VENTED EXPLOSION OF HYDROGEN / AIR MIXTURES: INFLUENCE OF VENT COVER AND STRATIFICATION

Vyazmina, E.[1], Jallais, S.[1] and Kuznetsov, M.[2]
[1] Centre de Recherche Paris-Saclay, AIR LIQUIDE Research & Development, 1BP 126, 78354, Jouy-en-Josas, France,
[2] KIT, Herman-von-Helmholtz Platz 1, 76344, Eggenstein-Leopoldshafen, Germany,
Elena.Vyazmina@airliquide.com Simon.Jallais@airliquide.com Mike.Kuznetsov@kit.edu

ABSTRACT

Explosion venting is a prevention/mitigation solution widely used in the process industry to protect indoor equipment or buildings from excessive internal pressure caused by an accidental explosion. Vented explosions are widely investigated in the literature for various geometries, hydrogen/air concentrations, ignition positions, initial turbulence, etc. In real situations, the vents are normally covered by a vent panel. In the case of an indoor leakage, the hydrogen/air cloud will be stratified rather than homogeneous. Nowadays there is a lack in understanding about the vented explosion of stratified clouds and about the influence of vent cover inertia on the internal overpressure. This paper aims at shedding light on these aspects by means of experimental investigation of vented hydrogen/air deflagration using an experimental facility of $1m^3$ and via numerical simulations using the computational fluid dynamics (CFD) code FLACS.

1.0 INTRODUCTION

A leakage in a confined enclosure is frequently considered for risk assessment studies for hydrogen energy application (refueling stations, electrolysers, small reformers ...). In presence of an ignition source, flame propagation results in an explosion. Internal explosions with a presence of an explosion vent are so-called “vented explosions”. In process industry explosion vents are commonly used to protect both internal equipment and the enclosure itself, allowing the pressure leave the closed domain, hence dropping the internal overpressure lower than the adiabatic limit. For special configurations vents also assist to an inflammable mixture partly leave the enclosure, therefore to reduce the explosion mass. As a consequence, it is crucial to be able to correctly size the explosion vents to reduce the consequences of the vented explosion.

Vented explosions were widely studied experimentally, numerically and analytically, see for instance ref [1-12]. However analytical models could not give the full overpressure field evolution in time outside and inside the enclosure. In other more complicated cases, for instance in the presence of flammable layer or stratification and vent covers, it is very difficult to find a proper analytical model giving reliable results in a wide spectrum of possible geometries. Thus these specific configurations must be further addressed by experimental investigations. Since it is not always possible to carry out an experiment in realistic dimensions, CFD can be used as a tool to predict the maximum internal and external overpressures, the length of the external flame and other important parameters, e.g. for the definition of the safety distances.

Nowadays there is a lack in understanding about the vented explosion of stratified clouds and about the influence of vent cover inertia on the internal overpressure. This paper aims at shedding light on these aspects by means of experimental investigation of vented hydrogen/air deflagration using an experimental facility of $1m^3$ and via numerical simulations using a computational fluid dynamics (CFD) code FLACS.

2.0 EXPERIMENTAL SET-UP

2.1 Brief description of the experimental facility

The KIT experimental facility is built inside the Test Chamber at the Hydrogen Test Centre HYKA of the IKET (Institute for Nuclear and Energy Technologies) at the KIT (Karlsruhe Institute for Technology). The chamber has dimensions 5.5 x 8.5 x 3.4 m (160m^3), see Fig. 1.

The test enclosure used in experiments (Fig. 2) is almost cubic with inner dimensions of 1000 x 960 x 980 mm³ (H x W x L), located in the above test chamber. In current experiments the vent area is chosen to be 0.01m^2 (10 x 10 cm) and 0.25 m^2 (50 x 50 cm). It is located in the centre of the front wall. Since Vyazmina et al.[3] demonstrated that nowadays CFD is hardly applicable for small vent area, for benchmark only vent area of 0.25 m^2 is used.

