [3]. The scale given should be reconsidered, since the inner diameter of the tube is known to be 5 mm, but according to the scale given on photographs an outer diameter of the tube is equal to 4.5 mm. From a private communication with Dr Mogi, it was clarified that the tube wall width was 4 mm. Thus, outer diameter of the tube shown in photographs was equal to 13 mm. Therefore, field of view in experimental photographs corresponds to 104 x 76.4 mm with tube bulging out by 14.6 mm.

After bringing the field of view to validated dimensions, another question should be answered – which simulation parameter should be taken to represent closely a visible flame registered in the experiment? While some works base their estimation of the visible flame length on temperature, for example in [20], in this study a flame is identified by the mole fraction of hydroxyl. Here we identify visible flame by the hydroxyl mole fraction higher than 0.001.

Comparison between experimental and simulated snapshots is shown in Figure 7. Numerical flame propagation can be referenced to experimental dimensions by vertical lines, which are positioned 10 mm apart. It can be seen that as the ignited jet exits the tube (0 μs) it develops into a cocoon of combusting mixture (50 μs). Shortly after this the annular vortex, which cannot be seen here (see Figure 6) causes the cocoon to break into upstream and downstream combusting regions (100 μs). As the downstream combustion region is blown away, the upstream region is stabilized near the tube exit (200 μs). The size of this region, however, is bigger in simulations. This can be explained by the difference in air entrainment in experiment and simulations. Indeed, simulations of hydrogen release were carried out not for the tube with 5 mm internal diameter and 4 mm wall thickness, but for the channel of 5 mm in a wall with "infinite" dimension. At earlier moments, the jet formation and combustion are dominated by the annular vortex. However, as the vortex propagates further downstream, its effect diminishes and entrainment rate starts to be dominant in defining the combustion of the stabilized flame, in particular its size.

Another reason for deviation in size of stabilised flame could be the wetting of the inside surface of the tube between the burst disk and the exit to the atmosphere by the aqueous Na_2CO_3 solution (1%) in order to allow visualization of the flame. This solution could have interfered with heat transfer and chemistry of hydrogen combustion and decreases the visible flame size. Additional simulations should be performed with reproduction of the real experimental geometry.

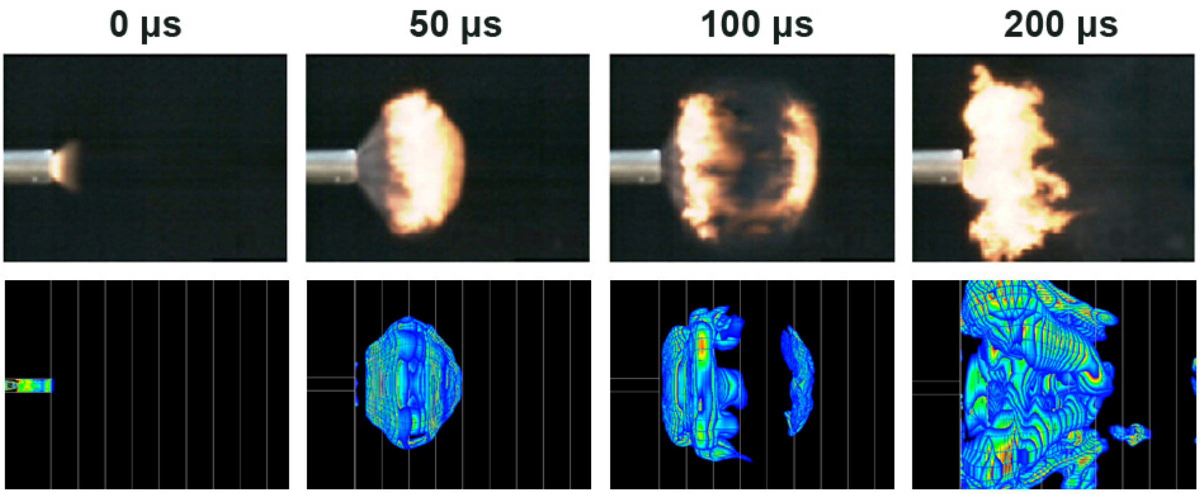

Figure 7. Comparison of high-speed video camera experimental photographs obtained by Mogi et al. [3] with numerical LES snapshots.

CONCLUSIONS

The LES model for numerical simulation of spontaneous ignition of high-pressure hydrogen release into downstream attachment filled with air at atmospheric conditions and dynamics of combustion outside the attachment is developed. The mechanism of spontaneous ignition in tubes downstream of a pressure relief device, e.g. the rupture disk, is investigated. Numerical experiments have demonstrated that ignition is initiated in a wall boundary layer. Results of simulations are in agreement with experimental data on the distance for spontaneous ignition from the rupture disk.

The mechanism of transition from spontaneous ignition inside of the tube into sustained jet fire is studied within computational limitations. It is assumed, following the experimental observations, that the transition to the sustained jet flame is largely dependent on the initial jet formation stage, where developing annular vortex pushes combusting mixture upstream into the recirculation zone. Once the flame is stabilised near the tube exit, it acts as a pilot flame and ignites jet fire later on.

The validated against experimental data LES model can be used for engineering design of innovative pressure relief devices.

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