



Grant agreement No: 325348

LECTURE – Hazards of hydrogen use indoors

Compiled by S. Tretsiakova-McNally; reviewed by D. Makarov (Ulster University)



Contents

Introduction	3
Objectives of the lecture.....	3
Hazards of hydrogen use indoors	3
Passive and forced ventilation	7
Well-ventilated fires.....	10
Under-ventilated fires.....	12
Self-extinction flame mode.....	12
External flame mode.....	16
Pressure peaking phenomenon	18
Summary	22
References	23

Introduction

This is the last lecture of HyResponse training programme. The topics discussed earlier such as unignited hydrogen releases and fires, harm criteria for humans and damage criteria for structures are relevant to the current lecture. The indoor use of FCH technologies is associated with the higher probability of hydrogen accumulation. Due to the growth of these technologies it is possible to find such FCH installations not only outdoors but also indoors. The examples include: FC forklifts inside warehouses; FC vehicles located in car parks, tunnels and garages; electrolyzers and fuel cells for home use etc. In case of an incident involving indoor FCH installations the following developments are possible: the occupants unable to leave a building/facility; First Responders unable to perform their duties without putting their own life at risk; the partial or complete demolition endangers the lives of both First Responders and members of the general public. Therefore, the topic of safe use of hydrogen and fuel cells indoors is of a high importance for First Responders. While for a hydrogen release outdoors buoyancy is a natural safety asset providing its rapid release/dispersion, for releases indoors this may not be the case. Fast hydrogen release indoors can lead to either a build-up of pressure or to its accumulation and hence to more severe consequences.

UU was one of the partners in the European funded project Hyindoor “Pre-normative research on safe indoor use of fuel cells and hydrogen systems” (www.hyindoor.eu). The main outcomes of this project led to a deeper understanding of the phenomena associated with the releases from hydrogen installations in the indoor settings and the guidance on hydrogen use indoors [1].

Objectives of the lecture

By the end of this lecture First Responders/trainers will be able to:

- Identify the main hazards of hydrogen use indoors
- Distinguish between passive and forced ventilation
- Describe the main regimes on hydrogen indoor fires
- Understand the effect of deflagration venting
- Explain pressure peaking phenomenon
- Use nomograms to evaluate the possibility of pressure peaking phenomenon (PPP)

Hazards of hydrogen use indoors

There is a range of scenarios involving FCH applications located indoors (see Deliverable D2.2 [2]). The total volumes of enclosures may vary, from a small garage to a box-like enclosure for a stationary fuel cell (FC), up to a large scale warehouse. Hydrogen release rates may vary as well, from a small mass flow rate release from a feed line to a FC up to a large-scale release from high pressure storage, for example a release from a FC car's PRD parked in a residential garage. In case of incidents or accidents occurring on FCH systems located indoors the priorities for First Responders are: to save human life, to protect property and the environment. Harm criteria for humans and damage criteria for structures are discussed in detail in the relevant lecture.

The hazards related to an incident/accident on indoor FCH installations include:

- Oxygen depletion and a subsequent asphyxiation
- Effects of high temperature and heat flux from jet fires
- Cold burns from liquid hydrogen spill
- Overpressure effects

- Injury and a loss of life
- Structural collapse
- “Domino” effects
- Damage to the environment

Those who design/approve/own the indoor FCH installation should give careful consideration to the reduction of ‘the damage to infrastructure structures and equipment and to minimise disruption of business, preserve corporate image and reduce direct and indirect financial losses’ [3, 4]. ‘Attention should be paid to preventing the escalating effects of objects, events and layouts on damages and to value and importance of the property in and around a facility’ [3].

In the event of a release whether big or small there are a number of potential phenomena which may happen. They may include:

- Unignited hydrogen release. If this happens indoors, the issues which need to be considered include: evaluating the size of the flammable envelope; determining the level of potential overpressure (without ignition); assessing the relationship between the ventilation rate and the release.
- Ignited release. If release is ignited with a formation of a jet fire a range of issues should be considered such as: the heat transfer to the surroundings; sustainability of a fire (i.e. is there a sufficient amount of oxygen to support it or will it go off); relationship between the ventilation and fire behaviour; possibility of fire reigniting.
- Explosion: Here, the questions should be asked: if an unignited release accumulates and subsequently ignites resulting in either a deflagration or detonation what are the consequences? What is the relationship between venting and the deflagration overpressure?

Hydrogen has a high propensity to leak and this can become a problem in an indoor environment. Obviously, hydrogen accumulation indoors can lead to the formation of a flammable mixture with the air (or oxygen). There are also other issues associated with unwanted releases such as pressure peaking phenomenon (PPP) and effect of oxygen depletion. An adequate ventilation can mitigate against these effects. If a hydrogen leak is ignited the fire (jet fire or plume) will spread and grow within an enclosure. In addition to the flame and hazards associated with it such as temperature and heat flux, there will be hot combustion gaseous products formed which may also represent a hazard. As these gaseous products rise a hot layer of gases may be formed under the enclosure ceiling. The way of fire growth will depend on the type of combustion, the interaction with the surroundings and access to oxygen [5]. Depending on the size and the location of the leak the flame itself may impinge on construction elements of enclosure.

Safety related phenomena and potential consequences associated with indoor incidents/accidents involving FCH systems are summarized in the diagram shown in Figure 1.

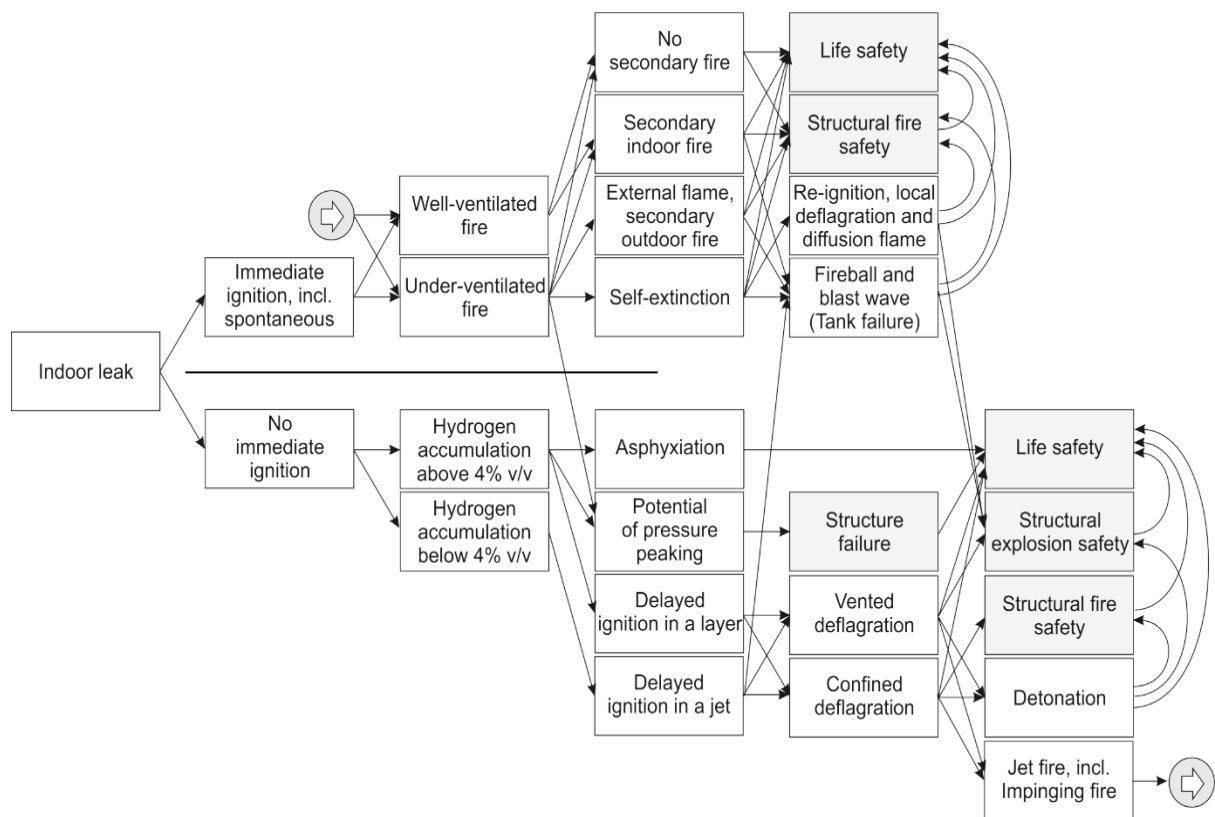


Figure 1. Safety related phenomena and consequences. White boxes correspond to hydrogen phenomena; grey boxes – to the consequences [4].

Following a hydrogen leak indoors two options are possible: no immediate ignition (bottom branch of the diagram) and immediate ignition including spontaneous ignition (top branch of the diagram). The ignition of a hydrogen leak can be caused by the presence of an open fire, a hot surface, an electric or mechanical spark and other factors, as well as hydrogen-specific phenomenon of *spontaneous ignition* (within air-filled piping) by so-called diffusion mechanism [6].

If the leak is ignited immediately, a subsequent fire can develop in two modes: *well-ventilated* and *under-ventilated*. *Well-ventilated fire* is characterized by a relatively low hydrogen release rate and complete combustion of hydrogen within the enclosure. The hazards associated with the well-ventilated fire include: direct effect from the flame and hot combustion products current, radiation from the hot layer formed under the ceiling and hot solid surfaces such as roofs, structural failure of load bearing construction elements due to direct flame impingement, etc. An increase in hydrogen release rate can result in the transition to *under-ventilated fire*, when oxygen is consumed at a faster rate than it can be replenished through the ventilation if possible at all. This in turn may lead to two sub-regimes: *an external flame* occurring in the vents (with no combustion inside the enclosure) and full *self-extinction* of fire within the enclosure. The additional actions are required from First Responders after the self-extinction of fire, e.g. in a FC container, to ensure hydrogen is not accumulated above the hazardous limit in the enclosure accommodating the FC.

