# Hydrogen Safety Engineering: Overview of Recent Progress and Unresolved Issues

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# ABSTRACT

This paper gives an overview of recent progress in hydrogen safety research at the HySAFER Centre in the University of Ulster and highlights some unsolved issues, which are mainly related to the indoor use of hydrogen and fuel cell technologies. The similarity law for hydrogen concentration decay in momentum-controlled subsonic, sonic, and supersonic jets is explained and validated. The technique to distinguish between momentum- and buoyancy-controlled flow in expanded and underexpanded jets is presented. The decay of hydrogen in a plane jet of limited length-to-width ratio is discussed. The physical phenomenon of a 90 degree "twist" of plane jet is reproduced numerically. It is proved that concentration decay in plane jet with infinite length-to-width ratio does not follow the similarity law suggested by Chen and Rodi.

A correlation for jet flame length, derived by means of a similitude analysis and validated against experimental data for the widest known range of parameters, is shown. In addition, a comparison between two techniques to determine the length of a hydrogen jet flame is presented. The engineering nomogram for graphical calculation of the jet flame length using only storage pressure and leak diameter is given. Furthermore, a correlation between the location of the hydrogen jet flame tip and hydrogen concentration in a non-reacting jet at the same location from the same source is presented.

The phenomenon, unique to hydrogen of pressure peaking during a non-reacting release from a pressure relief device (PRD) in an enclosure with a small vent is described. Initial results of self-extinction of hydrogen jet fire in a garage-like enclosure are presented. Numerical reproduction of spontaneous ignition during a T-shape PRD activation at pressures as low as those observed in experiments, is briefly discussed.

# **1 INTRODUCTION**

Why a hydrogen economy? According to a variety of sources, including the World Coal Institute, existing reserves of fossil fuels, based on current production and use rates are predicted to last: coal – approximately 160 years, gas - 70 years, and oil - 40 years. Geopolitical fears exist as a consequence of fossil fuel depletion. Many countries within the European Union and around globe are investing heavily in renewable energy programmes in order to secure independence of energy supply and address the issues of environmental pollution and climate change. The key role of zero emission green hydrogen produced from renewable energy (wind, tide, solar, hydro), and fuel cell and hydrogen technologies cannot be overestimated.

Demonstration projects utilising hydrogen and fuel cell technologies such as stationary combined heat and power installations, hydrogen-powered vehicles and buses, refuelling stations for liquefied hydrogen and compressed hydrogen at 35 and 70 MPa have been deployed in practically all developed countries. Commercialisation of hydrogen, to include a

fleet of fuel cell cars is planned for 2015. Safety remains the main "non-technical" barrier for introduction of the hydrogen economy.

Hydrogen Safety Engineering (HSE) is the application of scientific and engineering principles to the protection of life, property and environment from adverse effects of incidents/accidents involving hydrogen. The aim of this paper is to give an overview of recent research findings in hydrogen safety research and engineering in the HySAFER Centre at the University of Ulster.

#### 2 NON-REACTING MOMENTUM- AND BUOYANCY-CONTROLLED JETS

A non-reacting leak of hydrogen is one of potential consequence in a failure scenarios. In order to predict hazardous distance and define where the flammable hydrogen-air mixture is formed it is important to know how concentration in a jet decays from 100% by volume at the nozzle (point of leak) to the lower flammability limit (LFL) of 4% by volume of hydrogen in air. Then it is important to understand, e.g. for downward directed leaks, at what position the initially momentum-controlled jet changes flow regime to buoyancy-dominated. In reality leaks are expected to occur from elongated cracks, or similar, as opposed to perfectly round orifices. It is for this reason that the performance of plane jets is of interest for hydrogen safety engineering.

#### 2.1 The Similarity Law

The similarity law for hydrogen concentration decay in momentum-controlled subsonic jets was published in 1980 by Chen and Rodi [1]. Fuel mean mass fraction on a jet axis can be calculated for round and plane jets as

$$\frac{C_{ax}^{m}(x)}{C_{N}(0)} = 5.4 \sqrt{\frac{\rho_{N}}{\rho_{s}}} \frac{D}{x} \quad \text{(round jet), and} \tag{1}$$

$$\frac{C_{ax}^{m}(x)}{C_{N}(0)} = 2.13 \sqrt{\frac{\rho_{N}}{\rho_{S}}} \sqrt{\frac{D}{x}} \text{ (plane jet),}$$
(2)

where  $C_{ax}(x)$  is the mass fraction of leaking gas at a distance x from the nozzle,  $C_N(0)$  is the mass fraction of leaking gas at the nozzle exit at x=0 (can be omitted in the majority of cases as  $C_N(0)=1$  for a pure hydrogen leak),  $\rho_N$  and  $\rho_S$  are the density of gas in the nozzle and the density of the surrounding gas respectively, and D is the nozzle diameter.

