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ABSTRACT

Sudden releases of pressurised hydrogen may spontaneously ignite by the so-called "diffusion ignition" mechanism. Experimental and numerical studies have been performed on spontaneous ignition for compressed hydrogen at ambient temperature. There is a lack of knowledge of the phenomenon for compressed hydrogen stored at cryogenic temperatures. This study aims to close this knowledge gap by using a validated computational fluid dynamics (CFD) model to assess the effect of temperature decrease from ambient 300 K to cryogenic 80 K on the ignition dynamics. Previously used in our studies T-shaped channel system is selected as a configuration for the numerical analysis of cryogenic hydrogen ignition. The cryo-compressed hydrogen is initially separated from the air in the T-shaped channel system by an inertial burst disk (diaphragm). Simulations were carried out to determine the pressure limit leading to ignition in the configuration under investigation. It is found that the pressure limit for the cryo-compressed hydrogen at 80 K is 9.4 MPa, which is more than 3 times larger than for spontaneous ignition in the same setup for ambient temperature hydrogen (2.9 MPa).

KEYWORDS: "Diffusion ignition" mechanism, spontaneous ignition, cryo-compressed hydrogen, computational fluid dynamics.

NOMENCLATURE

b thickness of the diaphragm (m)
d diameter of the diaphragm (m)
k constant (0.92)
P diaphragm burst pressure (Pa)
t diaphragm opening time (s)

Greek

ρ density of the diaphragm material (kg/m^3)

INTRODUCTION

A sudden hydrogen release from a high-pressure vessel or equipment through the piping with air can be spontaneously ignited at comparatively low pressures of about 3 MPa (hydrogen at ambient temperature). This mechanism was postulated in 1973 by Wolanski and Wojcicki [1], following their observations on ignition occurrence when high-pressure hydrogen was admitted to a shock tube filled with air or oxygen. The authors suggested that ignition was caused by the high-temperature gradient at the contact surface where the oxygen heated by the primary shock wave, mixed and reacted with hydrogen due to diffusion. Experiments conducted by Bazhenova et al. [2] showed that an increase of the fuel initial temperature may cause an earlier ignition or ignition at lower pressures. Similar conclusions were reached by Golub et al. [3]. The authors investigated experimentally the effect of hydrogen pressure, temperature, and shock tube characteristics on the occurrence of spontaneous ignition. It was found that a shock tube diameter should be larger than 3 mm to obtain the ignition at hydrogen pressure below 40 MPa at ambient temperature. The authors observed a strong dependence of spontaneous ignition parameters on the initial temperature. For hydrogen pressure equal to 20 MPa, an increase of temperature from 300 K to 400 K caused a decrease in minimum shock tube diameter leading to ignition from 3 mm to 2 mm. Further experiments were conducted by Golub et al. in 2008 [4] to find the limit pressure for ignition in tubes of different lengths and cross-sectional shapes. The test on a tube with 5 mm diameter and 65 mm extension was selected by Bragin and Molkov [5] for

CFD modelling using a Large Eddy Simulation (LES) approach with Eddy Dissipation Concept (EDC) combustion sub-model with chemical kinetics. The minimum storage pressure leading to spontaneous ignition was found to be 2.04 MPa. In the following work [6], Bragin et al. simulated the experiments conducted by Golub et al. [7] on the sudden release of hydrogen from a high-pressure system into a T-shaped channel following the inertial flat burst disk rupture. Numerical simulations showed that the dynamics of the flat burst disk rupture process affects the potential for ignition and follow-up combustion, as a consequence of the difference between mixing processes of air with hydrogen for real inertial burst disk opening and idealistic instantaneous opening. Gong et al. [8] found that the shock pressure in a tube is a function of not only the storage to ambient pressures ratio, but depends also on the ratio of the characteristic shock propagation time to the burst disk (diaphragm) opening time. Overall, the mentioned experimental and numerical studies demonstrate that the pressure limit of hydrogen storage leading to spontaneous ignition depends on hydrogen temperature, the geometry of the system, the opening time of a rupture disk, etc. This work is not intended to give a comprehensive overview of spontaneous ignition studies but focuses on the effect of initial hydrogen temperature on the pressure limit for the ignition.