Both types of fire can result in the ignition of flammable materials inside the enclosure, generating *secondary indoor fire*. Thus, the fire will continue to burn even after hydrogen release is being stopped e.g. by shutting of safety valves, and additional hazards, such as release of toxic fumes, are possible.


The under-ventilated fire is characterised by relatively high hydrogen release rate. Thus, there is a potential for PPP, endangering structural integrity of the enclosure [6, 7]. It is worth noting that both unignited and ignited releases can generate hazardous overpressure due to PPP. However, calculation of the overpressure due to PPP is different for unignited release and jet fire. The under-ventilated fire may also lead to an external flame, i.e. *secondary outdoor fire*.

If both types of fires as well as secondary fires are not extinguished and continue to burn, this potentially may lead to a catastrophic failure of storage tank(s) located indoors, resulting in a rapid release of energy followed by ignition of large quantities of hydrogen, producing *fireball* and *blast wave*. External flame and secondary outdoor fires can also result in failure of outside hydrogen storage tank(s). Thus, measures should be taken to prevent this, e.g. by placing external hydrogen storage vessels at a distance from the enclosure vents.

The self-extinguished under-ventilated fire may re-ignite when a fresh supply of air enters the enclosure. It can potentially lead to a *localized deflagration* and a diffusion flame in the zones containing hydrogen above the Lower Flammability Limit (LFL), i.e. 4 vol. %. All types of fires present *life safety* hazards (direct thermal damage from the flame, radiation thermal damage, overpressure due to the PPP, and toxicity of combustion products produced by secondary fires) and *structural fire safety* hazards (weakening of the structural integrity and eventual collapse of the enclosure due to prolonged fires) [4].

If hydrogen leak is not ignited immediately upon the release, it would lead to a gradual hydrogen accumulation within the enclosure. The release with high flow rate exceeding ventilation capacity can produce hydrogen concentration above the LFL, which creates the possibility for the *delayed ignition in a layer* and its deflagration. Additionally, high flow rate release can result in asphyxiation and PPP. Although hydrogen is not poisonous/toxic it does not support metabolism. Similar to any other gas (with the exception of oxygen) a risk of asphyxiation exists mainly in confined areas as a result of oxygen depletion [8]. Hydrogen release with a lower rate, which does not lead to the accumulation of hydrogen above 4 vol. % in a layer, can still result in a *delayed ignition in a jet*. Both types of delayed ignition can result in deflagration of hydrogen-air mixture with overpressure, which potentially can destroy the enclosure. Mitigation of explosions by deflagration venting is a wide spread technique. When the enclosure is equipped with the vents, which provide a relief of deflagration overpressure, *vented deflagration* may happen. A *confined deflagration* differs from the vented deflagration by the absence of significant openings leading to the atmosphere, thus preventing pressure relief in the enclosure. The pressure peak in a closed vessel for a stoichiometric hydrogen-air mixture, initially at NTP, can reach up to 815 kPa [9], which would destroy any civil structure (generally able to withstand overpressures of about 10-20 kPa).

In some cases, deflagration can result in a transition to *detonation*. Due to the higher flame propagation velocity and higher levels of overpressure detonations present greater hazards compared to deflagrations. Both deflagration and detonation pose *life safety* hazard through the pressure and thermal effects. They also present *structural explosion safety* hazard, in the worst case scenarios leading to the collapse of the enclosure. Finally, both delayed ignition events discussed earlier can be associated with jet fires, including *fire impinging* effect on walls and/or ceiling of the enclosure. Once the jet fire is established, it can burn in either well-ventilated, or in under-ventilated regime, and the subsequent phenomena and safety consequences would follow the pattern indicated in the top

branch of the diagram (Figure 1) corresponding to immediate ignition as illustrated by the arrow in a circle pictograms 

Passive and forced ventilation

Ventilation can be *natural/passive* or *forced/mechanical/active*. Natural ventilation is a preferable option as it is cheap and reliable, it does not depend on a power source and is always operational. Natural ventilation is provided through permanent vents. The location of these vents is important and should ensure maximum air flow and dispersion of the flammable gas. With hydrogen a combination of upper and lower vents is recommended. If it can be verified, natural ventilation should be permitted to provide all required ventilation and makeup air.

The neutral plane (NP) is a horizontal plane where pressure inside and outside the enclosure are equal. Below the NP air enters the enclosure and above the NP lighter hydrogen-air mixture exits the enclosure. For natural ventilation the NP is at half vent height (Figure 2a). In the case of passive ventilation of the enclosure with release of gas lighter than air, the NP is located at or below the half height of the vent for steady-state conditions as shown in Figure 2b.

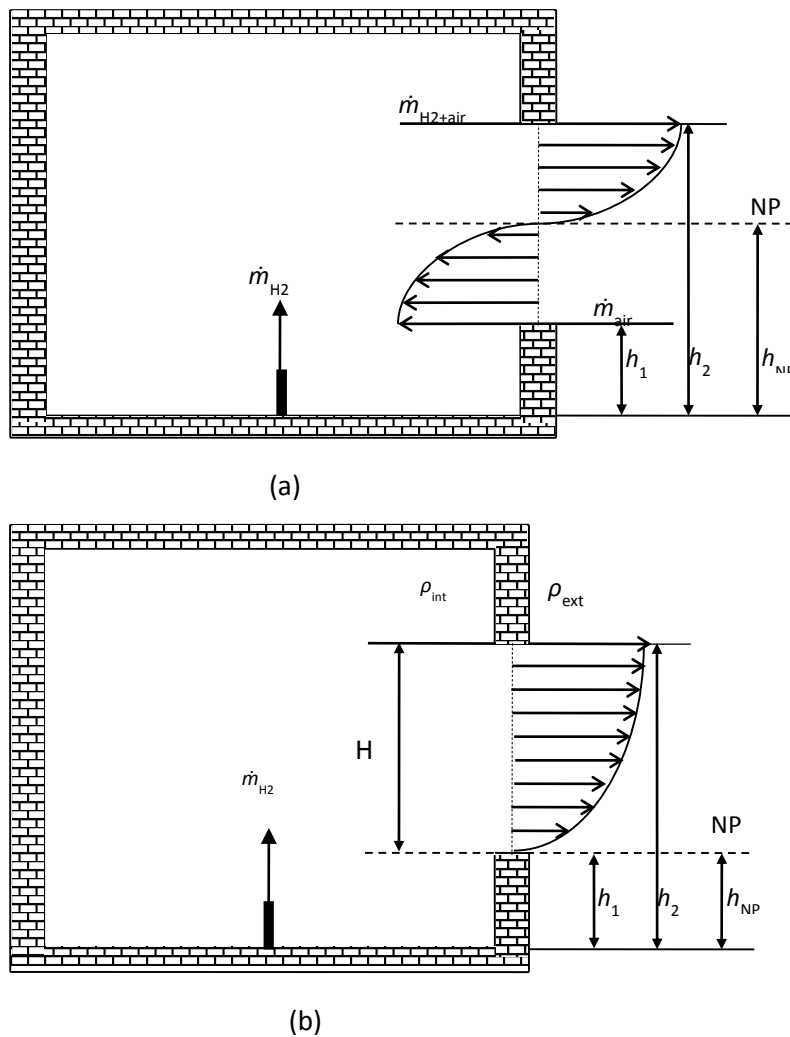


Figure 2. Flow velocity through the vent for natural (a) and passive (b) ventilation.

Natural ventilation equations for the air ventilation are derived in the assumption of the equality of flow in and out of the enclosure. In the case of passive ventilation, the NP for lighter than air gases can be anywhere below a half of vent height.

Maximum hydrogen concentration level in the enclosure with one vent in the assumption of sustained leak can be evaluated using the following equation [10]

$$X = f(X) \cdot \left[\frac{Q_0}{C_D A (g' H)^{1/2}} \right]^{2/3}, \quad (1)$$

where X is the hydrogen volume fraction, Q_0 is the release rate (m^3/s), C_D is the discharge coefficient, A is the vent area (m^2), H is the vent height (m), g is reduced gravity (m/s^2), $g' = g(\rho_{\text{air}} - \rho_{\text{H}_2}) / \rho_{\text{air}}$ (m/s^2), ρ_{air} and ρ_{H_2} are density of the air and hydrogen, respectively, (kg/m^3) and $f(X)$ is function equal to:

$$f(X) = \left(\frac{9}{8} \right)^{1/3} \cdot \left\{ \left[1 - X \left(1 - \frac{\rho_{\text{H}_2}}{\rho_{\text{air}}} \right) \right]^{1/3} + (1 - X)^{2/3} \right\}. \quad (2)$$

The equation (1) is derived in assumption that:

- the release flow rate remains constant;
- gas mixture is uniform across the enclosure, i.e. hydrogen concentration is not a function of location inside the enclosure.

A comparison with experiments had shown, however, that the equation (1) can be used to predict the maximum hydrogen concentration in the case of hydrogen forming layers [10], i.e. it can be considered conservative. Based on the equations of (1) and (2) an engineering nomogram for calculation of sizes (height and width) of a vent in case of a uniform mixture in the enclosure with a single vent [10] was developed (Figure 3). Note, that although in practice hydrogen-air mixture can form layers even in the enclosure with one vent, equations and the nomogram in Figure 3 will provide results close to the maximum concentration values, i.e. it is conservative and can be applied to non-uniform mixtures. The nomogram can be used to calculate hydrogen maximum concentration at steady state condition by known height and width of a vent and release rate. The nomogram is valid for both uniform and non-uniform mixtures in an enclosure with one vent. The procedure for hydrogen concentration calculation (red arrows) is as follows:

1. Select the mass flow rate of hydrogen leak at the vertical axis of the lower panel of the nomogram and project it horizontally until intersection with one of the diagonal lines corresponding to different vent heights. There are 15 such lines in the nomogram in Figure 3, covering practically all possible vent heights ranging from 0.5 mm to 10 m.
2. From the point of intersection, draw a vertical line up until it intersects one of the diagonal lines in the top right panel of the nomogram, which corresponds to different vent widths. There are 15 such lines in the nomogram in Figure 3, covering vent widths in the range between 0.5 mm and 10 m.
3. From the point of intersection, draw a horizontal line left until intersection with the function curve in the top left panel of the nomogram.
4. Draw a vertical line from the point of intersection to the horizontal axis of the top left panel. The value on the horizontal axis correspond to the hydrogen concentration in vol. %.