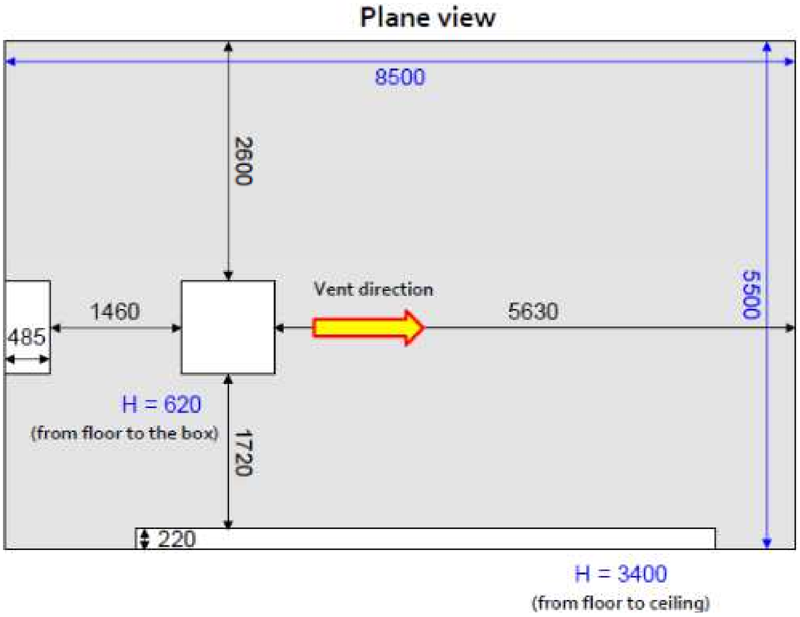

Fig. 1: Sketch (top view) of the enclosure position inside the experimental facility.

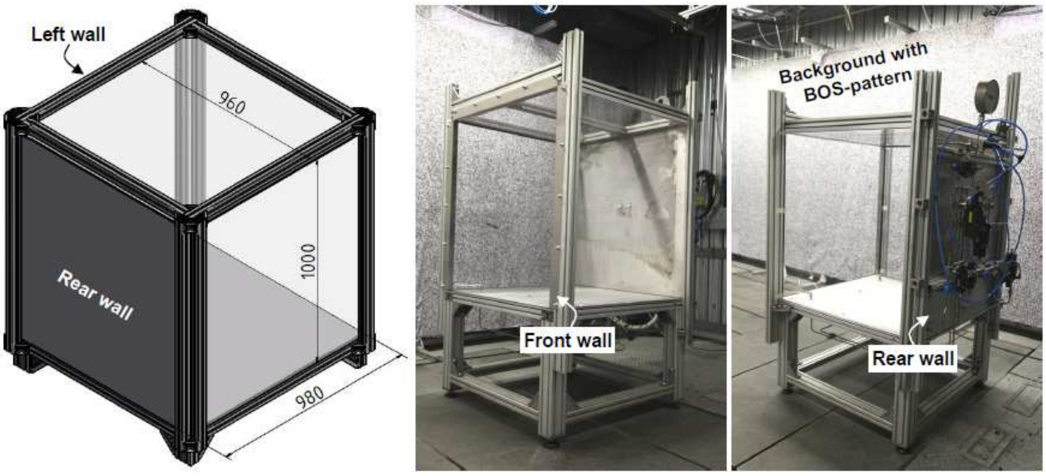

Fig. 2: Sketch and two views of the test enclosure inside the Test-Chamber.

For the preparation of all test-mixtures hydrogen containing precursor-mixtures with defined concentration are needed. Such precursor-mixtures are generated by mixing defined gas flows of H_2 and air that are controlled by two mass flow controllers (Tylan). To fabricate the different test mixtures with these precursor-mixtures different procedures and functionalities of the enclosure are needed.