However, there is no validation published on the application of this similarity law for sonic and supersonic highly underexpanded jets. The publication by Birch et al. [2] in 1987 did not add to the understanding of how the similarity law (1) should be used for jets originating from high pressure gas storage. Indeed, the following formula presented in [2] for underexpanded jets, has three distinct differences with the similarity law suggested by Chen and Rodi [1]

$$C_{ax}^{V}(x) = 5.4 \sqrt{\frac{\rho_{s}}{\rho_{N}}} \frac{D_{eff}}{x}, \text{ where notional nozzle diameter } D_{eff} = D \cdot \sqrt{\frac{p_{R}}{p_{s}} \left(\frac{2}{\gamma+1}\right)^{1/(\gamma-1)} \frac{1}{(\gamma+1)}}, \quad (3)$$

In equation (3),  $p_R$  and  $p_S$  are storage pressure and atmospheric pressure respectively, and is the ratio of specific heats. The three key differences are as follows: (1) Birch et al. [2] used volumetric fraction instead of mass fraction in the original work by Chen and Rodi [1]; (2) the

density ratio under the square root in [2] is the reciprocal of that used in [1]; and (3) a notional nozzle diameter was used by Birch and colleagues [2] instead of the real nozzle diameter used by Chen and Rodi [1].

It was suggested in [3], when considering the case of underexpanded jets, to apply the similarity law for round jets (1) in absolutely the same matter as for subsonic and expanded sonic jets. The only unknown parameter in equation (1) for underexpanded jets is the density of hydrogen in the nozzle  $\rho_N$ . To calculate this density an original phenomenological theory for underexpanded jets of non-ideal gas was developed [4] and applied to correlate available experimental data. Figure 1 demonstrates the good agreement between the similarity law (solid line), applied according to the methodology described above, and experimental data on axial hydrogen concentration decay published by different research groups for both subsonic and underexpanded jets at pressures up to 40 MPa and orifices diameter from 0.25 mm to 25 mm.



*Fig. 1. The similarity law (solid line) and experimental data on axial concentration decay in momentumcontrolled hydrogen jets.* 

The similarity law, if applied as described in [3], closely reproduces experimental data and thus can be considered as an engineering tool to predict concentration decay in momentumcontrolled hydrogen jets. It is worth noting that all experimental data are below the similarity law line in Fig. 1. This may be explained as the calculation applied to determine hydrogen density in the nozzle, which uses the theory of underexpanded jets, does not take into account friction and minor losses. Thus, the similarity law gives conservative predictions. A theory describing underexpanded jets accounting for losses can be found in [5].

Figure 1 demonstrates how to determine graphically the distance where concentration in a momentum-controlled jet is 4% or 1% by volume of hydrogen. The procedure can be reduced further to a simple engineering equation for calculating the location of the LFL (4% by

volume):  $x = 1708 \cdot \sqrt{\rho_N} \cdot D$ , in which *D* is the real nozzle diameter and hydrogen density in the real nozzle  $\rho_N$  is calculated using the underexpanded jet theory [4].

#### 2.2 Momentum and Buoyancy-Controlled Jets

For the development of a hydrogen safety engineering system it is important to know whether a leak is originally momentum- or buoyancy-controlled, or at which concentration the flow regime changes from momentum to buoyant for the same jet. The technique presented below to distinguish between momentum- and buoyancy-controlled flow in expanded and underexpanded jets is based on the approach developed by Schevyakov et al. [6] for expanded jets.

The results are presented in Fig. 2 in logarithmic coordinates of distance to diameter x/D (ordinate) and Froude number  $U^2/gD$  (abscissa), where U is velocity at the nozzle, g is gravitational acceleration, and D is diameter. For underexpanded jets the notional nozzle diameter and the velocity in the notional nozzle were applied in the Froude number and in the dimesionless ratio x/D, and calculated by the phenomenological theory [4]. Figure 2 shows theoretical curves by Schevyakov et al. [6], their experimental data for expanded jets, and data of other authors for underexpanded jets. Both expanded and underexpanded jets obey the same functional dependence.