The nomogram in Figure 3 can also be used for the opposite evaluation, i.e. for the calculation of the vent size required to ensure that for the given hydrogen release rate the concentration will not exceed a specified value (blue arrows in Figure 3). In this case the process of calculation is performed in the reverse order, starting with the desirable concentration value (see example with 2 vol. % mixture in Figure 3). If it is required to evaluate the dimensions of the vent, which will provide hydrogen volume percentage below a certain level, e.g. below 2 vol. % (blue arrows) one would start with the desired volume percentage value at the horizontal axis of the upper left panel and draw vertical line until the intersection with the Function curve in this panel. From this intersection point one can draw horizontal line to the right towards upper right panel, passing across the vent width curves. Next, one should select the release mass flow rate (e.g. 0.2 g/s) in the lower left panel of the nomogram, drawing horizontal line to right across lower right panel, passing through the vent height curves. It is now possible to determine the dimensions of the vent required for the enclosure as to provide hydrogen concentration not exceeding 2 vol. % for a specified hydrogen release. In the example demonstrated in Figure 3, to keep hydrogen concentration below 2 vol. % with the given release rate 0.2 g/s the enclosure should be equipped with the vent 1 m in height and 1 m in width.

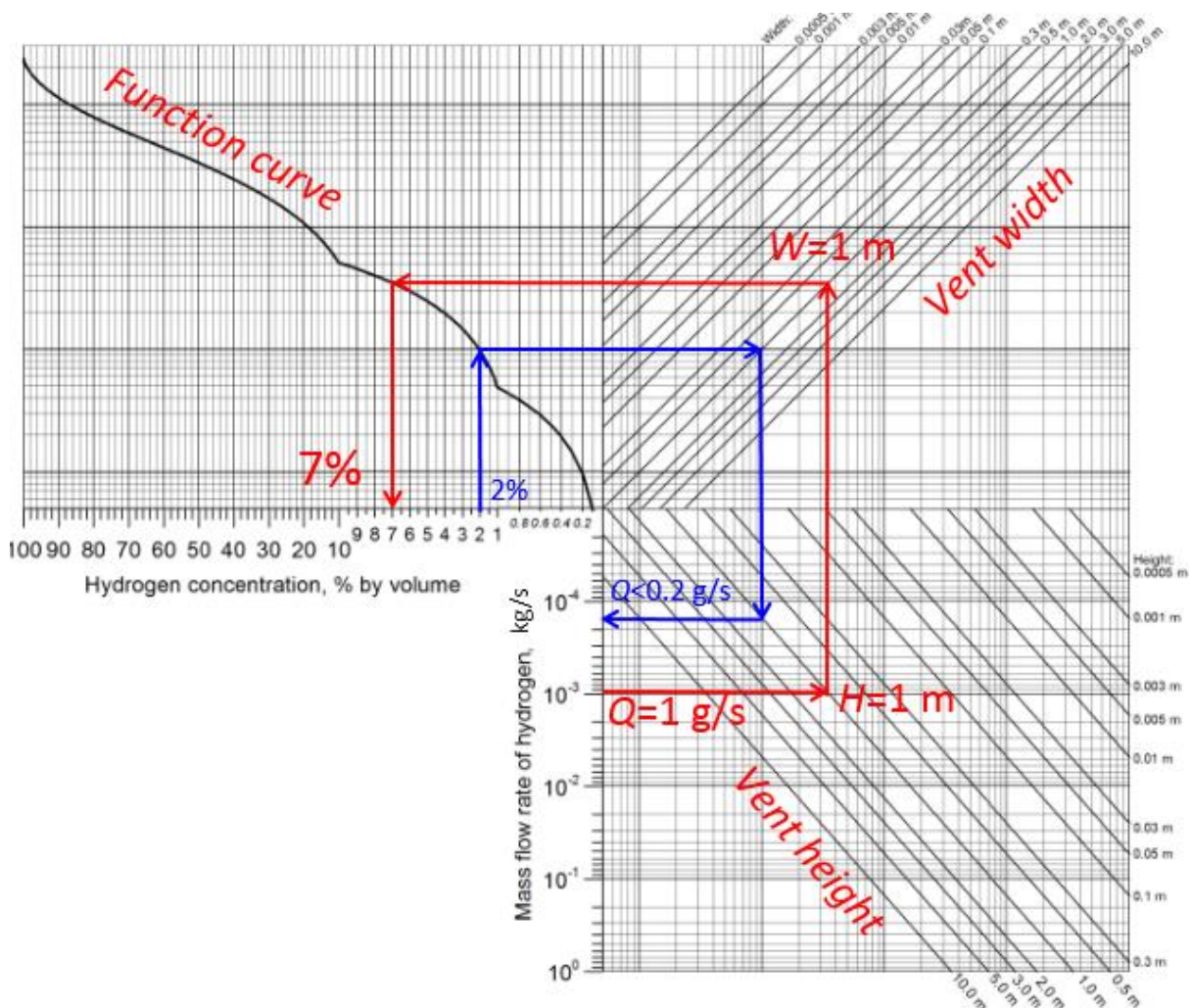


Figure 3. An engineering nomogram for calculation of the maximum value of steady-state concentration of hydrogen in the enclosure with one vent (discharge coefficient $C=0.6$).

Well-ventilated fires

The topic of hydrogen fires was discussed earlier in the relevant lecture. In the case of indoor hydrogen fires, if the fire is sufficiently short and if it does not impinge on a wall or any other surface the nomogram presented in the previous lecture is applicable for predicting the flame length. The work described in the lecture 'Hydrogen fires' on the effects of walls and barriers is also relevant to jet fires impinging directly on obstacles within the enclosure. A hydrogen release in the enclosure frequently occurs near, or along a wall or a surface, which can increase the length of the jet flame or the extent of unignited jet, by reducing the entrainment of the air. Thus hazard distances can increase. This is important when considering the position of equipment and hydrogen storage (particularly the location of PRDs on any storage) in relation to walls, and to the ground. Behaviour of the fire also depends on the release conditions and geometry of the enclosure and the ventilation. Indoor hydrogen fires can be well-ventilated and under-ventilated. If the enclosure is equipped with the ventilation, oxygen required to sustain hydrogen combustion will enter the enclosure through the vents. If there is sufficient ventilation in the enclosure, the flame will be fuel-controlled and can be considered to be well-ventilated [11].

The general rule for an indoor fire with one upper vent is as follows: the increase of hydrogen release flow rate changes the fire regime from

- well-ventilated fire (for small flow rates), to
- under-ventilated fire with external flame (for moderate flow rates), to
- under-ventilated fire with self-extinction of combustion (for higher flow rates), and again to
- under-ventilated fire with external flame (for very high flow rates).

A numerical study was carried out with the use of a contemporary model to understand underlying physical phenomena of the indoor hydrogen fire. The CFD model used has been described in [12, 13]. Seven numerical experiments with a single vent were performed for a FC-like enclosure with the dimensions $L \times W \times H = 1 \times 1 \times 1$ m and with the vent located centrally at the top of one wall (Table 1). The release was directed vertically upwards. Hydrogen release pipe was of 10 cm length with internal diameter of 5.08 mm located in the centre of the enclosure floor, 10 cm above the floor. The thickness of the enclosure aluminium walls was 2 cm. Further details on the calculation domains can be found in [13].

Table 1. Details of the numerical experiments [13].

No.	Vent size, HxW	Velocity, m/s	Flow rate, g/s	Result
1	Horizontal 3x30 cm	600 m/s	1.0857	Self-extinction
2	Horizontal 3x30 cm	300 m/s	0.5486	Self-extinction
3	Horizontal 3x30 cm	150 m/s	0.2714	External flame
4	Vertical 30x3 cm	600 m/s	1.0857	External flame
5	Vertical 30x3 cm	60 m/s	0.1086	Well ventilated
6	Vertical 13.9x3 cm	600 m/s	1.0857	Self-extinction
7	Vertical 13.9x3 cm	300 m/s	0.5486	External flame

Figure 4 shows the dynamics of well-ventilated hydrogen jet fire in the numerical experiment No. 5, with the lowest velocity of the release, 60 m/s. The vertical vent is located at the left wall. At the end of numerical experiment, the fire was at quasi-steady state conditions. The reaction zone, which is

associated with the presence of hydroxyl radicals OH, increases slightly in the time period from 10 s to 65 s (Figure 4a). There is practically no hydrogen leaving the enclosure (Figure 4b). Hydrogen mole fraction in the vent is negligible of the order of 2×10^{-4} . This indicates that the fire is well-ventilated in the conditions of simulation No. 5.

