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Molkov, V., Shentsov, V., Brennan, S., & Makarov, D. (2013). Dynamics of Hydrogen Flame Self-Extinction in a Vented Enclosure. In *Unknown Host Publication* University of Maryland. https://doi.org/10.3850/978-981-07-5936-0_14-03

[Link to publication record in Ulster University Research Portal](#)

Published in:
Unknown Host Publication

Publication Status:
Published (in print/issue): 10/05/2013

DOI:
[10.3850/978-981-07-5936-0_14-03](https://doi.org/10.3850/978-981-07-5936-0_14-03)

Document Version
Publisher's PDF, also known as Version of record

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Dynamics of Hydrogen Flame Self-Extinction in a Vented Enclosure

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ABSTRACT

The phenomenon of hydrogen jet flame self-extinction in an enclosure with one vent is simulated numerically for the first time. The eddy dissipation concept model of combustion with a full chemistry scheme is applied along with the renormalization group theory for turbulence modelling within RANS approach. The analysis of temporary profiles of temperature and species (hydrogen, oxygen, hydroxyl, water) concentrations in the numerical experiment, as well as velocity through the vent, shed a light on the dynamics of under-ventilated hydrogen fire the self-extinction process in the enclosure with one horizontal vent located under the ceiling. The self-extinction is a process rather than an instance. The analysis of under-ventilated fire based on parameters averaged throughout the enclosure can give a good indication of the moment when combustion essentially reduces due to lack of oxygen, yet it can mislead in interpretation of the moment when combustion is fully ceased. It is shown that the pressure peaking phenomenon is more pronounced for jet fire compared to unignited release from the same source (by factor 100 in this particular experiment, i.e. about 300 Pa and 3 Pa respectively). The separation distances from the enclosure are estimated for this indoor fire scenario. The maximum length of hot gases jet escaping the enclosure was about twice of the enclosure size. The simulations demonstrated a complex flow dynamics through the vent in both directions during the self-extinction process. This is thought due to the interaction between processes of sustained hydrogen leak, combustion, and heat transfer to the enclosure walls. The separation distances from the enclosure are estimated for indoor fire scenario.

KEYWORDS: Self-extinction, hydrogen flame, under-ventilated fire, numerical experiment, species concentrations.

INTRODUCTION

Indoor use of hydrogen and fuel cell systems poses a number of safety issues in case of unscheduled leak. One possible accident scenario is hydrogen jet fire in an enclosure. Knowledge about hydrogen jet flame behaviour in confined space is practically absent. Before safety strategies and engineering tools for indoor hydrogen fires are developed underpinning physical phenomena have to be understood. This paper is focused on understanding of under-ventilated hydrogen fire dynamics, and especially on the process of flame self-extinction. The study includes a numerical experiment exploiting the most advanced modelling techniques and its analysis.

The CFD solver of the ANSYS FLUENT software based on Reynolds Averaged Navier-Stokes (RANS) equations is applied. The eddy dissipation concept [1] is exploited for simulation of combustion with a full chemistry scheme, and the renormalization group theory [2] is used for the sub-grid scale modelling of turbulence. A similar approach has been successfully applied recently for the simulation of spontaneous ignition of a sudden hydrogen release in a T-shaped pressure relief device [3]. However, compared to the study of spontaneous ignition the reaction scheme for indoor fire simulations excludes NO_x chemistry. Previous work [3] can be considered as an implicit validation of the approach and sub-models in absence of hydrogen indoor fire experiments planned for 2013-2014 within the HyIndoor project (www.hyindoor.eu).

NUMERICAL EXPERIMENT DESCRIPTION

The simulations were carried out to investigate dynamics of self-extinction phenomenon in a fuel cell like enclosure of size $L \times W \times H = 1 \times 1 \times 1$ m with one horizontal vent of size $H \times W = 0.03 \times 0.3$ m located in a wall centre just under the ceiling. Hydrogen leak mass flow rate was 1.085 g/s, which corresponds to flow velocity 600 m/s at temperature 273 K through a pipe of 5.08 mm internal diameter. This is a characteristic mass flow rate for a 50 kW fuel cell. The leak from the pipe was directed vertically upward. The pipe exit was 10 cm above the floor. Hydrogen was released in the numerical experiment from a boundary that is a cross-section of the pipe located 5 cm within the pipe with the uniform sub-sonic velocity of 600 m/s. The pipe was initially filled in by air. The composition of air in the simulations is taken as 20.7% by volume of oxygen and 79.3% by volume of nitrogen. Initial temperature of air was 293 K throughout a calculation domain, i.e. 20 degree higher than leaking hydrogen. The mass flow rate and the temperature of leaking hydrogen were both kept constant during the simulations.