Fig. 2. The dependence of dimensionless jet length (x/D) on the Froude number  $(U^2/gD)$ .

Let us describe the meaning of graphs in Fig. 2. Five solid lines or curves can be seen in the Figure in addition to the data points. Four of these curves in Fig. 2 (denoted as 4%, 17%, 30%, and 60% of hydrogen by volume) are similar in shape and comprise a section which ascends with the Froude number (buoyancy-controlled flow) and a plateau section which represents the momentum-controlled regime. In a buoyancy-controlled regime the dimensionless distance from the nozzle to a particular concentration grows with increasing Froude number. In a momentum-controlled regime the dimensionless distance to a particular concentration does not change with further increase in the Froude number. The distance at which a downward directed jet reverses due to buoyancy is also shown in Fig. 2. It is

represented by the fifth solid line which intersects the other four lines at the exact point where the momentum-controlled regime changes to buoyancy-dominated flow. Buoyant jets (lower velocities) are always shorter compared to momentum-dominated jets (high velocities) from the same nozzle.

Two examples using Fig. 2 are as follows: (1) A jet with exit Fr=1000 (Log Fr = 3) is momentum-controlled when the axial concentration is above 60% by volume, and buoyancy-controlled at hydrogen concentrations below 60% downstream the jet when Log (x/D)>1, i.e. x>10D; (2) A Jet with Log Fr = 7 is momentum-controlled from the exit to an axial concentration of 4% by volume (LFL), which propagates as far as  $x/D = 10^{2.6}$ , i.e. about 400 nozzle (notional nozzle) diameters.

### 2.3 Plane Jet Behaviour

There are two issues relevant to the understanding of plane jet behaviour. The first is related to the prediction of concentration decay in hydrogen jets from realistic leaks which are expected in many cases to be in the form of a crack rather than rounded orifice. The second is important for the development of innovative pressure relief devices with shorter safety distances compared to current PRDs available on the market [7].

In this section initial results of numerical simulations of hydrogen concentration decay in a plane jet of limited length-to-width ratio are presented. The physical phenomenon of a 90 degree "twist" of the plane jet is revealed in simulations. The decay of concentration in the finite length-to-width ratio jet does not follow the similarity law suggested by Chen and Rodi for a plane jet with infinite length-to-width ratio and expressed by equation (2). Figure 3 demonstrates changes in jet shape with distance from the nozzle.



*Fig. 3. The shape of a jet from the plane slot of the length-to-width ratio of 200 (flow field up to 40 cm, yellow colour – 8.5% of hydrogen by volume, grey colour – 4% by volume).* 

Numerical simulations were performed for the following conditions: there is a slot of 20 mm length and 0.1 mm width (L:W=200) in a pipe of 5 mm internal diameter and 10 mm external

diameter. The area of this rectangular nozzle is equal to the cross-section area of a round nozzle of diameter 1.59 mm. In Fig. 3 the internal yellow contour corresponds to a volumetric concentration of hydrogen in air of 8.5% and the external grey shows where the lower flammability limit of hydrogen-air mixture (4% by volume) is located.

It is clearly seen in Fig. 3 that the underexpanded jet from an internal pipe pressure of 350 bar, "twists" perpendicular to the slot direction following release. This means that if the initial length-to-width ratio (L:W=200) is renamed as Y:X=200:1, where Y is size along the pipe axis (slot length) and X is size perpendicular to the pipe axis (slot width), then at a very short distance from the nozzle the ratio drops below 1. For example, at a distance of 5 cm from the plane nozzle this ratio is about Y:X=1:6, and at distance of 40 cm from the exit it is still below 1, i.e. about Y:X=1:3.6. However, the ratio tends to 1 in the far field from the nozzle.

Indeed, simulations demonstrated (see Fig. 4) that at a sufficiently large distance from the nozzle the jet becomes practically round. In order to conclude on the similarity in the far field of round and plane jets which have the same cross-sectional area at the nozzle exit, more research is needed. In particular, the profiles of hydrogen distribution in the radial direction should be compared for these two types of jets. However, a preliminary conclusion for hydrogen safety engineers is that the hazards from both types of jets in the far field appear to be quite identical.