Hydrogen may be stored in cryo-compressed conditions, i.e. storage temperature below 120 K as generally considered for cryogenics [9] and pressures up to 35 MPa [10]. Cryo-compressed hydrogen (CcH2) storage at pressures below 20 MPa is considered to provide a better gain in gravimetric and volumetric capacities against the energy required for the compression and cooling down of the hydrogen gas [11]. Applications investigated in [12]–[14] involved insulated pressure vessels refuelled with cryogenic hydrogen at 80 K pressurised up to 30 MPa. Thus, the temperature of 80 K will be considered in the present study as representative for cryogenic releases. Following the trends observed in experimental studies on spontaneous ignition for hydrogen at temperatures higher than ambient [3], it would be expected that a decrease of temperature of compressed hydrogen to cryogenic values would require a higher pressure to obtain spontaneous ignition. However, the impact of increased density of cryogenic releases on the shock ignition process and the trade-off against the increased difficulty of igniting colder gas is unclear. A better understanding of this phenomenon is crucial for hydrogen safety engineering and the inherently safer deployment of CcH2 systems and infrastructure. To the best of the authors' knowledge, neither experimental nor numerical studies are available on the spontaneous ignition of CcH2. The present study aims to close this knowledge gap for the first time by using CFD modelling to assess the effect of temperature decrease from ambient to cryogenic 80 K on the pressure limit for spontaneous ignition and combustion dynamics. This numerical study is carried out for hydrogen releases in a T-shaped channel filled with air following an inertial flat burst disk rupture.

PROBLEM FORMULATION AND NUMERICAL DETAILS

Problem formulation

The case selected for the numerical analysis is the sudden release of hydrogen from a high-pressure system into a T-shaped channel following the inertial flat burst disk rupture. The geometry of the system is shown in Fig. 1a. It reproduces the experimental setup [7] and follows the previous numerical study at ambient temperature [6]. The high-pressure system is composed of a 210 mm long tube with 16 mm internal diameter (ID), connected to a 280 mm long tube with 10 mm ID. The flat burst disk is located at the end of the high-pressure tube and once ruptured releases hydrogen into the mock-up pressure relief device (PRD) open to the atmosphere. The PRD consists of an axial channel with a length of 48 mm and a diameter of 6.5 mm. The PRD has a flat end where two radial channels are located. These two radial channels vent hydrogen into the open atmosphere and have 6.25 mm length and 4 mm ID. A description of this hydrogen release system can be found in [6].

Simulations are performed for both ambient and cryogenic temperature to find the pressure limit leading to ignition. Table 1 shows the matrix of simulations. The resulting pressure limits for ambient temperature hydrogen are compared then to experimental and numerical tests performed in [7] and

[6] respectively. Light sensors were used in the experiments [7] to register the occurrence of spontaneous ignition. The authors [6] reported that no ignition was recorded for pressure 1.2 MPa, whereas the light was registered for tests at pressures in the range 2.43-2.90 MPa.

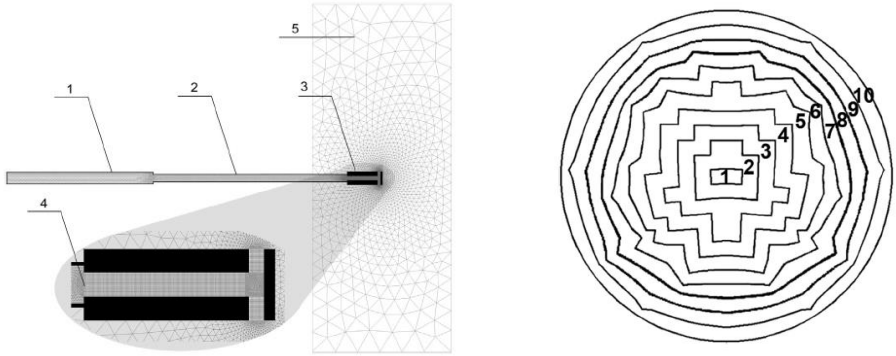
Table 1. Storage pressure and temperature for selected scenarios.