The vent size was pre-calculated using theory [4] to ensure that there is no air ingress into the enclosure through the vent when the enclosure is fully occupied by hydrogen in a case of unignited release, and that the pressure peaking phenomenon [5] does not generate overpressure above 10 kPa that all civil structures can withstand without destruction (windows can be broken in some cases by pressures as low as 2 kPa). The overpressure due to the pressure peaking phenomenon for the unignited release in the enclosure was estimated as insignificant 3 Pa.

The calculation domain was a hexahedron of size $L \times W \times H = 7 \times 6 \times 4$ m that included the enclosure and free space around. The enclosure walls were “made” of aluminium with thickness of 20 mm. Heat transfer to the enclosure walls, ceiling and floor was simulated by means available in ANSYS FLUENT. The simulations were performed for 145 s of real time after the beginning of the release, including stages of the short unignited release, the numerical ignition of the hydrogen jet, the initial stage of combustion that is “well-ventilated”, the under-ventilated jet fire with flame self-extinction, and finally the stage of non-reacting hydrogen release into the hot combustion products and its cooling.

The block-structured hexahedral grid generated by ICEM CFD 13.0 is shown in Fig. 1. The calculation domain counts a total number of control volumes (CVs) 1,530,987. The hydrogen inflow boundary was a cross-section area of 45 CVs and 450 CVs in total within the pipe. The total number of CVs in the enclosure is 229,746. The wall thickness is resolved with 4 cells and there are 73,274 CVs inside walls. The number of CVs along the vent width is 33, and along the vent height is 5 (depth of the vent is the same as walls - 4 cells). There are 660 CVs in the vent.

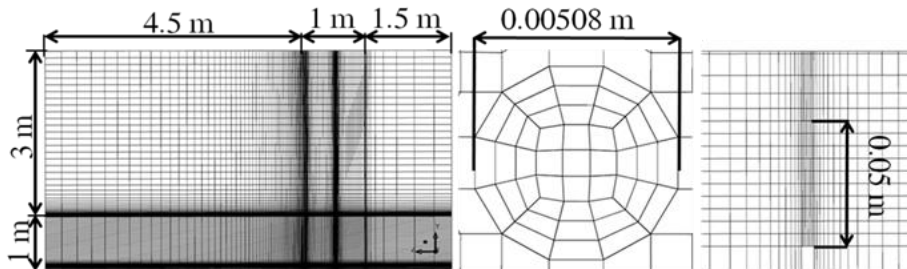


Figure 1. Calculation domain and computational mesh: general view (left), pipe cross-section (centre), pipe side view (right).

RESULTS AND DISCUSSION

Unignited release stage and numerical ignition

The unignited release stage had continued in this numerical experiment for the first 0.3 s. The contours of hydrogen jet development during this period are shown in two first snapshots in Fig. 2 (top). Numerical ignition was initiated at 0.3 s after the beginning of the release when the initial hydrogen jet reached about 80% of the enclosure height (snapshot “0.3 s” in Fig. 2, top).

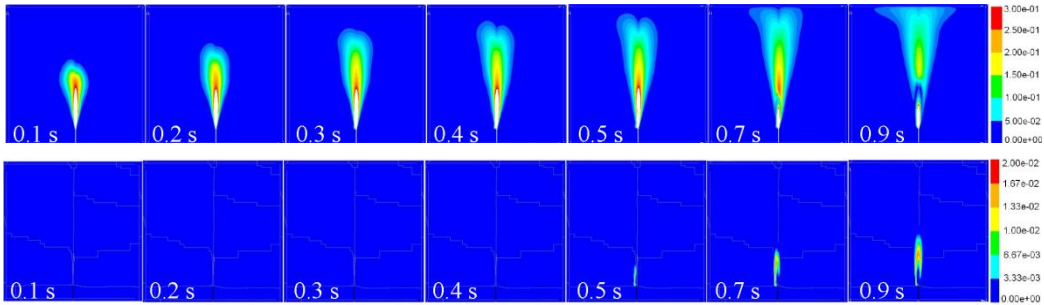


Figure 2. Contours of hydrogen (top) and hydroxyl (bottom) mole fractions in 2D slice along the pipe axis.

The duration of numerical ignition was 0.2 s: from 0.3 s to 0.5 s. The numerical ignition source was a patch with temperature 3000 K over the zone $LxWxH=1x0.25x1$ cm that occupies 62 control volumes (CVs) and touches the pipe on its left side (see Fig. 2, top, snapshots “0.3 s” and after). The zone was chosen to include a region with near stoichiometric hydrogen-air mixture to facilitate the numerical ignition. Snapshots “0.7 s” and “0.9 s” in Fig. 2 (top) clearly demonstrate that the flow is affected by the initiated combustion.