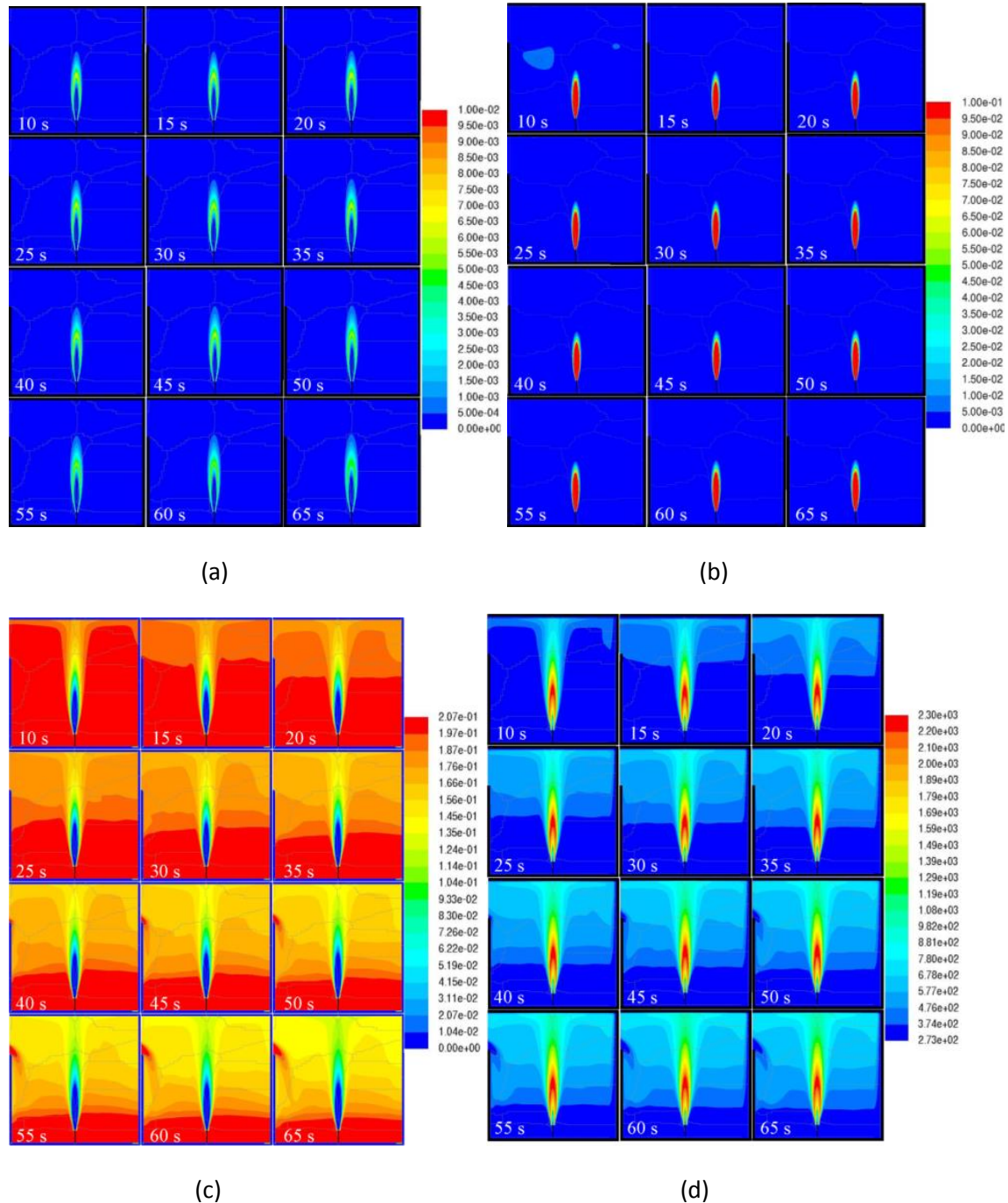


Figure 4. 2D slice along the enclosure centre-line, simulation No. 5 (well-ventilated fire) [13]: (a) OH radicals mole fraction, (b) H_2 mole fraction, (c) O_2 mole fraction, and (d) temperature.

Figure 4c demonstrates a very slow depletion of the initial oxygen layer at the bottom of the enclosure that can be explained by the fact that an intake of oxygen from outside through the lower part of the vent sustains the flame (the intake of air is clearly seen in snapshots). Temperature contours (Figure 4d) confirm the presence of the layer at the bottom of the enclosure, where the initial temperature is

preserved. In a room-like enclosure this would create favourable conditions for the evacuation of the occupants. It is worth noting that radiation is not accounted for in this model that would affect acceptability of a safety engineering design based on harmful criteria of thermal radiation flux. The temperature decays from 2300 K in the flame to about 750-1000 K in the hot current under the ceiling. This temperature is probably insufficient to ignite any combustible materials especially in the presence of water vapour (H_2O mole fraction under the ceiling is in the range 0.11-0.13 at 65 s). Yet some components within the FC box could be destroyed. The only difference of numerical experiment No. 4 is a tenfold increase of the hydrogen release flow rate. The well-ventilated fire is observed for hydrogen release velocity of 60 m/s, and an under-ventilated fire with transition to an external flame is observed for release velocity of 600 m/s.

Under-ventilated fires

In the case where there is insufficient ventilation the flame will be ventilation-controlled and could be considered as *under-ventilated*. In the case where the flame is under-ventilated all hydrogen will not be consumed in the vicinity of the leak and will only burn where oxygen is available, therefore there will be both hot products and potentially hydrogen or an external flame at the vent [14].

The development of a hot layer at the ceiling depends on the size and the location of the vents (if any) relative to the size of the leak. In the case of insufficient ventilation relative to the leak the hot layer will grow downwards through the enclosure. This presents both thermal and asphyxiation hazards.

As the flame becomes increasingly under-ventilated the level of oxygen is decreased in the enclosure until the moment when oxygen and hence combustion are present in the vicinity of the vent producing an external flame. There may be little or no combustion in the rest of the enclosure where hydrogen will accumulate. In this case if the leak were subsequently stopped (shut-off) or reduced through blow-down then the external flame may burn back into the enclosure where a premixed flammable atmosphere may potentially exist, leading to an explosion [14].

If the enclosure has no ventilation then it will not be possible for oxygen to enter the enclosure, thus the flame will deplete the oxygen in the enclosure until either fuel or oxygen is consumed and the flame extinguishes [14].

The product of hydrogen combustion is water, thus it is possible in the case of minimum ventilation and a small flame, that water vapour produced by hydrogen combustion combined with the depletion in oxygen may lead to a self-extinguishment of the flame. If self-extinguishment was to occur and the hydrogen leak was not stopped at the point of extinguishment, then a scenario would develop whereby the enclosure would be filled with unburnt hydrogen. If the leak was subsequently shut off the hydrogen was blown-down then a premixed flammable atmosphere would develop in the enclosure. The presence of hot surfaces or a similar ignition source could lead to re-ignition and a potential explosion. At the limit of an under-ventilated case the external flame exists at the vent. In the case of self-extinguishment, no flame exists, either internally or externally. The details of numerical experiments (Table 1) on under-ventilated hydrogen jet fire and self-extinction dynamics in an enclosure are extracted from [13] and described below.

Self-extinction flame mode

Let us consider a scenario with a jet fire from a TPRD in a small garage with sizes $L \times W \times H = 4.5 \times 2.6 \times 2.6$ m and volume 30.4 m^3 . A single vent equivalent in the area to a typical brick $L \times H = 25 \times 5$ cm is located

flush with the ceiling and excludes consideration of pressure effects. Hydrogen is released through the 5.08 mm pipe at the rate 390 g/s. Combustion of the released hydrogen within the garage consumes oxygen in the air and produces water. A self-extinction of hydrogen in the enclosure could be expected shortly. Indeed, numerical simulations of this scenario demonstrated a decrease in temperature within the enclosure as shown in Figure 5 and the regions of OH associated with reaction zones after 3 s already.

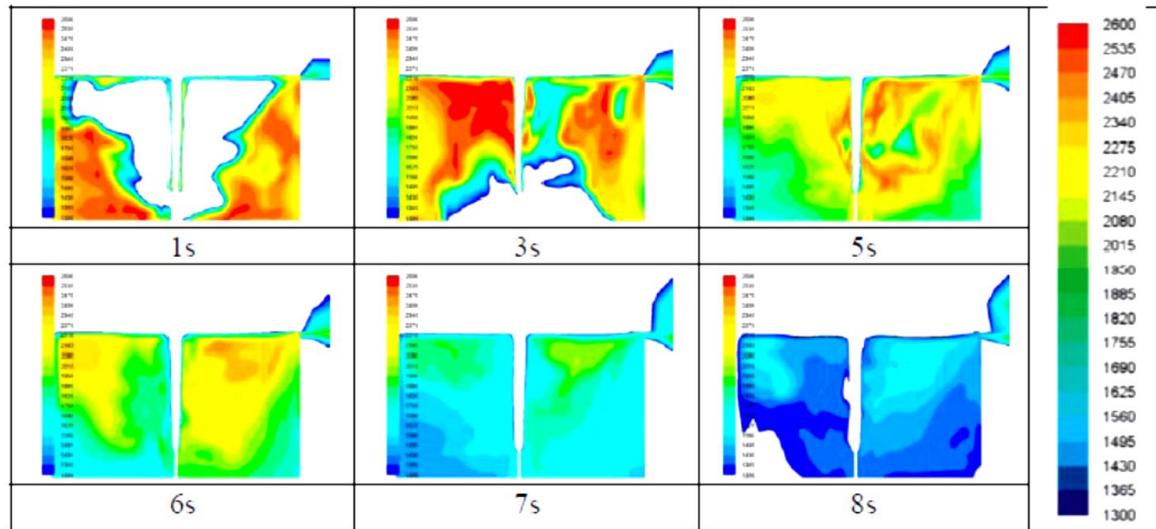


Figure 5. Contours of static temperature ranging from 1300 to 2600 °C corresponding to the visible flame (2D slice through centre of the garage) [15].

The self-extinction of a hydrogen flame in the enclosure with one horizontal vent located at the top of one wall was reported for the first time in [12]. The analysis of the numerical experiment, especially of hydroxyl (OH) concentration, assisted in understanding of the self-extinction process. The use of averaged throughout the enclosure volume parameters during the under-ventilated fire can give an indication of the moment when combustion is reduced, however it can underestimate significantly the timing when the flame is fully ceased. The numerical experiments demonstrated a complex pattern of flow through the vent in both directions during the under-ventilated fire. The complete self-extinction was observed when the entire vent area was occupied for a finite period of time by the air intake into the enclosure. The reason of this observation was assumed to be the cooling of hot combustion products by the sustained hydrogen release and, to some extent, by heat transfer to the enclosure walls. The work [13] expands the initial numerical experiments and aims at understanding of indoor hydrogen fires in the enclosure with one horizontal or vertical vent located at the top of one wall and a sustained hydrogen release of constant flow rate and temperature.