The signals of all sensors involved in the mixture preparation (gas analysing system, mass flow controllers) together with the thermocouples installed to the enclosure are recorded with a “slow” data acquisition system (recording frequency 1 Hz) which is based on an interface and an in-house KIT developed LabView-program.

During the filling procedure of the chamber with a vent opening it is necessary to use a thin plastic film as hermetic cover for the opening to avoid hydrogen accumulations outside the enclosure. Such hydrogen accumulations outside the enclosure may lead to dangerous situations, especially when flammable concentrations are reached. To assure the absence of flammable mixtures outside the enclosure gas sensors (Honeywell, Type Sense- and Signalpoint with measuring ranges of up to 2500 ppm and 4 vol.% H_2 respectively) are installed to the ceiling of the Test-Chamber that provide an alarm when a H_2-concentration of 1 vol-% (25% of the Lower Flammability Limit (LFL) of hydrogen in air) is reached. Prior to the ignition, when the desired concentration inside the enclosure is reached, the thin film has to be removed or destroyed to avoid any influence of it on the results of the experiments. In current experiments the film is broken by a set of two cutting wires that are activated (heated) electrically. Immediately after the destruction of the film the mixture is ignited by a spark generated between two electrodes inside the enclosure. Ignition is performed at two positions: BackWall (X=50mm; Y=0mm; Z=0mm) and BackTop (X=50mm; Y=0mm; Z=450mm).

To record the overpressure history during an experiment a set of 8 fast pressure transducers (PCB M113B and Kulite XTEH types) and one fast acoustic pressure sensor (PCB M113B12 type) is used, see Table 1 for their locations. The centre of the back wall is taken as the beginning of coordinates.

Table 1. Position of pressure sensors.

P 01	P 02	P03	P04	P09	P05	P 06	P 07	P08
X=746 Y=0; Z=-500	X=0; Y=0; Z=0;	X=494; Y=0; Z= -500;	X=0; Y=0; Z=250;	X=1220; Y=0; Z=0;	X=1720; Y=0; Z=0;	X=2220; Y=0; Z=0;	X=2720; Y=0; Z=0;	X=3220; Y=0; Z=0

2.2 Stratified mixtures

For the experiments with non-uniform test-mixtures different hydrogen containing precursor-mixtures are prepared in a mixing vessel and then injected into the enclosure from different positions, in different directions, and during different times. Several concentration measurements at the same time are required to determine the shape of the concentration gradient or the jet plume at a distinct point in time. This is achieved by installing several remote controlled sample taking cylinders outside the enclosure that take samples from the inside in different positions simultaneously. These probes are then analysed offline. This method is quite time consuming and needs several measurements under the same conditions to assure reproducibility of the procedure before experiments with an ignition of the mixture can be performed.

The test matrix with a stratification and layer of H_2-air mixture is shown in Table 2. Experiments correspond to two different stratified layers of H_2 air mixture partially filled the test chamber with a maximum concentration at the top and zero concentration in the bottom to produce a large layer of 50 cm (L-Layer) and of a small layer of 25 cm (S-Layer) of relative uniform mixture. Ignition point was located at the upper position close to the middle of back wall.

Table 2. Test matrix for stratified hydrogen layers.

Type of stratification	max-min %H_2	Ignition	Number of experiments
L-Layer	15%	BackTop	1
	20%	BackTop	2
	25%	BackTop	2
S-Layer	15%	BackTop	1
	20%	BackTop	2
	25%	BackTop	1

Figure 3 shows the measured concentration profiles for L- and S-layers.