Figure 2 (bottom) shows areas within the enclosure with high concentration of hydroxyl where combustion takes place. The mole fraction of hydroxyl of about 0.01 is usually accepted as associated with the combustion zone at normal atmospheric conditions [6]. There is a clearly seen zone with no hydrogen in the jet at snapshot “0.9 s” (Fig. 2, top) when the reaction zone is already established and consumes hydrogen (Fig. 2, bottom). There is a flammable non-uniform hydrogen-air cloud above the reaction zone at this moment with the highest concentration of about 16% of hydrogen by volume in air. The established non-premixed turbulent flame does not present an ignition source for the premixed hydrogen-air cloud above the flame, which would be expected to deflagrate in fractions of seconds if ignited. This is in agreement with the knowledge that hydrogen jet flame tip is located where the concentration in unignited jet from the same leak source decays to 8-16% by volume, and that non-premixed turbulent combustion does not propagate downstream to areas with smaller hydrogen concentrations [7].

However, a presence of an ignition source of sufficient energy in this initial premixed hydrogen-air could probably initiate deflagration of this non-uniform mixture created during the short (0.3 s) period of unignited release. In 2 s after the release initiation the flammable hydrogen-air cloud dissipates below the lower flammability limit (see Fig. 3, top left). This implies that spontaneous ignition of a sudden hydrogen release by the diffusion mechanism [3] could be an effective technique to reduce pressure effects and thus negative consequences of unscheduled indoor release of hydrogen. The validity of this safety strategy has to be proved by further research.

Jet flame development

Figure 3 shows the dynamics of temperature and mole fractions of hydrogen, oxygen, and water within the enclosure during the first 60 s of the process. The flame length grows after the ignition source was switched off (see also Fig. 4). High temperature reaches the ceiling at about 2 s, combustion products start to descend at about 4 s, and after 10-15 s practically the whole volume

of enclosure is occupied by hot products creating intolerable temperature conditions. During the first 10 s of combustion the temperature reached the maximum value above 2200 K, and began to decrease after this time due to dilution of the combustion zone by entrained combustion products.