Number of simulations	Storage temperature, K	Storage pressure, MPa
6	300	1.35, 1.65, 2.43, 2.60, 2.80, 2.90
5	80	5.00, 7.50, 8.75, 9.40, 10.00

CFD model and numerical details

The CFD model employed in the present study is based on the Large Eddy Simulation (LES) approach validated against tests on spontaneous ignition in different release geometries (see [4], [6]). The choice of the CFD sub-models was aimed to better represent the physical phenomenon independently from the specific features of the test geometry. In the present study, the approach was updated by using a different combustion sub-model. Simulations were carried out using ANSYS Fluent v.17.2 as a computational platform. The CFD model solved the conservation equations for mass, momentum, energy and species. The renormalization group (RNG) theory was used to model sub-grid scale turbulence, given its capability to reproduce turbulent, transitional and laminar flows [15]. The finite rate chemistry (FRC) model was used for combustion, which choice was justified by the small control volume size throughout the numerical grid. Hydrogen combustion in the air was simulated by a chemical kinetics mechanism that includes 37 elementary reactions and 18 species [16].

Figure 1a shows details of the numerical domain. A control volume (CV) size equal to 250 μm was employed at the burst bisk area whereas CV size 400 μm was maintained along the axial channel. An hexahedral mesh was employed in the axial channel, as in this portion of the TPRD it could be expected a reasonable alignment of the flow with the structured mesh. This choice was deemed to limit an eventual "numerical diffusion". CV size of 200 μm was used in the zone of intersection between the axial and radial channels. A tetrahedral mesh with smaller CV size was implemented at the intersection, as deemed to better represent the expected more complex structure of the flow and the shock in comparison to the axial channel. CV size was gradually increased to 10 mm in the far-field from the PRD. The total number of CVs was 417,685.



(a) (b)

Fig. 1. a) Central cross-section of the computational domain and numerical grid: 1 and 2 - high-pressure tubes, 3 - PRD, 4 - burst disk, 5 - external domain [6]; b) Sections of the burst disk used in the simulations to mimic its rupture process (opening in time): 1-10 are sections of the burst disk that open in series [6].

The external domain limit was modelled as non-reflecting pressure far-field boundary. Tube walls were modelled as non-slip isothermal surfaces for the case with ambient temperature hydrogen, whereas they were modelled as coupled walls made of steel for the case with cryogenic hydrogen. The specific heat at constant pressure for hydrogen at cryogenic temperatures was defined according to the NIST database [17], as a polynomial function of temperature: $c_{p,H2} = 6.97 \cdot 10^{-6}T^4 - 5.23 \cdot 10^{-3}T^3 + 1.31T^2 - 107T + 13300$. The initial air composition in the PRD (right from the burst disk) was composed of oxygen and nitrogen with mass fractions 0.23 and 0.77 respectively. At the initial moment, the ambient temperature and pressure were equal to 300 K and 101325 Pa respectively. The high-pressure tube was modelled as filled with hydrogen (mass fraction 1.0), and pressure and temperature as in [6]. An explicit method was used to solve the governing equations and a four-step Runge-Kutta algorithm was employed for the time advancement of simulations. The time step was determined from an imposed Courant Friedrichs Lewy (CFL) number of 0.3. A second-order upwind scheme with Advection Upstream Splitting Method (AUSM) was applied for flow discretisation. In the cases involving cryogenic hydrogen, it is considered that the air mixing with the expanding cold hydrogen within the TPRD will be highly heated by the shock wave at the considered pressures. Thus, the eventuality of the air components phase change was not taken into account in the present model.

Bragin et al. [6] highlighted the importance of modelling the inertial opening of the burst disk as it was found to generate more intense mixing between hydrogen and air and affect the temperature of the heated by shock air. The authors [6] simulated the non-instantaneous diaphragm opening by subdividing the flat burst disk area into 10 sections (see Fig. 1b) and by opening them in sequence. The same technique was employed in this study. The opening time, *t*, was calculated as [18]:

$$t = k\left(\frac{\rho b d}{P}\right)^{1/2}, \quad (1)$$

where k is a constant equal to 0.92 (range 0.91-0.93), ρ is the density of the diaphragm material, assumed to be annealed copper (8900 kg/m^3); b and d are the thickness and diameter of the diaphragm, equal to $5 \cdot 10^{-5}$ and $6.5 \cdot 10^{-3}$ m respectively; P is the burst pressure (Pa). The diaphragm section opening time for each of the ten sections (for all 11 simulated burst pressure scenarios) is given in Table 2.