*Fig. 4. The shape of a jet from the plane slot of the length-to-width ratio of 200 (flow field up to 350 cm, yellow colour – iso-surface 8.5% of hydrogen by volume, grey colour – iso-surface 4% by volume).* 

# **3 JET FIRES**

Jet fire is a typical scenario following an accident involving hydrogen. Hydrogen is currently stored onboard at pressures up to 70 MPa. Potentially a leak could occur from a small crack or a full bore of a piping system. To understand and tackle jet flames, including those arising from high pressure hydrogen storage where the effects of non-ideal gas behaviour cannot be ignored, it is important for hydrogen safety engineers to know the length of a jet flame. In

particular, this is one of the factors which affects the safety distance (see for example NFPA 55 standard [8]).

#### 3.1 A Correlation for Jet Flame Length

A correlation for hydrogen jet flame length derived by the similitude analysis and validated against experimental data for the widest known range of parameters has been published recently [3] (see Fig. 5). It was argued in [3] that the flame length correlates not just with nozzle diameter, as was thought previously [9], or just with mass flow rate as in an empirical correlation [10], developed recently, rather it correlates on both these parameters.

It was shown that the flame lengths of subsonic, sonic, and supersonic jets obey the same dependence that can be expressed by the following equation  $L_F = 76 \cdot (\dot{m} \cdot D)^{0.347}$ , where  $\dot{m}$  is mass flow rate in kg/s and D is real nozzle diameter in meters. This is a best fit equation of 95 experimental data points from different authors. A conservative estimate for the flame length is 50% longer and can be calculated by the equation  $L_F = 116 \cdot (\dot{m} \cdot D)^{0.347}$ . The mass flow rate  $\dot{m}$  was calculated from the phenomenological theory of underexpanded jet [4] used above to verify the similarity law for underexpanded non-reacting jets.



Fig. 5. A correlation for hydrogen jet flames [3].

#### 3.2 Comparison Between Two Techniques for Jet Flame Length Calculation

A comparison between two techniques to calculate hydrogen jet flame length is carried out in this section. In general, the jet flame length is a function of Re, M and Fr numbers. There can not be a "perfect" correlation based on only one of these numbers. The idea that experimental jet flame length can be correlated by only the Fr number has a long history, for example: Baev at el., 1974 [11], Shevyakov and Komov, 1977 [12], Delichatsios, 1993 [13], and Schefer et al., 2006 [14].

The one of approaches to correlate dimensionless flame length with only Fr number suggested by Delichatsios for plumes and expanded jets [13] was recently upgraded by Schefer et al. [14] for underexpanded jets using their own theory of underexpanded jet which accounts for non-ideal behaviour of hydrogen at high pressures. However, this approach does

not seem to work well in the momentum-controlled regime when more experimental data are analyzed. Indeed, we have applied the methodology [14, 13] and using [4] for the calculation of the notional nozzle parameters as above, to the same 95 experimental data points shown in Fig. 5 plus 28 experimental data points by Shevyakov et al. [12], and Imamura et al. [15]. The result demonstrated higher scattering of experimental data points (see Fig. 6) compared to our approach (see Fig. 5).

In the momentum-controlled regime where there are large flame lengths the scattering of experimental data increases to about 20% using the new method [3] (see Fig. 5), when flame length data are correlated with the similarity group  $\dot{m} \cdot D$ , to about 50% when the data correlated against the Froude number [14, 13] (see Fig. 6). In fact, Fig. 6 demonstrates that there is no clear transitional area from buoyancy to momentum-dominated jet flames and additionally there is no clear "plateau".

The recent correlation [3] (see Fig. 5) better predicts the flame length when compared to the correlation previously used of flame length against the Froude number [14, 13] (see Fig. 6), particularly in the momentum-controlled regime. It should be noted that momentum-dominated jets are the most relevant to hazard and risk assessment of hydrogen systems and infrastructure.



Fig. 6. A correlation for hydrogen jet flames following methodology [14, 13].

#### 3.3 The Engineering Nomogram

The use of the correlation for jet flame length shown in Fig. 5 requires calculation of a mass flow rate by the phenomenological theory of underexpanded jets [4] in each particular case. This is not always a convenient way of flame length assessment, for example by regulators

involved in the permitting process for fuel cell and hydrogen systems. To assist different stakeholders, including the general public, in the quick and reliable calculation of the flame length using available leak parameters the simple nomogram was developed (see Fig. 7). The nomogram is derived from the universal correlation for jet fires (Fig. 5).