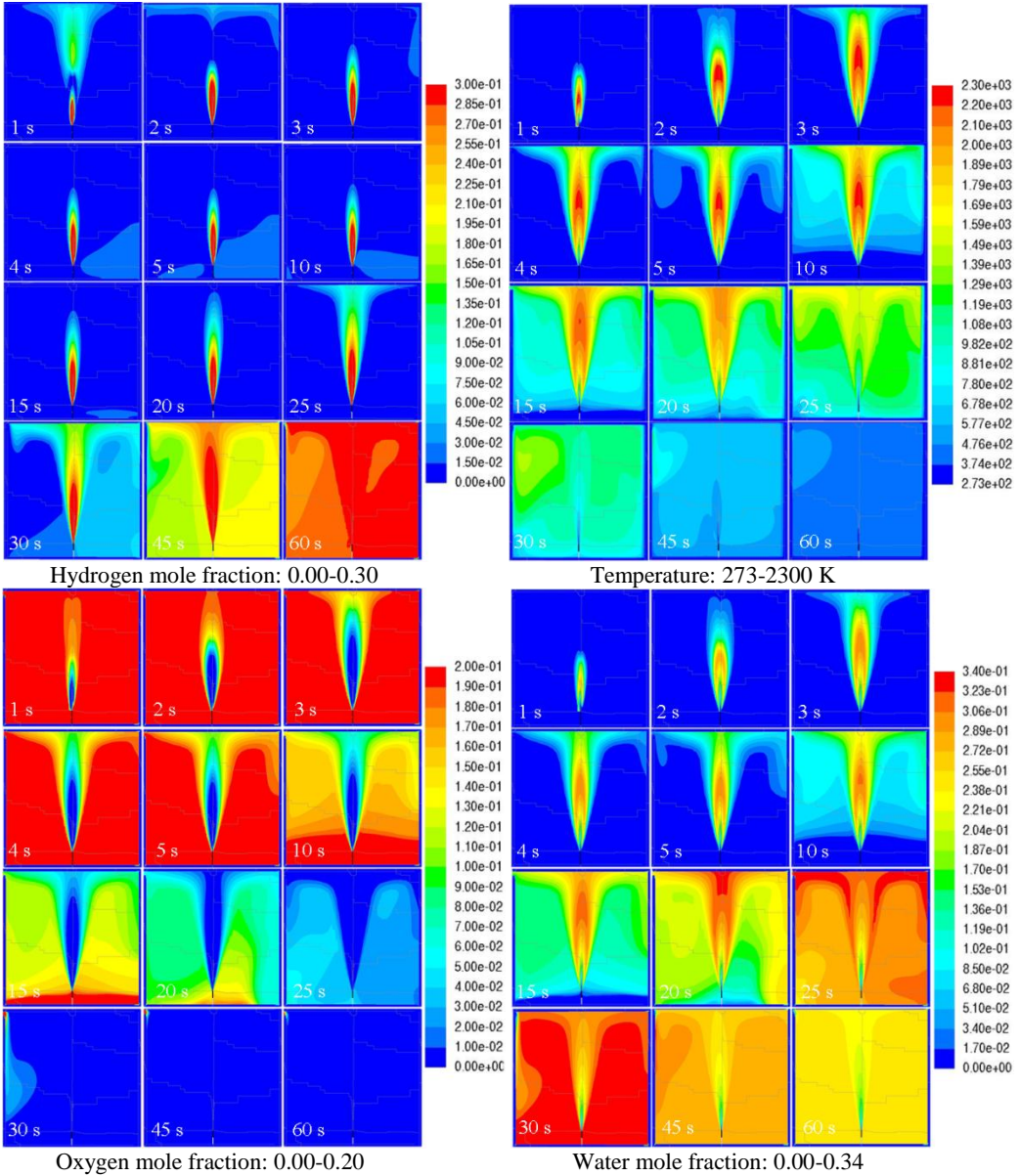


Figure 3. The simulated dynamics of hydrogen flame self-extinction in the enclosure with one vent. From left to right: hydrogen mole fraction (in the range 0.00-0.30), temperature (273-2300 K), oxygen mole fraction (0.00-0.20), water vapour mole fraction (0.00-0.34).

Numerical simulations demonstrated that hydrogen flame grows until about 10 s when there are distinct areas of hydroxyl (OH) mole fraction about 0.01 (Fig. 4, left). Then the hydroxyl mole fraction starts to decrease and practically vanishes at the central (along the pipe) 2D cross-section of the enclosure at time about 45 s (Fig. 4, right).

Hydrogen mole fraction distribution in the enclosure is quasi-steady from about 4 s to 10 s (Fig. 3, top left) when the regime of combustion is of well-ventilated fire. Hydrogen envelope and hydroxyl zone start to grow after about 10 s that indicates that there is not enough oxygen entrained into the hydrogen jet to complete combustion in vitiated atmosphere at the same flame length as before. Indeed, Fig. 3 (left bottom) shows that oxygen molar fraction drops practically throughout the whole enclosure at 10 s except a narrow region close to the floor.

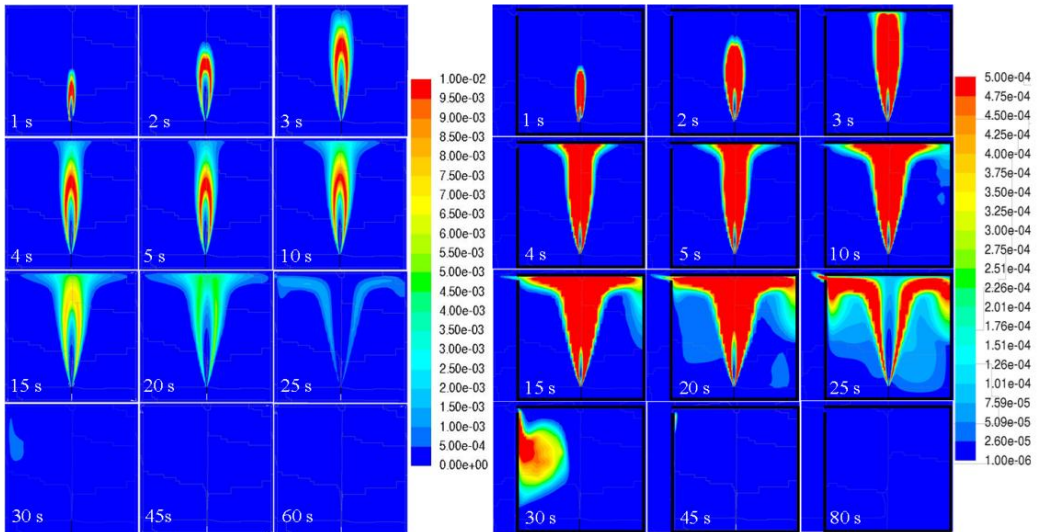


Figure 4. Contours of hydroxyl (OH) mole fraction in a 2D slice along the pipe axis in the range: 0-0.01 (left), and $1\text{E-}06 - 5\text{E-}04$ (right).