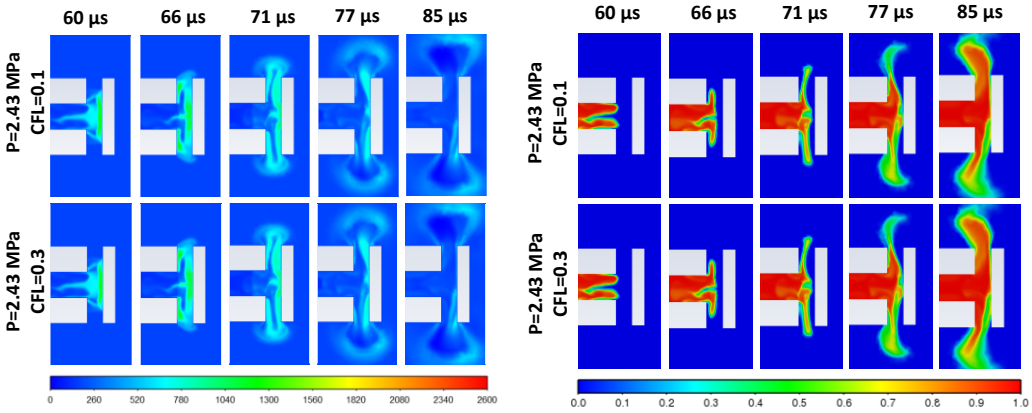
Table 2. Opening times of ten burst disk sections (see Fig. 1b) for 11 simulated cases.

Burst disk section No.	1	2	3	4	5	6	7	8	9	10
Pressure, MPa	Opening times, μs									
1.35	0	4.7	9.5	14.2	18.9	23.7	28.4	33.1	37.9	42.6
1.65	0	4.2	8.6	12.8	17.1	21.4	25.7	29.9	34.3	38.5
2.43	0	3.5	7.1	10.6	14.1	17.7	21.2	24.7	28.3	31.7
2.6	0	3.4	6.9	10.2	13.6	17.1	20.5	23.8	27.3	30.7
2.8	0	3.3	6.6	9.9	13.1	16.5	19.7	23.0	26.3	29.6
2.9	0	3.2	6.5	9.7	12.9	16.2	19.4	22.6	25.9	29.1
5.0	0	2.4	4.9	7.4	9.8	12.3	14.8	17.2	19.7	22.1
7.5	0	2.0	4.0	6.0	8.0	10.1	12.0	14.0	16.1	18.1
8.75	0	1.8	3.7	5.6	7.4	9.3	11.2	13.0	14.9	16.7
9.4	0	1.8	3.6	5.4	7.2	9.0	10.8	12.5	14.4	16.1
10.0	0	1.7	3.5	5.2	6.9	8.7	10.4	12.2	13.9	15.6

RESULTS AND DISCUSSION

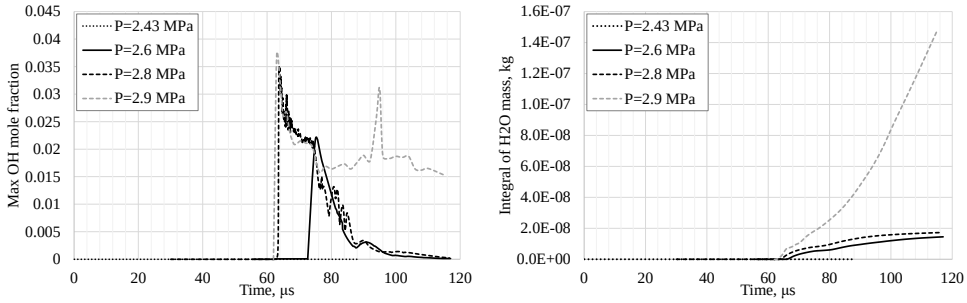
For hydrogen at ambient temperature, an initial storage pressure in the range 1.35 MPa - 2.9 MPa has been investigated. Pressure equal to 2.43 MPa is observed to not lead to the ignition. Temperature