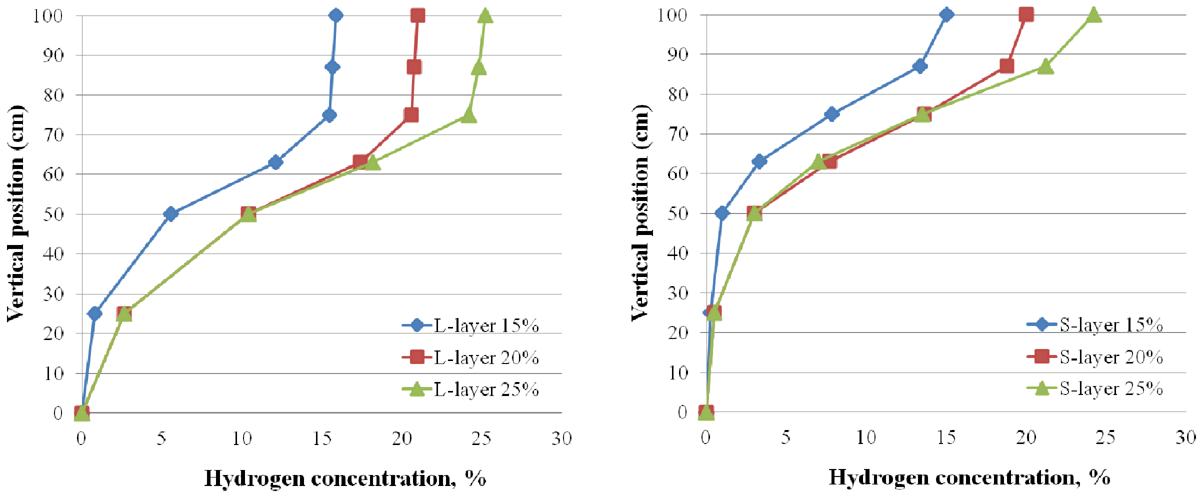

Fig. 3: Measured concentration profile for L- and S-layers.

2.3 Post-processing of the overpressure signal

An influence of mechanical vibrations of the chamber on the pressure signal appeared as a high frequency oscillations of the pressure signal at the time more than 100 ms after the flame released through the vent. A filtered pressure signal with FFT low pass filter of 200, 400 and 1000 Hz is used for the further analysis. A frequency of 400 Hz is chosen for filtering of the pressure signal, see Fig. 4. The characteristic length for the BackWall ignition is 1m, the speed of sound is ~400m/s for the unburned gas, and hence the characteristic frequency of a layer of a fresh gas is approximately 400Hz. Therefore this frequency is chosen for filter

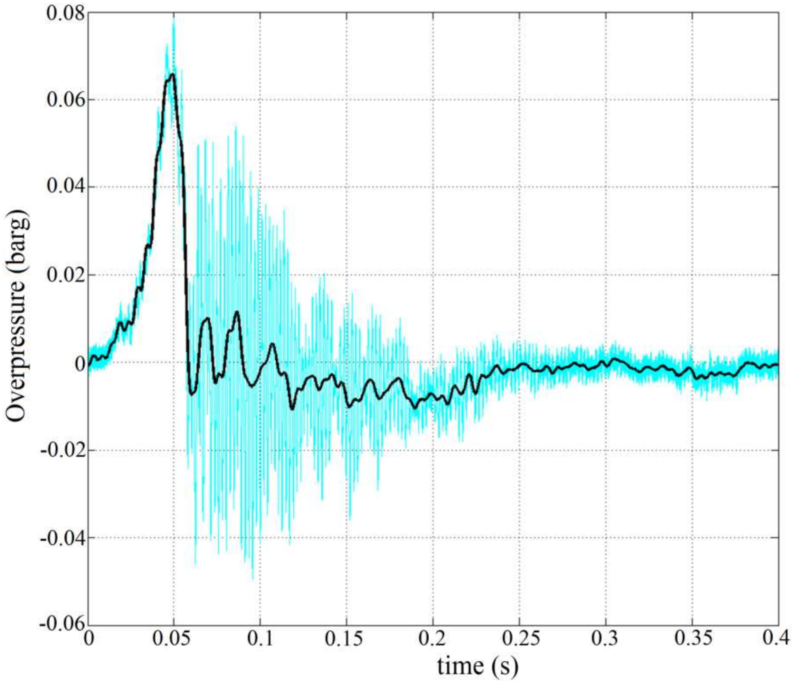

Fig. 4: Post-processing of the overpressure signal: exp S-Layer 25%, pressure sensor P01: raw signal (in cyan) vs. filtered signal (in black).