Combustion products (see water mole fraction in Fig. 3, bottom right) reach the ceiling at about 2 s then spread as a ceiling jet for couple of seconds. After that combustion products begin to descend and extend downward to the level of the release point at 10-15 s. The entrainment of water into combusting hydrogen jet dilutes reaction. At the same time oxygen mole fraction reduces due to combustion and lack of air intake into the enclosure through the vent (Fig. 3, bottom left).

High descending temperature (Fig. 3, top right) presents a hazard for equipment and life safety, e.g. it would impair evacuation in room-like enclosure. This must be considered when carrying out hydrogen safety engineering. The temperature throughout the enclosure is around 1000 C at time 15-25 s. This is a characteristic temperature for fire transition to the flashover regime.

There is a potential “ambiguity” in interpretation of snapshots in Figs. 3 and 4 as follows. There is a decrease of temperature and OH concentration from snapshot “25 s” to snapshot “30 s” yet the amount of water vapour is increased during the same period. The answer to this “ambiguity” can be partially drawn from Fig. 5 and the fact that visualisation of parameters in these figures is in 2D slice only. The maximum concentration of water in central 2D slice is at the intermediate snapshot “27.5 s” rather than “30 s”. It will be demonstrated below that weak reactions will continue in some isolated areas within the enclosure up to 80 s.

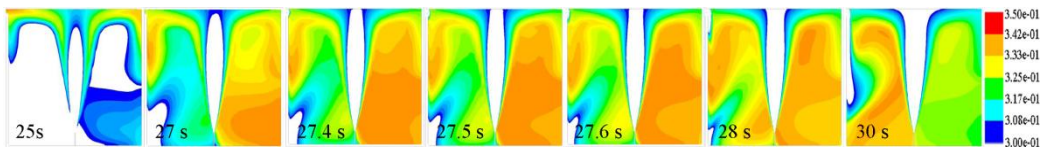


Figure 5. Contours of water mole fraction in a 2D slice along the pipe axis in the range 0.3-0.35.

Self-extinction of under-ventilated fire

Dynamics of field parameters within enclosure

Self-extinction of hydrogen flame is not an instant process. The rate of combustion reactions is affected with time by the consumption of oxygen initially available in the enclosure, and by dilution of the reaction zone by entrained combustion products, i.e. water vapour and nitrogen.

At time 10 s the initial concentration of oxygen is present only in a quarter of the enclosure volume near the floor (Fig. 3, bottom right). From 10 s to 25 s the oxygen mole fraction drops from the initial value of 0.207 to less than 0.05. This oxygen concentration is known to be insufficient to sustain hydrogen combustion in air at normal pressure and temperature. However, a different value of oxygen concentration could be characteristic for a vitiated atmosphere and elevated temperature. Figure 4 (left) shows that there are regions with small amount of hydroxyl radicals implying ceasing yet presence of reaction (OH is visualised in the range 0.00-0.01 in Fig. 4, left).

Figure 4 (right) is a visualisation of hydroxyl mole fraction in the range $1\text{E}-06 - 5\text{E}-04$ to “zoom-in” and see regions of weak reaction in a central cross-section of the enclosure. The location of reaction zone before it ceases in this 2D slice is near the vent (snapshots “30 s” and “45 s” in Fig. 4, right). This “late” reaction within the enclosure close to the vent is due to air ingress into the enclosure that starts at about 26.8 s through the lower part of the vent in its corners (Fig. 6).

Figure 6 shows horizontal velocities at the vent exit to the atmosphere. White colour indicates areas where gas flows out of the enclosure, black colour shows areas through which gas enters the enclosure, and gray colour points out regions where velocity is about zero. There is a range of velocities indicated for each snapshot. Positive limit, if any, indicates a maximum velocity of out flowing gases and negative limit, if any, indicates a maximum velocity entering the vent. For selected conditions of the numerical experiment it is not trivial that there is a period from 26.8 s to about 85 s during which gases flow in both directions through the vent or only into the enclosure (sub-period from 27.5 s to about 70 s). This flow pattern essentially affects the under-ventilated fire and the self-extinction process.