and hydroxyl (OH) mole fraction profiles are analysed to gain insights into the ignition dynamics. The mole fraction of OH is usually used as an indicator of the location of chemical reactions. Figure 2a shows the temperature profile across the symmetry plane of the axial channel. Maximum temperature reaches approximately 1500 K in the area of shock wave reflection where no hydrogen is present, see Fig. 2b. Temperatures in areas of hydrogen mixed with air are not sufficient to lead to the ignition. This is confirmed by the maximum hydroxyl mole fraction dynamics in time, which, as shown in Fig. 3, is rather negligible (horizontal line) during the entire process time when the ignition is expected (up to 90 μs). Results for storage pressures 1.35 MPa and 1.65 MPa are not shown as leading to similar results as 2.43 MPa. The absence of ignition for pressure 2.43 MPa somehow differs from the numerical study [6] where ignition was observed, even being rather weak and later self-extinguished. This non-critical difference could be associated with the difference in combustion models employed for the simulations, and the multiple modifications of the Fluent sub-models and schemes between versions v.6.3 and v.17.2. Experiments also confirmed the observations of the numerical study in [6], by recording ignition for this pressure [7].



(a) Temperature, K (b) Hydrogen mole fraction

Fig. 2. Temperature (a) and hydrogen mole fraction (b) profiles on the symmetry plane for storage pressure of 2.43 MPa, CFL number equal to 0.1 and 0.3. The initial temperature of hydrogen is 300 K.

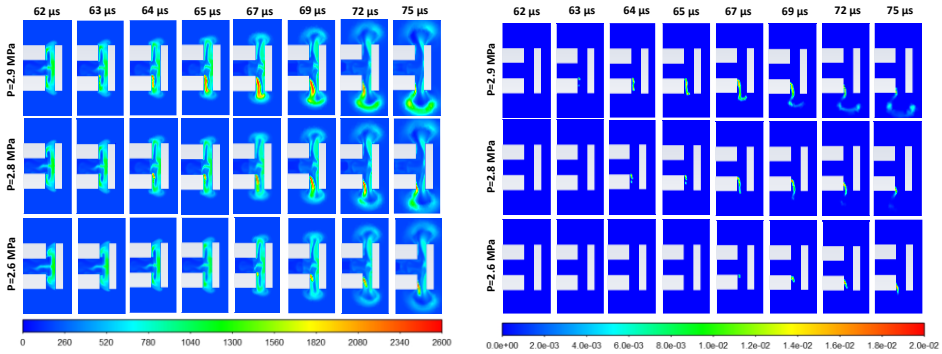


(a) (b)

Fig. 3. Dynamics in time across the computational domain: (a) maximum hydroxyl mole fraction, (b) integral of water vapour mass. The initial temperature of hydrogen is 300 K.

A simulation is performed for a CFL number decreased from 0.3 to 0.1 to assess time convergence of the simulation results. Figure 2 shows that the dynamics of temperature (a) and OH mole fraction (b) distributions for CFLs equal to 0.1 and 0.3 do not present any relevant and detectable difference, proving the time convergence of simulation results. Therefore, CFL=0.3 is used for the following simulations.

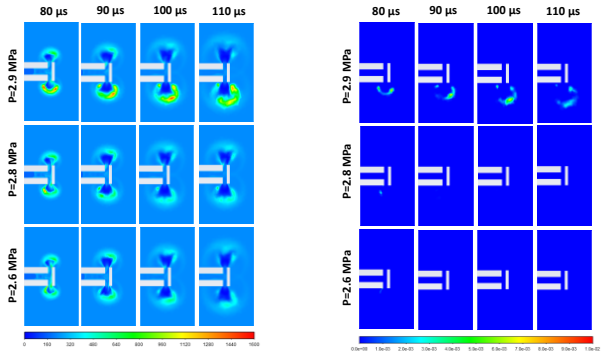
To find the pressure limit providing ignition, the hydrogen pressure is increased from 2.43 MPa to 2.6 MPa. Figure 4 shows the temperature and hydroxyl mole fraction in the time range 62-75 μs. Temperatures up to 2600 K are reached in the radial channels of the PRD. In the high-temperature zone, an OH mole fraction is starting to manifest local ignition at about 67 μs.