Self-extinction of hydrogen flames indoors was also simulated in the numerical experiment No. 1 with the horizontal vent (Table 1) [12].

Let us consider the dynamics of self-extinction observed in the simulation No. 2 (the release velocity of 300 m/s) and compare it with the simulation No. 1 (the release velocity of 600 m/s). Figure 6 shows the dynamics of OH mole fraction for simulation No. 2 in 3D (Figure 6a) and 2D (Figure 6b). The reaction contour (OH mole fraction iso-surface of 1×10^{-4}) shows location of flaming combustion and moves out of the enclosure at about 30 s. This zone of the reaction outside the enclosure separates from the reaction zone inside the enclosure at 45 s and exists until about 56 s. The size of this external

small reaction zone does not exceed two vent heights. At about the same time of 56-57 s there is air ingress into the enclosure that supports a weak reaction just below the vent. This internal reaction zone practically ceases at about 120 s. Contrary to the experiment No. 4 with the external flame, in the simulation No. 2 with the self-extinction, the combustion in the jet ceases first on the left side, which is closer to the vent, at 55-56 s. This can be explained and consistent with the presence of a bit larger amount of oxygen at this time at the bottom on the right hand side of the jet (Figure 6a).

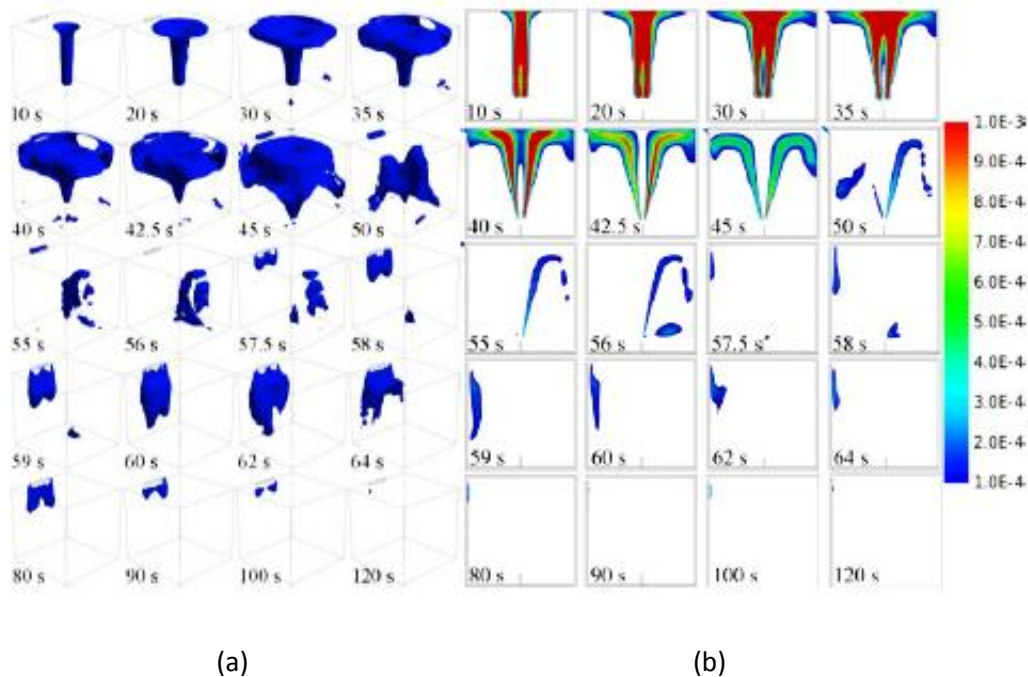


Figure 6. Hydroxyl OH mole fraction in $1 \times 1 \times 1$ m enclosure, simulation No. 2 (hydrogen jet fire self-extinction) [13]: (a) 3D view of iso-surface of OH 1×10^{-4} , (b) 2D slice along the enclosure centre-line.

The small size of the reaction zone outside of the enclosure in the period 30-56 s can be explained by analysis of species concentrations presented in Figure 7. Indeed, during this period hydrogen concentration in the flow out of the enclosure does not exceed about 7-10 vol. %, concentration of water is increasing from about 15 to more than 34 vol. %, and oxygen concentration drops from about 10 vol. % to 0 vol. %. The flammability diagram shows that this mixture with the air is just on the border of the flammable region [16]. In the simulation No. 2 this mixture reacts with air in conditions when temperature of the mixture is quite high and drops to about 800 K only at the end of this period.

As it follows from Figure 7 the flow out of the enclosure finishes after 50 s and there is only inflow into the enclosure (see the snapshots corresponding to 57.5 s through to 120 s). Thus, in the agreement with simulation No. 1 for the self-extinction to happen there has to be a prolonged period of time when, after the initial stage of internal combustion followed by the cooling of hot products by “cold” hydrogen, there is an intake of air through the whole area of the vent into the enclosure.

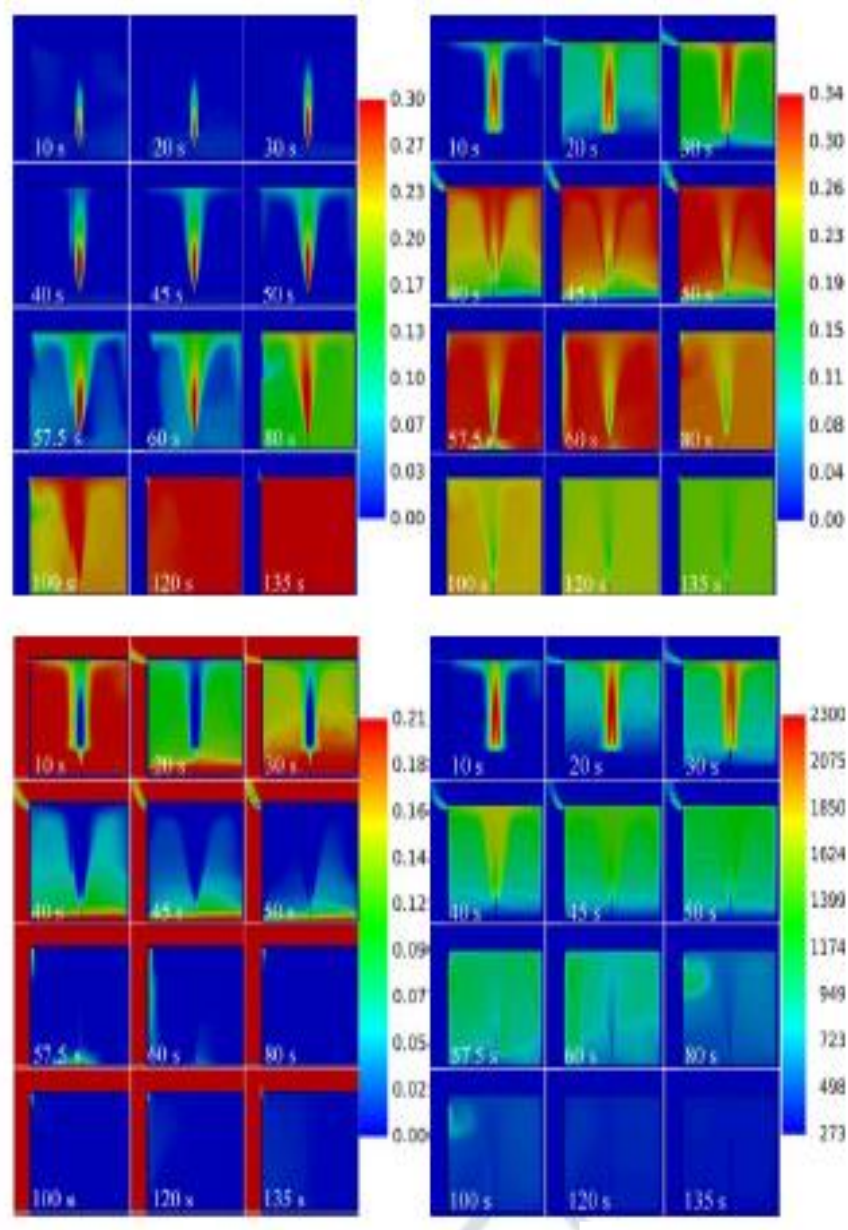


Figure 7. 2D slice along the enclosure centre-line simulation No. 2 (hydrogen jet fire self-extinction) [13]: (a) H₂ mole fraction, (b) H₂O mole fraction, (c) O₂ mole fraction, and (d) temperature.

Figure 7 (a) shows that after 2 minutes of the release the enclosure is filled in with hydrogen with mole fraction above the stoichiometric level, > 0.30 . Similar to the simulation No. 4 with the vertical vent the jet is slightly inclined to the wall with the vent. The maximum mole fraction of water is observed at 50-60 s. There is a strong “stratification” of oxygen at the time of 40-50 s, with practically zero concentration at the top and practically initial concentration of oxygen of 20.7 vol. % at the bottom. Temperature falls down to about 100 degree above initial temperature after 2 minutes of ignited release. This result can be used as an indication of fire resistance time to components within the fuel cell enclosure.

The former conclusion that the self-extinction is always observed when there is a period of time when there is air intake into the enclosure through the whole vent area is confirmed in experiment

corresponding to conditions of simulation No. 6 (Table 1) with the vertical vent of the smallest area. To further support this rule, in the simulation No. 7 (external flame) there was no such period.