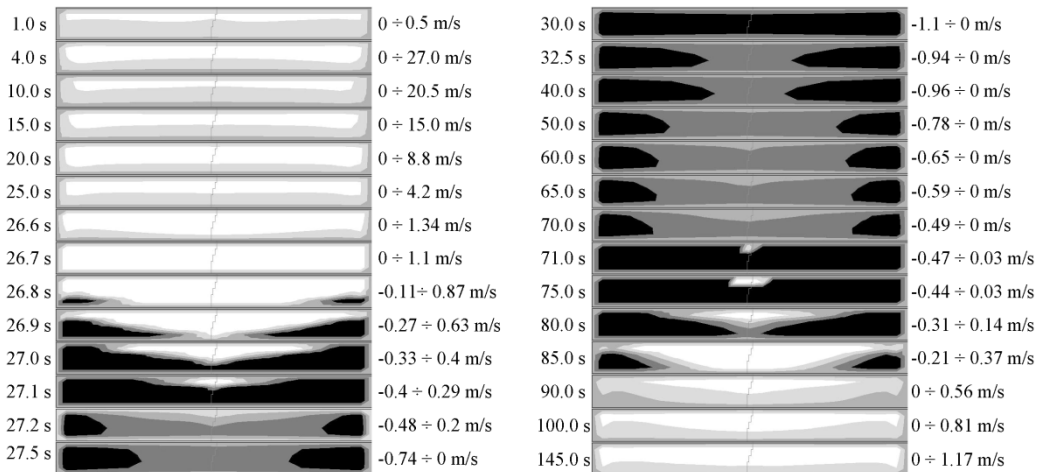


Figure 6. Velocities trough the vent: white – outflow, black – inflow.

Figure 3 shows that 60 s after the release there is practically no oxygen within the enclosure, temperature decreased in most of regions to 150-200 C due to sustained release of hydrogen with temperature 273 K and heat losses from hot gases to walls. Hydrogen concentration went up to 30% by volume at 60 s, and water vapour concentration dropped from 25-34% by volume at 25-

30 s to 20-25% at 60 s. This is due to water entrainment into the pure hydrogen jet and flow of this mixture out of the enclosure through the vent.

Figure 7 shows maximum volumetric fraction of hydroxyl radical OH within the enclosure as a function of time. The peak of OH mole fraction above 0.02 at time less than 1 s after the release is associated with the numerical ignition and high temperature of the patch of 3000 K above the adiabatic flame temperature. From about 3 s to about 8-10 s the mole fraction of OH is stabilised at a level of just above 0.01 that is a characteristic mole fraction for hydrogen combustion in air at normal conditions. This stage of combustion is similar to a free jet flame in the atmosphere as depletion of oxygen and dispersion of combustion products in the enclosure are negligible to this moment. After 8-10 s the maximum mole fraction of hydroxyl OH reduces monotonically to a small value of about 0.001 at about 25-30 s and stays at this level up to 80 s when it drops to zero. Thus, we can conclude that the flame self-extinction period spreads from about 10 s to 80 s.

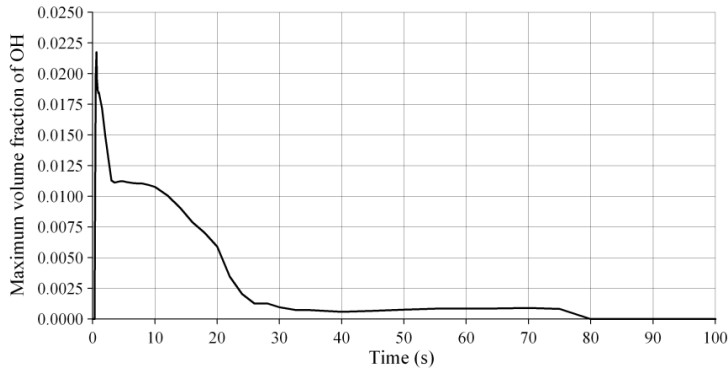


Figure 7. Maximum volumetric fraction of hydroxyl (OH) in the enclosure as a function of time.

Dynamics of averaged parameters during flame self-extinction

Figure 8 shows average volumetric fractions of water (H₂O), hydrogen (H₂), and oxygen (O₂). In agreement with results presented in Fig. 5 the maximum of average water concentration in the enclosure is at time 27.5 s after the start of the release. This time coincides with time when the average oxygen concentration decreased below the level that is able to sustain combustion (Fig. 8, right), and hydrogen concentration starts to increase as its consumption due to combustion stopped (Fig. 8, centre). Conclusions about flame self-extinction based on average values of species in the enclosure should be done with care. Indeed, Fig. 7 shows that there are areas in the enclosure where reaction continues up to 80 s.

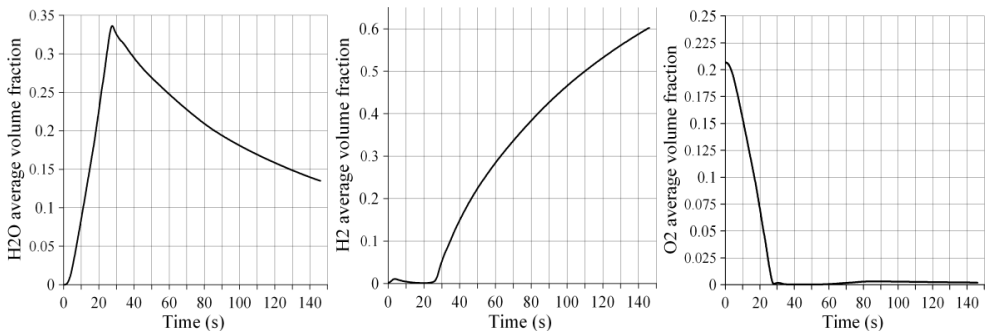


Figure 8. Species average volumetric fraction in the enclosure as a function of time: water (left), hydrogen (centre), oxygen (right).