(a) Temperature, K (b) OH mole fraction

Fig. 4. Profiles on the symmetry plane for storage pressures 2.6, 2.8 and 2.9 MPa in time range 62-75 μs: (a) temperature, (b) hydroxyl mole fraction. The initial temperature of hydrogen is 300 K.

Figure 5 focuses on the combustion dynamics outside the PRD and shows how the OH mole fraction has completely disappeared from the symmetry plane by 90 μs for storage pressure 2.6 MPa.



(a) Temperature, K (b) OH mole fraction

Fig. 5. Dynamics on the symmetry plane for storage pressures 2.6, 2.8 and 2.9 MPa in time range 80-110 μs: (a) temperature, (b) hydroxyl mole fraction. The initial temperature of hydrogen is 300 K.

Figure 6 provides a view of the reacting zone in the whole domain. It shows the volumetric distribution of OH mole fraction above the limit of 0.001, which is generally accepted as an indicator of a reacting zone in hydrogen-air flames [19]. This view gives insight into the location of any reacting zone beyond the symmetry plane. For storage pressure 2.6 MPa, at 90 μs combustion is present in a small zone just outside the bottom radial channel, and at 110 μs this has completely disappeared. This is fully in line with the maximum OH mole fraction recorded in the calculation domain and presented in Fig. 3a, which shows a peak at about 75 μs, to then decrease to zero within the following 20 μs except the case of 2.9 MPa.

90 μs **110 μs**

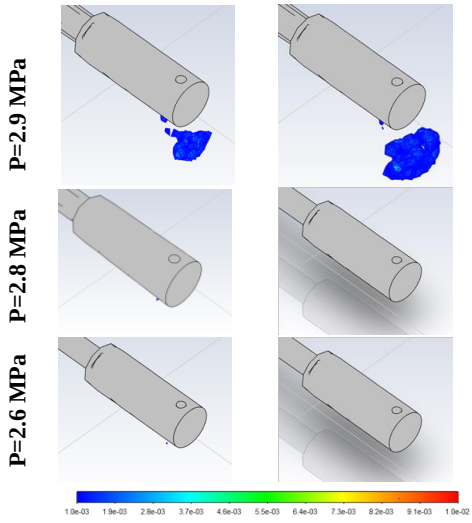
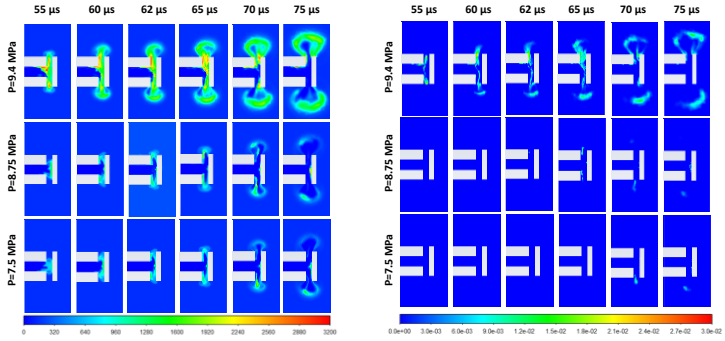


Fig. 6. Hydroxyl mole fraction 3D distribution for storage pressures 2.6, 2.8 and 2.9 MPa. The initial temperature of hydrogen is 300 K.

Therefore, numerical simulations demonstrate ignition at a pressure of 2.6 MPa, followed by self-extinction of reaction. The difference of 7% with the pressure limit for ignition of 2.43 MPa observed in experiments is considered of acceptable accuracy for complex engineering problems like this one. Numerical simulation for initial pressure equal to 2.8 MPa demonstrates a slightly larger and longer presence of ignition and combustion zones, but also in this case there is self-extinction of the reaction. For the initial storage pressure of 2.9 MPa, the combustion is initiated in the bottom radial channel of the PRD (see Figs. 4 and 6). A larger high-temperature zone can be observed for 2.9 MPa, with combustion initiated in a few localised spots as shown by the OH mole fraction in Fig. 4b. These mainly depend on the hydrogen concentration in the air in those locations, which is deemed to be closer to the stoichiometric concentration. Combustion develops with time into a cocoon outside the PRD, leading to sustained combustion and likely transition into a jet fire (see Fig. 5). Combustion is confirmed by the continuous presence of OH and the increase of water vapour mass in the domain (see Fig. 3). It can be observed that for all pressures in the range 2.6-2.9 MPa, the ignition process is asymmetrical and that the ignition spots are mainly concentrated in the lower radial channel. For a pressure of 2.9 MPa, external combustion is seen to be more enhanced towards the bottom side of the PRD. The asymmetry of the ignition and combustion process is deemed to be caused by the inertial and asymmetrical opening of the burst disk (see Fig. 1b). The simulation results well agree with the experimental evidence [7] and numerical study [6] demonstrating ignition and sustained reaction at initial storage pressure of 2.9 MPa.