External flame mode

Figure 8 demonstrates the results of the simulation No. 4 for the release with the velocity of 600 m/s, when a transition of an internal jet fire in the enclosure to an external flame mode occurs. The mole fraction of hydroxyls in the flame at 10 s is equal 0.01, which is characteristic for combustion at normal atmospheric conditions (not shown in Figure 8). Then, the maximum OH mole fraction reduces along with shrinking of the zone where the highest mole fraction of OH is present. This is thought due to dilution of the jet flame by entrained combustion products. The maximum mole fraction of OH does not exceed 7.5×10^{-3} at time of 20 s.

Figure 8a shows the evolution of the reaction zone during the transition of the internal combustion to the external flame by visualization of OH mole fraction in the range from 1×10^{-6} to 5×10^{-4} , whilst an image in Figure 8b corresponds to the range 5×10^{-4} - 1×10^{-3} . There is no or very little reaction outside the enclosure up to 20 s. While the combustion rate inside the enclosure decreases after 20 s the reaction zone starts to move out of the enclosure through the vent with the external flame being visible above the enclosure after 50 s. Figures 8a and 8b clearly show that the reaction ceases first on the jet flame side that is opposite to the vent which is located at the top of the left wall. Figure 8b demonstrates that there is a continuous reaction zone on both sides of the vent. This zone connects the internal reaction in the area where fresh air is entering the enclosure with the external flame of flowing out of the enclosure mixture of hydrogen and combustion products in the atmospheric air. These two opposite flows through the vent create a reacting eddy that seats within the enclosure close to the vent and stabilises the lower flame edge. The upper edge of the external flame is attached to the top edge of the vent.

The evolution of hydrogen mole fraction in the enclosure is shown in Figure 8c. Fire is in the well-ventilated regime until about 20 s when there is no hydrogen leaving the enclosure due to its complete combustion inside. The accumulation of hydrogen is somewhat higher at the side of the jet opposite to the wall with the vent. There is some inclination of the jet towards the vent (see the snapshot at 50 s). The mole fraction of hydrogen is above 0.30 practically throughout the whole enclosure at time of 65 s with exclusion of small region close to the vent where the air is entering. The mole fraction of hydrogen at 110 s is 0.48 to 0.50 at floor and ceiling levels respectively.

The maximum amount of water vapour is observed at 27-30 s (Figure 8d), similar to the simulation No. 1 with a horizontal vent of the same area reported in [12]. After this, the mole fraction of water is monotonically decreases in time due to water entrainment into the sustained hydrogen jet and flow out of the enclosure (as a part of flammable mixture).

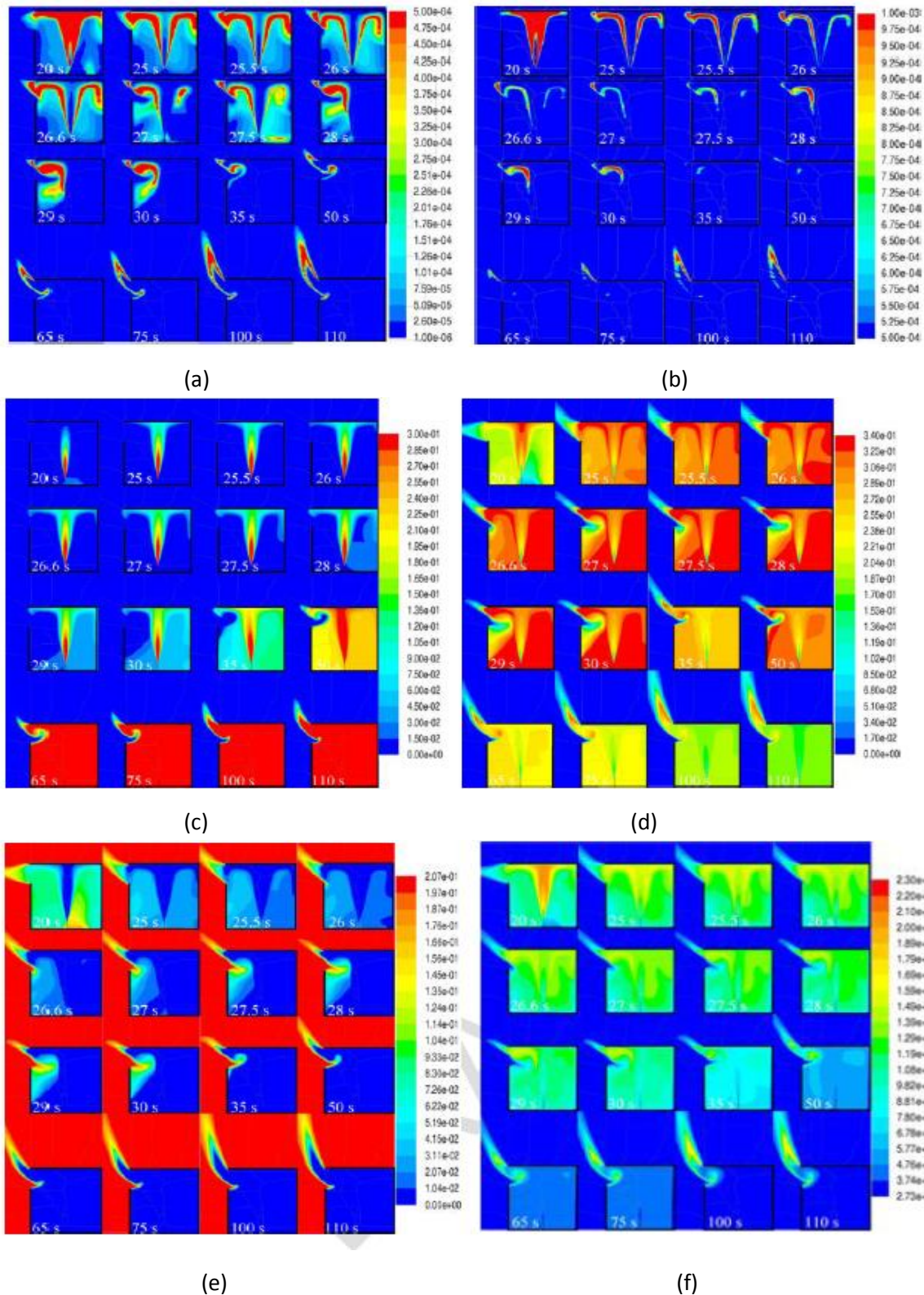


Figure 8. 2D slice along the enclosure centre-line, simulation No. 4 (hydrogen jet fire external flame mode) [13]: (a) OH mole fraction, range 1×10^{-6} – 5×10^{-4} , (b) OH mole fraction, range 5×10^{-4} – 1×10^{-3} , (c) H_2 mole fraction, (d) H_2O mole fraction, (e) O_2 mole fraction, and (f) temperature.

At a critical for flame “survival” time point of about 50 s, when the transition to the external flame commences, the mole fraction of hydrogen in outflow increases to about 0.2, and that of water

(diluent) drops to 0.2-0.3. This mixture composition is deemed to be in the flammable range following the flammability diagram for hydrogen-air-diluent mixture at atmospheric pressure and temperature, if the effect of temperature is neglected. Thus, the availability of flammable mixture flowing out of the enclosure and the presence of reaction (ignition source) provide conditions for transition of combustion outside of the enclosure.

Figure 8e shows that oxygen mole fraction within the enclosure gradually decreases and is practically equal to zero at the time of 35 s, excluding a small area close to the vent. Then, the air entering the enclosure to some small depth burns and is immediately entrained into flow of hydrogen and combustion products flowing out of the enclosure through the upper part of the vent. Temperature dynamics inside and outside the enclosure is shown in Figure 8f. The snapshot corresponding to 50 s demonstrates an important role of the reacting eddy, which is formed in the vent shear layer between mixture leaving the enclosure and air entering the enclosure, on the flame sustainability and the transition of under-ventilated internal fire to the external flame mode.

For the horizontal vent of the same area the establishment of the external flame was observed in the simulation No. 3 at a lower velocity of hydrogen, 150 m/s. The same velocity of the release as in the simulation No. 4 (vertical vent), i.e. 600 m/s, for the horizontal vent resulted in the flame self-extinction (simulation No. 1). The self-extinction was observed also at the velocity of 300 m/s (simulation No. 2). Thus, a velocity limit separating the external flame mode and the self-extinction mode is between 150 m/s and 300 m/s for the given enclosure geometry.

The external flame is observed in the simulation No. 7 with a vertical vent of the smallest area and for the release velocity of 300 m/s. The increase of release velocity to 600 m/s (simulation No. 6) resulted in the self-extinction. It is noted that a characteristic feature of the self-extinction phenomenon is the existence of a period when there is air intake into the enclosure through the whole area of the vent (not a part of the vent area).

Pressure peaking phenomenon

Pressure peaking is the phenomenon observed for the gases which are very light (lighter than air), which can result in overpressure exceeding the structural strength limit of an enclosure or a building in the case of sufficiently high hydrogen release rate. Pressure peaking would occur if hydrogen release flow rate is high enough to result in complete displacement of the air from the enclosure, i.e., hydrogen concentration within enclosure must reach 100 vol. %.

It is known that in FC vehicles hydrogen is most commonly stored today as a compressed gas in tanks, which are equipped with pressure relief devices (PRDs) as per EU No 406/2010 Commission Regulation [17]. The PRD is fitted to the fuel tank and begins to release hydrogen when temperature of about 110 °C is reached, e.g. in fire conditions. The PRD can provide rapid release of hydrogen, if large orifice diameter is used, thus minimising the possibility of tank explosion during too long exposure to fire. High mass flow rates from PRDs are probably “acceptable” for outdoors. However, the hazards resulting from a rapid release indoors are different.