2.4 Vent cover

Effect of vent cover is investigated experimentally for two homogeneous concentrations: 10% and 12% H_2/air. For a vent cover a 5mm thick plate of stainless steel of size 50cm x 50cm is used. It is found that the presence of a vent magnify the maximum combustion pressure inside the vessel, see Table 3. For low concentrations and light vent cover the inertia of the cover plate increases the maximal internal overpressure by 15-20% compared to the case without a cover.

Table 3. Effect of vent cover on the overpressure inside the chamber.

Concentration, %	Vent cover	Ignition	Max Overpressure, (mbarg)
~10%	no	BackWall	8.6
	yes	BackWall	10.5
~12%	no	BackWall	32.7
	yes	BackWall	38.2

3.0 NUMERICAL APPROACH

For numerical simulations a commercial CFD code FLACS v10.5 [13] is used. FLACS is dedicated to the simulation of gas explosions in offshore oil and gas production platforms with high and medium obstruction. FLACS solves the compressible Navier-Stokes equations on a 3-D Cartesian grid using a finite volume method and RANS (Reynolds-Averaged Navier-Stokes) k-ε model for turbulence [14].

The SIMPLE pressure correction algorithm is used [15]. The combustion model is regarded as a collection of flamelets with one-step kinetic reaction. The laminar burning velocity is taken from pre-defined tables. The flame turbulent burning velocity is based on Bray's expression [16]. The reaction zone in a premixed flame is thin compared to the practical grid resolution. In FLACS, the flame zone is thickened by increasing the diffusion by a factor β and simultaneously reducing the reaction rate by a factor $1/\beta$, where β is chosen such that the flame thickness becomes 3-5 grid cells.

The computational domain is chosen to be approximately the same size as in the experimental facility. The computational domain is 8.3m long in the streamwise direction (from -1.5m up to 6.8m), 5.55 m in the cross-stream direction (from -3.1m up to 2.45m) and 3.4 m in the vertical direction (from -1.15m up to 2.25m). The cell size is chosen to be 2.5cm. Solution independence on the grid size is verified by comparison of simulation results with coarser grid of 5cm. In the simulations the centre of coordinates was chosen the same way as in the experiment (Fig 5). No initial turbulence is imposed in simulations. The concentration in H_2/air mixture is the same as in the corresponding experiments (see Table 1).

A standard pressure relieve panel is used to reproduce the effect of vent cover (see FLACS User's Manual [13]).