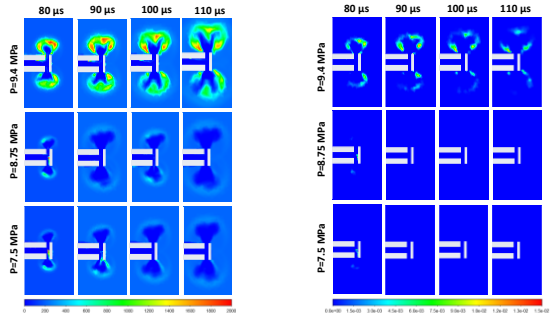
The same procedure is applied to determine the pressure limit of spontaneous ignition for hydrogen stored at a cryogenic temperature of 80 K. The initial storage pressure was changed in the range 5-10 MPa. Figure 7 shows the temperature and hydroxyl profiles across the symmetry plane for pressures 7.5, 8.75 and 9.4 MPa, being the pressures closer to the determined pressure limit. Asymmetrical distribution of temperature at 55 μs reflects the stronger shock wave and effect of the inertial and not fully symmetrical opening of the burst disk. The higher shock wave pressure results in a higher temperature of the heated by shock air (over 2000 K). For storage pressures of 7.5 MPa and 8.75 MPa, triggering of ignition in the radial channel can be observed at 70 μs and 62 μs respectively. However, the further mixing of hot temperature air with the cryogenic temperature hydrogen leads to self-extinction of combustion by the time of 90 μs. This is confirmed by the absence of hydroxyl on the symmetry plane (Fig. 8) and in the 3D domain (Fig. 9). For a storage pressure of 9.4 MPa, ignition happens much earlier in the axial channel of the PRD. Larger high-temperature zones can be observed in this case, as a consequence of the higher pressure of the shock wave and earlier development of

combustion reactions. Figure 8 shows a combustion cocoon formed externally to the PRD. The reaction is enhanced outside the top radial channel, which is different to what was observed for atmospheric temperature hydrogen at pressure 2.9 MPa. The authours believe that this behaviour is a consequence of the different opening dynamics of the burst disk for the limiting pressures associated to the two hydrogen temperatures. The opening time for a pressure of 9.4 MPa (16.1 μs) is almost half of the time required for a pressure of 2.9 MPa (29.1 μs, see Table 2). This causes the interval of time between the opening of one burst disk section to another (see Fig. 1b) to be different by the same order of magnitude. Being the burst disk sections asymmetrical, they can easily induce an enhanced development of combustion towards the top channel for cryogenic hydrogen rather than towards the lower channel as observed for ambient temperature hydrogen. Comparing Figs. 4 and 7, it is possible to observe a larger combustion and high temperature zone for T=80 K and P=9.4 MPa (Fig. 7) in comparison to the case with ambient temperature hydrogen and P=2.9 MPa (Fig. 4). This is a direct consequence of the higher storage pressure, which does not only compansate but overcomes the decrease in combustion rate associated with the lower hydrogen temperature. The combined effect of higher pressure and lower temperature causes the hydrogen density to be up to 12 kg/m^3 for T=80 K. This value is similar to the density of the air compressed by the shock at the intersection of the TPRD in the ambient temperature case. Velocity of the flow is particularly enhanced for the cryogenic case, creating zones with flow velocity up to 2400 m/s at the exits from the radial channels of the TPRD.



(a) Temperature, K (b) OH mole fraction

Fig. 7. Profiles for storage pressures of 7.5, 8.75 and 9.4 MPa in time range 55-75 μs: (a) temperature, (b) hydroxyl mole fraction. The initial temperature of hydrogen is 80 K.