Let us consider a hypothetical scenario involving a release from a typical on-board hydrogen storage tank at 35 MPa, through a 5.08 mm diameter orifice [18]. The release is assumed to occur vertically upward in the centre, 0.5 m above the floor, of a small garage of size $L \times W \times H = 4.5 \times 2.6 \times 2.6$ m [19] and volume of 30.4 m³ with a single vent equivalent in area to a typical brick $L \times H = 25 \times 5$ cm located flash

with the ceiling. A conservative approach is taken, i.e. a constant mass flow rate of 0.39 kg/s is applied (ignoring a pressure drop in the storage tank) after the PRD opening. Thus, a worst-case scenario i.e. high mass flow rate in a small garage with minimal venting is considered.

The application of mathematical models for the steady state subsonic release (when hydrogen fully occupies the enclosure) gives the predicted overpressure values in the enclosure in range between 15 (resulting from Bernoulli's equation with zero velocity in the vessel) and 17.9 kPa (from orifice flow equation for subsonic flow) for a discharge coefficient C in both cases taken as commonly recommended $C=0.6$ [20]. However, these estimates do not account for the initial state of injection of a lighter gas (hydrogen) into a heavier gas (air). The predicted transient pressure load in the vented enclosure is given in Figure 9.

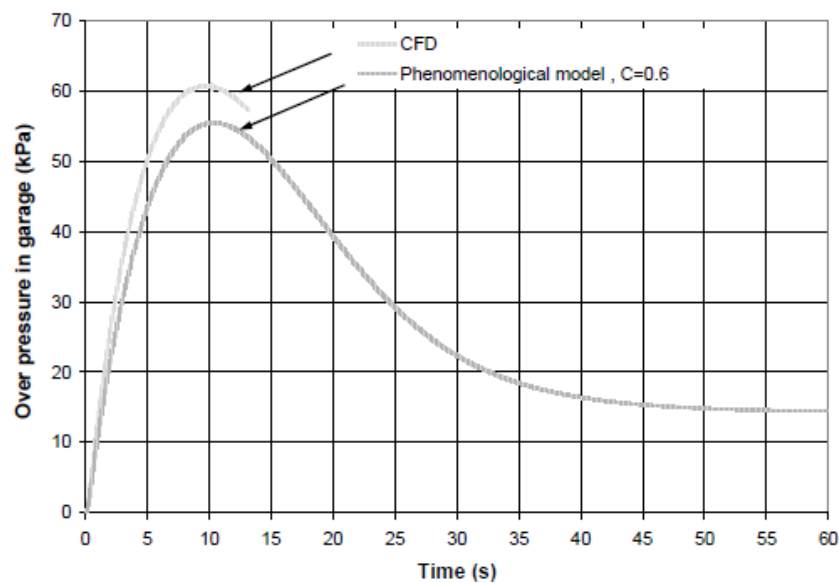


Figure 9. Predicted overpressure in the garage with time, a comparison between CFD and a phenomenological model [18].

Figure 9 illustrates how the overpressure within the enclosure resulting from the injection of hydrogen reaches a level capable of demolishing the garage [9] within only 3 s for the selected scenario. As it follows from Figure 9 if the garage is not destroyed first, the pressure within the garage, for this particular scenario, reaches a maximum level in excess of 60 kPa. The pressure then drops off and tends towards a steady state value, considerably lower, and equal to that predicted by the simple steady state estimations. Once again please note that this represents a worst case scenario with a constant mass flow rate. Therefore, continuation of a constant mass flow rate for 60 s included in Figure 9 is purely for illustrative purposes to show the time frame before steady state conditions are reached when practically all the garage is occupied by 100 vol. % hydrogen. It should also be noted how the maximum pressure is reached in less than 10 s: within this time the entire garage would be demolished, without even considering the consequences of ignition.

It should be noted that the overpressure level reached inside the garage increases with the decrease of molecular mass of the gas injected into the garage, i.e. lighter gas such as hydrogen results in a significantly higher pressure than a heavier one, e.g. propane. This should be taken into account when

designing PRDs for use with hydrogen, i.e. the same technology used for e.g. CNG should not be assumed to behave in the same way for hydrogen.

Figure 10 demonstrates the predicted overpressure values versus time for a range of gases with the same mass flow rate (0.39 kg/s) in the same garage-like enclosure (volume 30.4 m³, vent 0.0125 m²). Discharge coefficient $C=0.6$. The molecular masses of hydrogen, helium, methane and propane are 0.002, 0.004, 0.016 and 0.044 kg/mol, respectively. It is clear that the peak of overpressure drops with the increasing molecular mass of the gas. The higher the molecular mass of the gas, the closer the maximum pressure is to steady state values predicted using simple methods. The volumetric flow rate out of the enclosure is inversely proportional to the square root from the density of gas escaping the enclosure. Thus, in the beginning of the process when the density of the hydrogen-air mixture is very high and close to the density of the air, the constant volumetric inflow of pure hydrogen is essentially higher than the volumetric outflow of the heavier hydrogen-air mixture and this explains why the overpressure for lighter incoming gas grows to a higher level compared to that for a heavier incoming gas and pressure dynamics has a characteristic peak for hydrogen only.

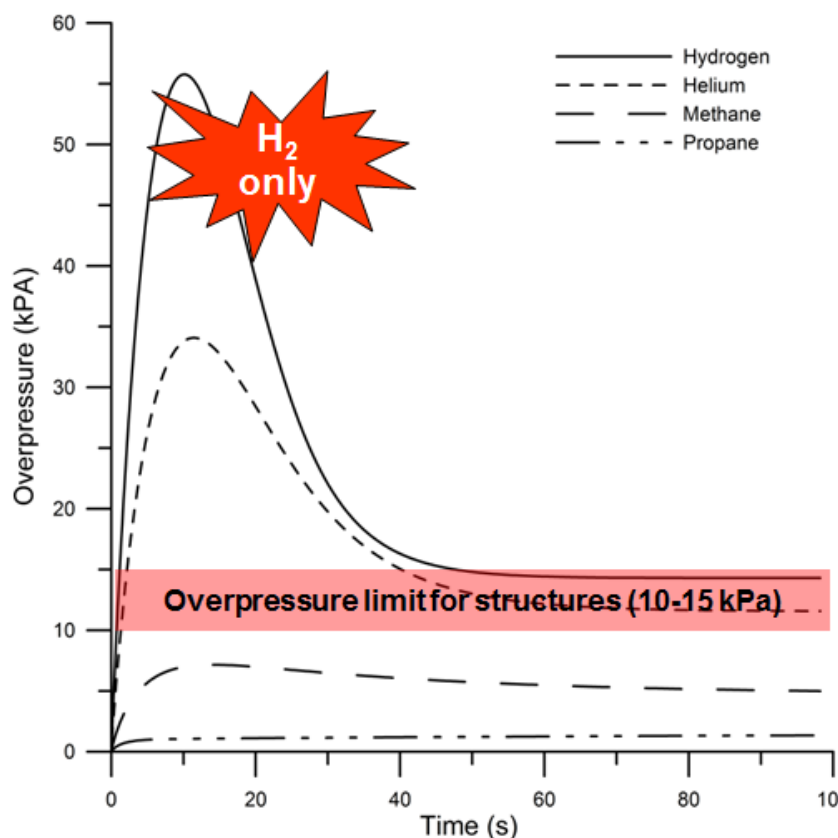


Figure 10. Predicted overpressure values for hydrogen, helium, methane and propane released in a garage versus time, release rate of 0.39 kg/s [18].

Pressure peaking phenomenon only occurs when hydrogen release rate is sufficiently high to completely displace air from the enclosure with time of sustained leak. Therefore, before estimating overpressure produced by PPP (and applying the engineering tool described later) it is necessary to confirm whether the release rate is sufficient to fill the enclosure with 100% of hydrogen if a leak is sustained. An engineering nomogram in Figure 11 can be used to verify this [10]. The nomogram allows one to calculate the maximum vent dimensions which for a given steady release will eventually result in a 100 vol. % hydrogen concentration in the enclosure. In order to find the maximum vent

dimensions, select hydrogen release rate on the vertical axis and draw a horizontal line until its intersection with one of the diagonal lines corresponding to an appropriate vent width. Draw a vertical line from the intersection point to horizontal axis to find the required vent height. Alternatively, the nomogram in Figure 11 can be used to find the minimum release rate for a known vent size when calculation of PPP is needed, in which case the above steps are reversed. If the release rate found through this nomogram is lower than the actual one, or the actual vent dimensions are smaller than found using nomogram in Figure 11, 100 vol. % hydrogen concentration will be reached and PPP can occur and the nomogram for PPP (Figure 12) should be used.

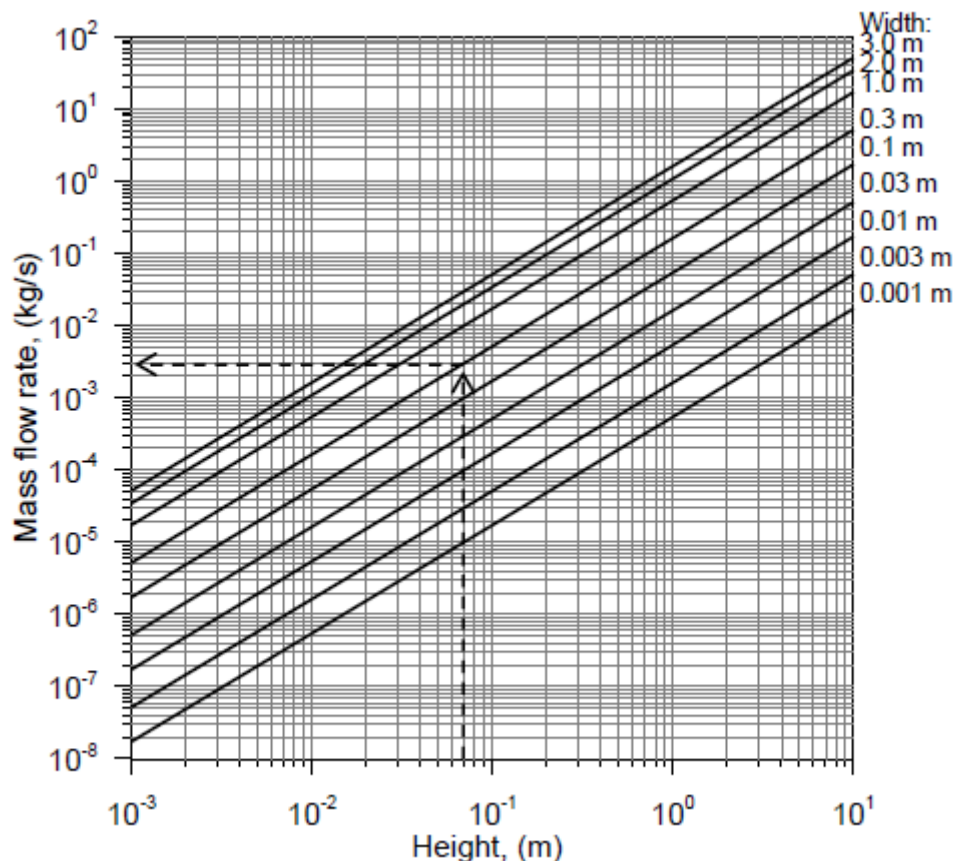


Figure 11. The nomogram for graphical evaluation of hydrogen leak mass flow rate in an enclosure with one vent, which leads to 100 vol. % of hydrogen concentration [10].