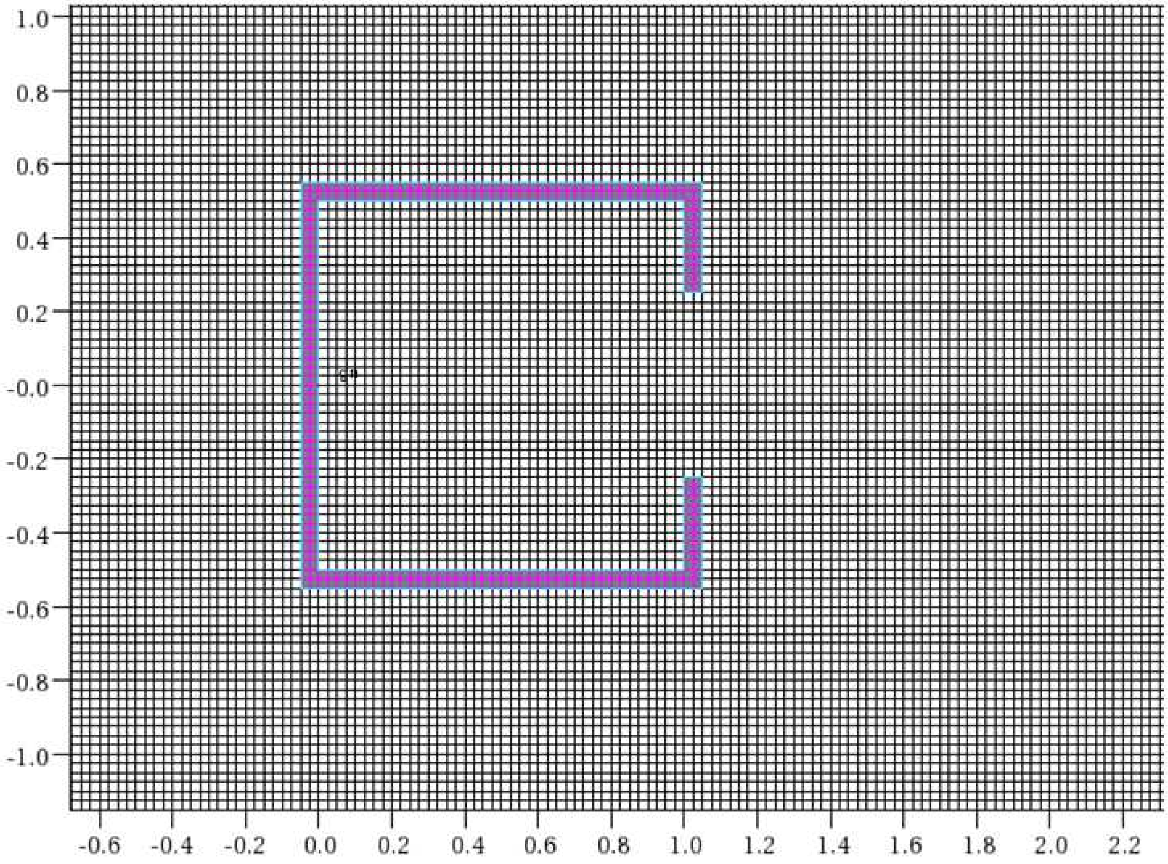

Fig. 5: The computational grid (the section correspond the centreline of the combustion vessel).

4.0 RESULTS

4.1 Stratified mixtures

The comparison of simulation results and experimental data is presented in the Table 4. Simulations are performed for the measured concentration profiles, see Fig 3.

Simulation results are always conservative. Simulations match better experiment in case of low reactive mixtures L-layers 15% and S-layers 15% than for 20% layers and for 25% layers. This can be explained by much higher mixture reactivity at 25%, i.e. a small error in the concentration strongly affects the obtained overpressure.

Simulations overestimate overpressure by ~30-40% for 20% H_2/air mixture and by a factor close to 2 for 25% H_2/air mixture. However since FLACS shows conservative results it application for gradient mixtures can be regarded as acceptable.

Table 4. Maximum overpressure inside the chamber for stratified mixtures: simulations vs experiment.

Type of stratification	max-min %H_2	Ignition	Experiment (mbarg)	Simulations (mbarg)
L-Layer	15%	BackTop	21	26
	20%	BackTop	94	160
	25%	BackTop	212	390
S-Layer	15%	BackTop	5	6
	20%	BackTop	33-34	50
	25%	BackTop	77	127

4.2 Equivalent concentration

It is difficult and time-consuming to correctly reproduce the stratification profile of hydrogen; hence it is interesting to find out the concentration of the homogeneous mixture, which gives the same overpressure. The standard approach is to take the overpressure corresponding to the maximum concentration. Using this approach, the overpressure is strongly overestimated and this is too conservative.