Fig. 7. The nomogram for graphical calculation of jet flame length by physical nozzle diameter and storage pressure [3].

The engineering nomogram, shown in Fig. 7, is designed for the graphical calculation of jet flame length using only two easily available parameters of a leak: storage pressure and physical orifice diameter. An example of the nomogram use is demonstrated in Fig. 7. Let us first choose the diameter of a leak nozzle, e.g. D=3 mm, and storage pressure, e.g. p=35 MPa (350 bar). To start graphical determination, let us draw a horizontal line from the diameter axis across until it intersects with the line denoted as 350 bar. Then, let us draw a vertical line from the intersection point upwards until intersection with the line denoted in the nomogram by the coordinates  $L_{F^-}(\dot{m} \cdot D)^{1/2}$ , which is in fact the best fit line of the correlation for jet flame length presented in Fig. 5. Finally, let us draw the horizontal line from this intersection to the left across to the intersection with the axis "Flame length  $L_F$ , m". Thus, the flame length from a leak of 3 mm in diameter from a hydrogen system at an internal pressure of 35 MPa will be 5 m. For the conservative estimate this flame length could be increased by 50% as explained above to be 7.5 m. The use of this engineering nomogram is simple and does not require any additional tools or knowledge other than leak diameter and storage pressure.

The nomogram incorporates a special feature based on results by Mogi et al. [10]: no stable flames were observed for nozzle diameters 0.1-0.2 mm as the flame blew off although the spouting pressure increased up to 40 MPa ("No flame" area in Fig. 7).

### 3.4 The Jet Flame Tip Location

To gain deeper insight into hydrogen safety science and be equipped to design robust safety engineering systems it is important to know the location of the tip of momentum-dominated jet flames i.e. the location of the maximum length of the visible flame from the source (with an intermittency of 50%). Is there any data explaining what is the hydrogen concentration in a non-reacting jet at a location which corresponds to the tip of a jet flame originated from the same leak source? For example, Bilger and Beck [16] suggested that the flame length is defined "for convenience" as the length on the axis to the point having a mean composition which is stoichiometric, i.e. hydrogen concentration is twice that of oxygen. This is similar to the widely spread point of view published in 1957 [17] and repeated later in 1976 [18] that the calculated flame length may be obtained by substitution the concentration corresponding to the stoichiometric mixture in the equation of axial concentration decay for a non-reacting jet. However, based on a limited number of experimental data it was estimated recently in [3] that the hydrogen non-premixed jet flame tip is located far above the location of axial stoichiometric hydrogen concentration in air of 29.5% by volume. It was found that at the location of the flame tip the concentration of hydrogen is close to the limit for downward and spherically propagating premixed hydrogen-air flames i.e. 8.5-9.5% by volume.

More experimental data were processed recently. The correlation between location of the hydrogen jet flame tip and hydrogen concentration in the non-reacting jet from the same source, i.e. the same leak diameter and pressure  $p_{cont}$ , is presented in Fig. 8. The experimental points in Fig. 8 represent the dimensionless flame length  $L_F/D$ , where D is physical nozzle diameter. The diagonal lines in Fig. 8 correspond to the dimensionless distance x/D to location of particular hydrogen concentration at the jet axis calculated using theory [4].

The conclusion can be drawn from Fig. 8 that for momentum-controlled jets the flame tip is located where the axial concentration of hydrogen in a non-reacting jet is between 8% and 16% by volume depending on experimental conditions. The best fit line is close to 11% by volume. This is far below the stoichiometric concentration of 29.5% by volume as was thought previously [17, 16, 18].



Fig. 8. The correlation between dimensionless the flame length  $Lf/d_{noz}$  and dimensionless distance to concentrations in the non-reacting jet from the same leak source  $x/d_{noz}$ .

### **4 TOWARDS INNOVATIVE PRESSURE RELIEF DEVICES**

Regulation requires the used of pressure relief devices for onboard storage of hydrogen. The performance of PRDs in the case of indoor non-reacting or reacting releases is not yet understood. Current PRDs are designed to blowdown hydrogen from the storage tank (usually Type 4 with limited fire resistance) quickly to prevent catastrophic failure of the high pressure storage in the case of external fire. Using the nomogram (Fig. 7), the flame for a pressure relief device with an orifice diameter of 5 mm at a pressure 70 MPa is estimated as 10 m (average value) or 15 m (conservative estimate). This high flame length can hardly be accepted by the public when assessing the risk of a hydrogen-powered car parked in a garage. Non-reacting releases from current PRDs are not less hazardous as will be shown further in this section. There is a clear need for innovative PRDs which will exclude the current level of hazards and associated unacceptable risk for consumers. However, let us first understand why the performance of existing PRDs is questionable.