Pressure peaking during jet fire

It has been mentioned previously that the calculation of pressure peaking phenomenon for unignited release in the enclosure with this vent size and this mass flow rate gives overpressure of 3 Pa [2]. For reacting release, i.e. jet fire, a maximum simulated overpressure in the enclosure is almost 100 times higher, i.e. about 300 Pa, for the same conditions. This pressure peak is reached at time of about 4 s (Fig. 9, left). The velocity of gases out of the enclosure reaches its maximum of 27 m/s at this moment (see Fig. 6). Pressure throughout the enclosure is practically uniform during the pressure peak 1-10 s (Fig. 9, right).

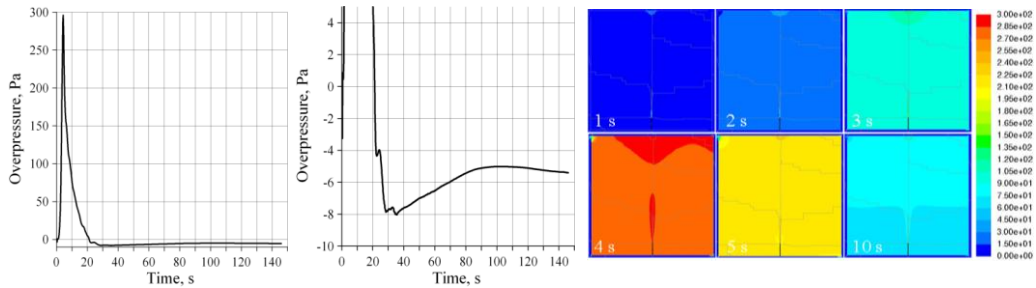


Figure 9. Average overpressure (relative to the operating pressure) within the enclosure (left, centre) as a function of time; pressure distribution within the enclosure (right).

Figure 9 (centre) shows that pressure drops to its minimum at 27-35 s when there is air intake into the enclosure (see Fig. 6). After that there is one more pressure peak of about 3 Pa at about 100 s (Fig. 9, centre) when there is no combustion any more. The averaged through the enclosure volume static pressure continues to stay below the operating pressure (initial pressure in the calculation domain without accounting for the hydrostatic pressure, $\rho g h$). This can be explained by the fact that for this numerical experiment the neutral plane location, i.e. the height at which pressure within and outside the enclosure are equal, is just below the lower edge of the vent. This means that hydrostatic pressure at the floor level within the enclosure is lower compared to pressure at the same level outside the enclosure due to difference in density in the hydrostatic equation. The averaging of overpressure throughout the enclosure volume then gives a negative value of the order of a few Pascals (Fig. 9, centre). Yet the pressure within the enclosure above the neutral plane is higher than outside with presence of 3D effects as demonstrated flow pattern through the vent (Fig. 6).

Weak combustion close to the vent and air ingress

Hydrogen combustion in a form of jet flame disappears between 25 s and 30 s that can be concluded from Fig. 4. Then combustion proceeds in the form of weak reaction zone close to the vent where oxygen ingress is taking place. The region of weak reaction is formed at the vent lower edge and is spread throughout the whole width of the vent up to 50 s. After time of 50 s this region degrades into two parts located at lower corners of the vent and at time about 80 s the combustion is fully complete in the whole domain (there is a couple of CVs with OH mole fraction 1E-06 at time 82 s). Indeed, there are no zones with hydroxyl OH (Fig. 7) and water generation during reactions (Fig. 10). Figure 10 shows maximum net reaction rate of water generation during combustion as a function of time.

Air intake into the enclosure after 26.8 s (Fig. 6), which keeps the weak reaction alive, is thought mainly due to the continuing release of cold hydrogen into hot combustion products. The small almost invisible flow out of the enclosure re-starts after about 70 s when temperature dropped down to 100-150 C. There are flows in opposite directions through the vent up to 90 s. From this time on the mixture of hydrogen, water and nitrogen flows out of the enclosure and there is no

inflow. With time this would eventually form 100% of hydrogen concentration in the enclosure. At 90 s the temperature drops to harmless 50-55 C throughout the enclosure. However, the absence of oxygen would be a reason for asphyxiation and death would people be present in scaled up enclosure similar to that under the investigation. Approximate composition of gases at 90 s is: 0.19 of water vapour, 0.43 of hydrogen, and 0.38 of nitrogen. The buoyancy drives this lighter than air mixture out of the enclosure.