(a) Temperature, K (b) OH mole fraction

Fig. 8. Profiles for storage pressures of 7.5, 8.75 and 9.4 MPa in time range 80-110 μs: (a) temperature, (b) hydroxyl mole fraction. The initial temperature of hydrogen is 80 K.

Figure 9 shows the volumetric development of the reacting zone by the hydroxyl mole fraction distribution. It is concluded that pressure of 9.4 MPa leads to spontaneous ignition and likely leads to a transition into a hydrogen jet flame. It follows that for cryogenic hydrogen at 80 K, the pressure limit of spontaneous ignition is more than 3 times larger than for ambient temperature hydrogen for the considered system of the T-shaped channel. It should be underlined that these conclusions are valid for the T-shaped channel with concrete burst disk. The storage pressure limit leading to

spontaneous ignition strongly depends on the geometry and characteristics of the release system and burst disk. Furthermore, the potential for ignition occurrence at a certain pressure can be affected by the behaviour and timing of the burst disk opening, as it will affect the primary and reflected shock, and the shock-shock interactions ([20], [21], [22]). A faster rupturing rate can increase the likelihood of spontaneous ignition occurrence for a given pressure close to the limit.

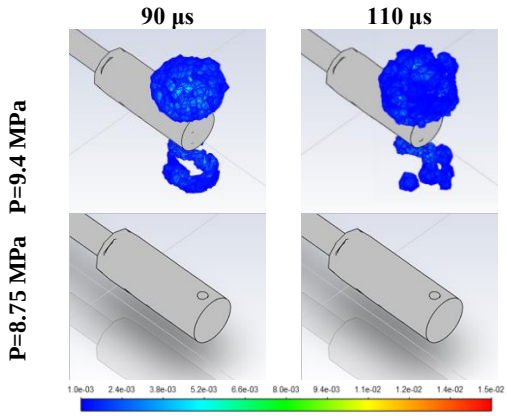


Fig. 9. Hydroxyl mole fraction 3D distribution for storage pressures of 8.75 MPa and 9.4 MPa. The initial temperature of hydrogen is 80 K.

CONCLUSIONS

The originality of the research is given by the numerical investigation of the spontaneous ignition for cryo-compressed hydrogen in a T-shaped channel. Ignition and combustion dynamics were assessed in terms of temperature and hydroxyl mole fraction distributions. The significance of the research is given by the provision of a validated contemporary tool for hydrogen safety engineering to determine the pressure limits leading to spontaneous ignition for compressed hydrogen at both ambient and cryogenic temperatures. For ambient temperature hydrogen (300 K), it was found that a pressure of 2.9 MPa is required to obtain spontaneous ignition and likely transition into a jet fire outside the T-shaped channel. Pressure in the range 2.6-2.8 MPa was found to trigger ignition, later resulting in self-extinction. Simulations closely reproduce the experimentally observed pressure limit of 2.43 MPa which was sufficient to provide ignition, but not sustained jet flame. Validation of simulations against experiments established the rigour of the research. For cryogenic hydrogen (80 K), it was found that a pressure approximately 3 times larger than for warm hydrogen is required to trigger ignition and sustain combustion outside the T-shaped channel, which could likely lead to a hydrogen jet fire. The pressure limit of 9.4 MPa was found to lead to ignition and sustained jet fire in the considered setup. Simulation results showed that below this pressure, e.g. at 8.75 and 7.5 MPa, there was an ignition in the T-shaped channel which then self-extinguished, as demonstrated by the disappearance of high-temperature regions and hydroxyl species.

ACKNOWLEDGEMENTS

This research has received funding from the Fuel Cells and Hydrogen 2 Joint Undertaking under grant agreement No 779613 (PRESLHY). The JU receives support from the European Union's Horizon 2020 research and innovation programme and the United Kingdom, Germany, Greece, Denmark, Spain, Italy, Netherlands, Belgium, France, Norway, Switzerland. The authors would like to acknowledge EPSRC for funding the project Kelvin-2 "Tier 2 High-Performance Computing Services", EP/T022175/1 and Innovate UK for funding the project "Northern Ireland Green Seas" (ID: 397841).

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