#### 4.1 The Pressure Peaking Phenomenon of Hydrogen Release in a Garage

Let us consider a non-reacting release of hydrogen from a typical PRD in a garage with a small vent of a size comparable with one standard brick. It could be expected that after the start of the release with a constant mass flow rate the gauge pressure in the garage will monotonically grow until it is stabilised at some level. Recent research has shown that this is not the case [19]. The phenomenon of pressure peaking during a non-reacting hydrogen release from a pressure relief device (PRD) in an enclosure with a small vent was discovered and explained.

Let us consider a small garage LxWxH=4.5x2.6x2.6 m with one opening area equivalent to that of a typical brick LxH=25x5 cm. Hydrogen is released from a typical onboard storage tank at 350 bar through a 5.08 mm diameter orifice PRD. A constant mass flow rate of 0.39

kg/s is assumed (hypothetical worst case scenario, conservative case). Hydrogen releases vertically upward in the centre, 0.5 m above floor. Opening time of PRD is 0.195 s. Volume of the vehicle occupying the garage was not accounted for and the introduction of 700 bar tanks will lead to higher mass flow rates for the same PRD. Simple methods, including orifice equations, predict an overpressure in the garage of 15-18 kPa. However, the maximum pressure peak is of the order of magnitude higher in the region of 56 kPa (see Fig. 9).

Figure 9 demonstrates that the phenomenon of pressure peaking is unique for hydrogen as a methane, the closest to hydrogen by molecular weight, has an undistinguished peak and a propane release produces no peaking effect at all. This finding is of importance for hydrogen safety engineering. The explanation of the phenomenon is quite simple. Indeed, the volumetric mass flow rate out of the enclosure is inversely proportional to the square root of the density of the gas escaping the enclosure. Thus, in the initial stages of the release, in assumption of uniform mixing of hydrogen with air, the density of the mixture within the garage is quite high and close to the air density. To compensate the volumetric inflow of pure hydrogen, a higher pressure within the enclosure is required at quasi-steady state for higher molecular mass gas escaping the enclosure (volumetric mass flow rate can be estimated as proportional to the square root of overpressure in the enclosure for subsonic flows).



Fig. 9. Peaking pressure dynamics of hydrogen release from PRD in a garage compared to pressure dynamics of methane and propane at the same mass flow rate of 0.39 kg/s.

Unfortunately, building constructions can withstand pressures only below 10 kPa. Higher pressures could destroy them if special measures are not undertaken. If we assume that typical garage structures can be destroyed by pressures in the region 15-20 kPa then simple engineering estimates could give the impression that a release from PRD at described conditions is safe. However, the pressure peaking effect shows that this is not the case and the garage would be destroyed in a couple of seconds for the scenario described. It means that hydrogen safety engineering practice should be reconsidered to account for this phenomenon. The straight forward way to address the safety issue of hydrogen-powered vehicle use in garages and parking that follows from the above results is reduction of the mass flow rate from the PRD and as a consequence an increase in fire resistance of onboard storage tanks. One possibility to be investigated is the use of potentially more fire resistant Type 4 tanks

with intumescent paint instead of Type 4 vessels made of carbon fibre and plastic liners which are not as fire safe.

### 4.2 Self-extinction of Hydrogen Flame in Enclosure

Hydrogen is unique in many senses. During combustion in air it produces a perfect, and indeed the widest spread, fire extinguishing agent "water". Let us consider a scenario with a jet fire from a PRD in the same garage as described in the previous section and exclude consideration of pressure effects (as it was shown above even a non-reacting release will destroy a garage in 2 s, thus in the case of a reacting jet this time would be an order of magnitude shorter). Combustion of released hydrogen within the garage will consume oxygen in air and generate water. Self-extinction of hydrogen in the enclosure could be expected shortly. Indeed, initial numerical simulations of this scenario demonstrates a decrease of temperature within the enclosure (see Fig. 10) and regions with OH associated with reaction zones after already 3 s.