Similar to Kuznetsov et al. [17, 18] the combustion behavior governs not by the average hydrogen concentration but by the maximum hydrogen concentration at the top of compartment. Six different stratified compositions with various linear gradients and maximum and minimum hydrogen concentrations are investigated (Figure 6). Figure 6 shows pressure records of uniform 10 % hydrogen-air mixture and stratified compositions with almost the same amount of hydrogen (Grad (17-4%H_2) and Grad (12-2%H_2). Two non-uniform compositions with close concentrations at the top (Grad (17-4%H_2) and Grad (10-5%H_2) and 7% H_2 of average concentration were also compared. The maximum pressure for non-uniform compositions (17-4%H_2) and (15-4%H_2) of almost the same average concentration will be 6 (!) times higher than for uniform composition of equal hydrogen concentration (10%H_2). Flame velocity will also be several times faster than for uniform composition because of higher reactivity at the top of the vessel and several times larger specific flame area.

Moreover, for two stratified compositions of 12-2%H_2 and 10-5%H_2 of the same average hydrogen concentration (~7%H_2) the mixture with higher concentration at the top burns two times faster than another one. Characteristic maximum combustion pressure in this case is more than 10 times higher than for uniform mixture of 7 %H_2.

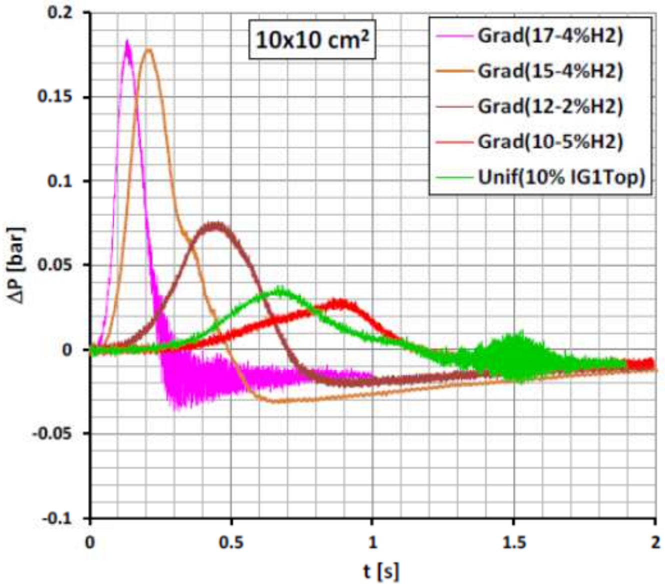

Fig. 6: The effect of mixture non-uniformity on maximum overpressure: experimental data.

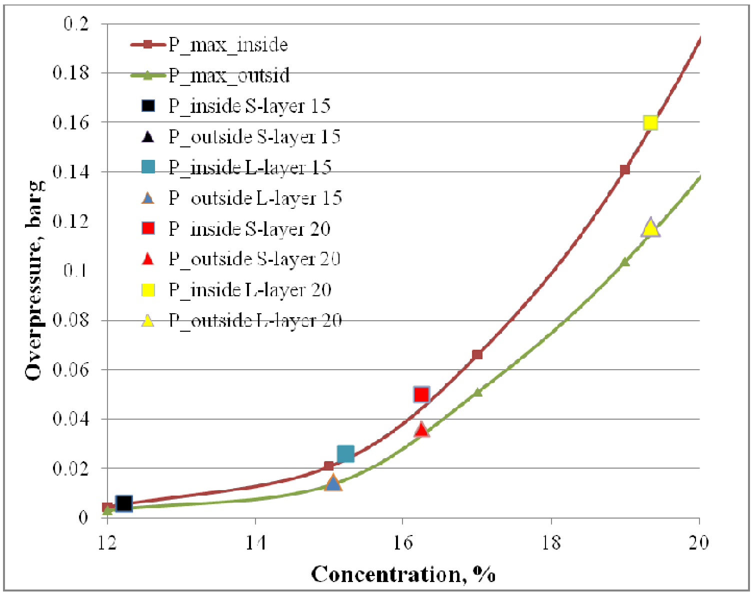

Fig. 7: The overpressure inside and outside the chamber for various concentrations of hydrogen for the BackTop ignition and vent area of 50x50cm: FLACS simulations.