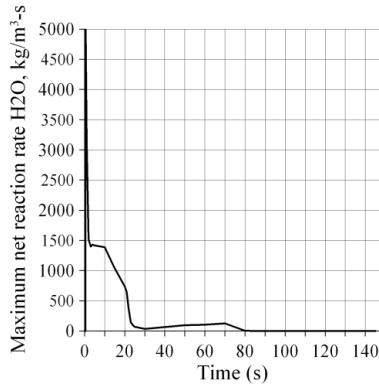


Figure 10. Maximum net reaction rate of water generation during combustion as a function of time.

Separation distance from the enclosure

Figure 11 shows the development of hot gases jet from the enclosure vent. There are three separation distances based on hot gases temperature [7]: 70°C - “no harm” limit (blue colour in Fig. 11); 115°C - pain limit for 5 min exposure (green colour); 309°C - “death” limit due to third degree burns for a 20 s (red colour).

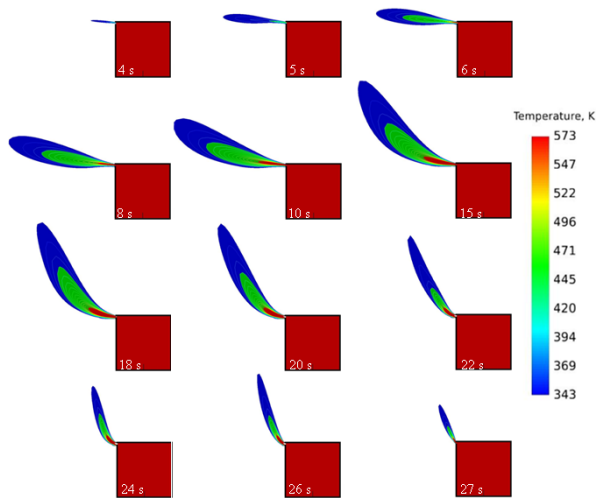


Figure 11. Contours of external jet of hot products: blue – no harm temperature (70°C), green – pain limit (115°C), red – third degree burn (309°C).

Figure 11 demonstrates that at initial stage the jet escaping the enclosure is in momentum-controlled regime due to higher velocity (Fig. 6) during the pressure peaking (Fig. 9, left). After the pressure peak at 4 s the velocity of gases flowing out of the enclosure significantly drops. Hot products and hydrogen are driven out of the enclosure by buoyancy after about 20 s. The maximum length of the external hot jet is about 2 m (no harm distance), i.e. two sizes of the

enclosure. The maximum length of the pain limit temperature is about 1.5 m. The third degree burn distance changes from zero at about 6 s to maximum of about 0.5 m at 15 s. Thus, approaching the fuel cell during this time could present real hazard for people. The “death” zone disappears after about 27 s when there is air intake into the enclosure (see Fig. 6).

CONCLUSIONS

The self-extinction of a hydrogen flame in an enclosure with one vent has been simulated for the first time with a full chemistry model, with application of the EDC model for combustion and the RNG theory for turbulence. These are pre-test simulations of experiments planned to be carried out in 2013-2014 as a part of the HyIndoor project (www.hyindoor.eu). The analysis of the numerical experiment assisted in understanding of the self-extinction process. The use of averaged throughout the enclosure parameters during under-ventilated fire can give a good indication of the moment when combustion essentially reduces however it can underestimate the timing when the flame is fully self-extinguished. The pressure peaking phenomenon for jet fires is shown to be more hazardous than for unignited release from the same source, e.g. in this particular experiment the overpressure is about 100 times larger for jet fire scenario (300 Pa and 3 Pa for jet fire and unignited jet respectively). The separation distance from the enclosure for this indoor hydrogen fire scenario is about twice of the enclosure size. Contrary to the expectation that gases will flow only out of the enclosure during the process, the simulations demonstrated a complex pattern of flow through the vent in both directions during the self-extinction process. The reason for this “unexpected” phenomenon is the interaction between sustained cold hydrogen leakage, creation of hot combustion products and their cooling after self self-extinction by cold hydrogen jet and heat transfer to the enclosure walls. The results of this study demonstrate the potential of the model to be used as a contemporary hydrogen safety engineering tool for real life applications.

ACKNOWLEDGEMENTS

The authors would like to express their gratitude to the Fuel Cells and Hydrogen Joint Undertaking for funding this research through the HyIndoor project (grant No. 278534).

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