Figure 12 shows a nomogram for PPP evaluation, which allows calculation of the maximum overpressure peak produced by high rate hydrogen release from the known mass flow rate and leak diameter. To use the nomogram in Figure 12, follow the following procedure:

- Start with the vertical axis on the lower panel of the graph and select storage pressure, read across horizontally to the leak diameter.
- Read vertically upwards to calculate the mass flow rate of the leak. Continue vertically upward from the mass flow rate to the point of intersection with the line for the appropriate vent area in the upper panel.
- Read horizontally to the left until the intersection with the vertical axis. The point of intersection provides the maximum overpressure in the enclosure.

Alternatively, the nomogram in Figure 12 can be used to determine the area of the vent required to keep the overpressure below the specified limit. In this case, follow the first two steps and then draw

a horizontal line from the desired overpressure value found on the vertical axis of upper panel of the graph. The closest to the intersection curve in the upper panel will correspond to the required vent area (if the intersection falls between two curves, use rightmost in order to obtain a conservative value).

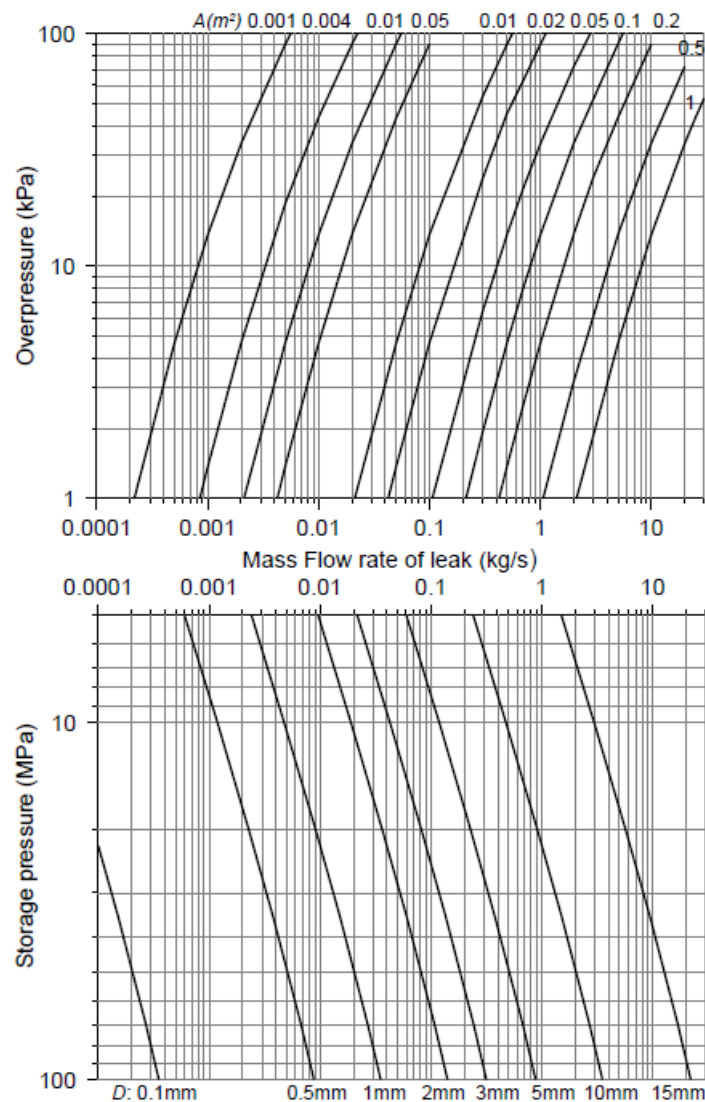


Figure 12. Pressure peaking nomogram for various release rates [4].

Summary

The final lecture provides First Responders with an overview of the indoor use of FC and hydrogen technologies. It is stressed that the information covered in the previous lectures is all applicable and thus only additional recent research is included here. This lecture highlights the specific hazards related to FCH systems located indoors. It covers the important topics of passive and forced ventilation, well-ventilated and under-ventilated hydrogen fires including two regimes of self-

extinction, and external flame. This lecture also discusses pressure peaking phenomenon, which is specific for hydrogen.

References

1. HyIndoor project. Available from <http://www.hyindoor.eu/> .
2. HyResponse Deliverable D2.2 - Detailed scenarios of typical accident for selected FCH systems and infrastructure (2016). Available from: <http://www.hyresponse.eu> [accessed 10.06.16].
3. Saffers, J-B and Molkov, V (2014). Hydrogen safety engineering framework. International Journal of Hydrogen Energy. Vol. 39, pp. 6268-6285.
4. HyIndoor Deliverable D5.1 – Widely accepted guidelines on FC indoor installation and use (2015). Available from: <http://www.hyindoor.eu> [accessed 23.05.16].
5. Karlsson, B and Quintiere, J (2000). Enclosure fire dynamics. CRC Press.
6. Molkov, V (2012). Fundamentals of hydrogen safety engineering, Part I and Part II. Available from: www.bookboon.com, free download e-book.
7. Brennan, S and Molkov, V (2013). Safety assessment of unignited hydrogen discharge from onboard storage in garages with low levels of natural ventilation. International Journal of Hydrogen Energy. Vol. 38, pp. 8159-8166.
8. ISO/TR 15916 (2004). Basic considerations for the safety of hydrogen systems. International Organization for Standardization. ISO Technical Committee 197 Hydrogen Technologies. International Organization for Standardization, Geneva.
9. Baker, WE, Cox, PA, Westine, PS, Kulesz, JJ and Strehlow, RA (1983). Explosion hazards and evaluation. Amsterdam: Elsevier Scientific Publishing Co, The Netherlands.
10. Molkov, V, Shentsov, V and Quintiere, J (2014). Passive ventilation of a sustained gaseous release in an enclosure with one vent. International Journal of Hydrogen Energy. Vol. 39 (15), pp. 8158– 8168
11. HyIndoor Deliverable D4.3 – Second intermediate report on analytical, numerical and experimental studies (2014). Available from: <http://www.hyindoor.eu> [accessed 20.05.15].
12. Molkov, V, Shentsov, V, Brennan, S, and Makarov, D (2013). Dynamics of Hydrogen Flame Self-Extinction in a Vented Enclosure. Proceedings of the 7th International Seminar on Fire and Explosion Hazards”, 5-10 May 2013, Providence, RI, USA.
13. Molkov, V, Shentsov, V, Brennan, S, and Makarov, D (2013). Hydrogen non-premixed combustion in enclosure with one vent and sustained release: numerical experiments. Proceedings of ICHS 2013, 9-11 September 2013, Brussels, Belgium.
14. HyIndoor Deliverable D4.1 – Detailed research program for hydrogen jet fires in a confined spaces (2013). Available from: <http://www.hyindoor.eu> [accessed 20.05.15].
15. Molkov, V, Bragin, M, Brennan, S, Makarov, D, and Saffers, J-B (2010). Hydrogen Safety Engineering: Overview of Recent Progress and Unresolved Issues. International Symposium of Combustion and Fire Dynamics, October 2010, Santander, Spain.
16. Trevino, C and Mauss, F (1992). Chapter 10 “Structure and Extinction of Non-Diluted Hydrogen-Air Diffusion Flames”, In: Peters, N., Rogg, B., Reduced Kinetic Mechanisms for Applications in Combustion Systems. Lecture Notes in Physics, Volume m15. Springer-Verlag, 1992.
17. EU No 406/2010, Commission Regulation of 26 April 2010 implementing Regulation (EC) No 79/2009 of the European Parliament and of the Council on type-approval of hydrogen-

powered motor vehicles. Official Journal of the European Union. Vol. 53, 18 May 2010. Available from: <http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2010:122:FULL:EN:PDF> [accessed on 13.02.14].

18. Brennan, S, Makarov, D and Molkov, V (2010). Dynamics of flammable hydrogen-air mixture formation in an enclosure with a single vent. Proceedings of the 6th International Seminar on Fire and Explosion Hazards, Leeds, April 2010.
19. SAE J2579 (2009). Technical information report for fuel systems in fuel cell and other hydrogen vehicles, SAE International, Detroit, Michigan, USA, January, 2009.
20. Emmons, DD (1995). Vent flows, SFPE Handbook, ed. P. J. Di Nenno, (2nd Edition). Society of Fire Protection Engineers, Boston, MA, USA.
21. Brennan, S and Molkov, V (2013). Safety assessment of unignited hydrogen discharge from onboard storage in garages with low levels of natural ventilation. International Journal of Hydrogen Energy. Vol. 38, pp. 8159-8166.