Fig. 10. Contours of static temperature in the range 1300-2600 C (2D slice through centre of 3D plane).

# 4.3 Spontaneous Ignition during PRD Activation

PRD activation could initiate spontaneous ignition of hydrogen in air by a so-called "diffusion" mechanism first investigated by Wolanski and Wojcicki in 1972 [20]. There are a number of excellent paper on experimental and numerical studies of spontaneous ignition during a sudden release of hydrogen. In this overview we would like to discuss only the experimental observation of spontaneous ignition of hydrogen at storage pressure as low as 1.35 MPa reported recently by Golub et al. [21, 22]. Figure 11 shows the geometry of the high pressure system and a T-shape PRD, taken from the study [21, 22].

The high pressure system consisted of a 210 mm long tube with a 16 mm internal diameter (1) followed by a 280 mm long tube with a 10 mm internal diameter (2) at the end of which the burst disk (5) followed by a T-shape PRD (3) was installed (Fig. 11). The mock-up PRD had a 6.5 mm internal diameter main cylindrical channel with a flat end and two side openings connecting the main channel to two exit tubes, each with a 4 mm internal diameter.

The experimental study demonstrated that when the initial pressure of hydrogen in the chamber did not exceed 1.2 MPa, a light sensor did not record the ignition. When the initial

pressure in the chamber was 2.9 MPa, a light sensor registered the ignition. It is not clear from the experimental publication what exactly was observed at intermediate pressures even if 1.35 MPa was reported at a conference presentation [21] as a minimum pressure for the ignition.



Fig. 11. The scheme of experimental high pressure system, which includes chambers (1) and (2), T-shape mockup PRD (3) [21, 22], burst disk (5) between high pressure system and PRD, and mesh of the computational domain (4).

Numerical simulations demonstrated that ignition, which was identified when the mole fraction of radical OH reached an order of  $10^{-3}$ , can be seen at the initial hydrogen storage pressure of 1.65 MPa. However, this initial ignition spot at this pressure disappears with time. Simulations at an initial pressure of 2.4 MPa showed no extinction of the initial ignition spot which is larger compared to that in the case of an initial pressure of 1.65 MPa. Computational fluid dynamics enables insight into the process. In particular, the location of ignition in the T-shape PRD was identified (see Fig. 12).



Fig. 12. Location of spontaneous ignition in T-shape mock-up PRD [21, 22](temperature scale).

#### **CONCLUDING REMARKS**

An overview of recent research performed in the HySAFER Centre at the University of Ulster is presented. The methodology to apply the similarity law for non-reacting momentumdominated releases describing the decay of hydrogen concentration in both expanded and underexpanded jets is presented and validated. The technique enabling definition of the axial concentration at which a momentum-dominated jet comes buoyancy controlled is suggested. This method can be used to determine the length of the hydrogen jet directed vertically downwards. Behaviour of a plane jet in the near field and far field is analysed. The phenomenon of the jet's 90 degree "twist", i.e. perpendicular to the slot nozzle direction, is revealed for high pressure releases. Two correlations for hydrogen jet flame length are compared. It is shown that the correlation based on a new similarity group, which is the product of mass flow rate and physical nozzle diameter, reproduces experimental data with better accuracy. The simple engineering nomogram for graphical determination of hydrogen jet flame length using only two easily available leak parameters, i.e. physical nozzle diameter and storage pressure, is described and examples of its application are given. It has been shown that the non-premixed jet flame tip is located at a distance where the hydrogen concentration in a non-reacting jet from the same source is in the range 8-16% by volume. The phenomenon of pressure peaking during hydrogen releases in a vented enclosure, which is characteristic for hydrogen only, is briefly discussed. Initial results of numerical simulations of the phenomenon of self-extinction of hydrogen jet fire in an enclosure are shown. Finally, the physics of spontaneous ignition in a T-shaped mock up PRD was investigated using numerical methods. Simulation results were found to reproduce experimental data. Computational fluid dynamics provided a unique means to gain insight into the phenomenon occurring in the complex geometry, notably identification of the mechanism and the precise location of spontaneous ignition. This knowledge could be applied in the design of new generation PRDs.

These results are relevant to safety engineering design of hydrogen and fuel cell systems for indoor use and found a basis for development of innovative PRDs to reduce hazards and associated risks of existing PRDs.

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