FLACS simulations also illustrate the same behavior, see Figure 7. For the gradient L - layer of 15% the maximum overpressure computed in FLACS 10.5 is 26 mbarg, where for homogeneous mixture 15% is approximately 140 mbarg. For the gradient L - layer of 20% the maximum overpressure is 160 mbarg, where for homogeneous mixture 20% it is 190 mbarg. Taking the average concentration for L - layer of 15% (~ 7.6 %H_2) and L - layer of 20% (~ 11 %H_2) will give a much lower overpressure of a couple of 7 and 8 mbarg correspondingly.

Table 5. Equivalent concentration for stratified mixtures: simulations.

Real concentration	Average concentration %	Equivalent concentration, %
S-Layer 15%	4.3	12
L-Layer 15%	7.6	15
S-Layer 20%	6.15	16
L-Layer 20%	11.2	19

Figure 7 shows that gradient layers give higher overpressure than the average homogeneous mixture. This comparison demonstrates that for S- layer 15% in terms of the generated overpressure equal to 12% of H2/air mixtures. Table 5 gives the average and equivalent in terms of overpressure concentration for each stratified mixture. The equivalent concentration is approximately twice the average concentration.

4.3 Vent cover

An effect of vent cover on maximum overpressure is shown in Table 3. The effect of vent cover on maximum combustion pressure looks quite evident: the presence of the vent cover enhances the maximum overpressure inside the enclosure.

Experimental observations demonstrate that in case of a vent cover, there is an enormous negative pressure impulse due to release of combustion products from test vessel and the following closing of the vent for entering of ambient air, see Figure 8. Two stainless plates of 2 and 5 mm thick for the vent 50 x 50 cm^2 are investigated. The thicker the vent cover is, the higher maximum combustion pressure occurs inside the vessel.

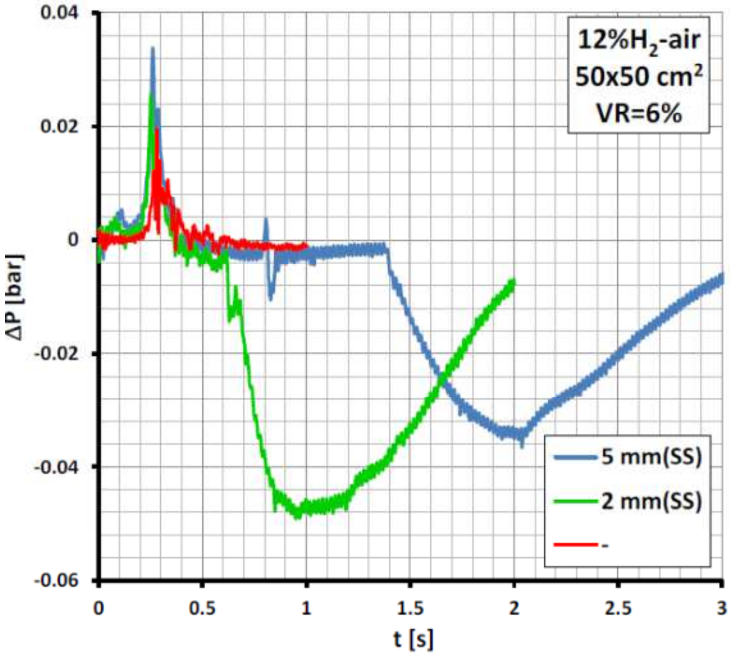

Fig. 8: Effect of cover on maximum overpressure inside the chamber: experimental results.

Simulations are also performed to model vent cover. They show a quite good agreement with experimental data in terms of the maximum overpressure, see table 6.

Table 6. Maximum overpressure inside the chamber for geometries with and without vent covers (homogeneous mixtures): simulations vs experiment.

Concentration, %	Vent cover	Experiment (mbarg)	Simulations, (mbarg)
10.33	no	9	8
9.99	5mm (SS)	11	11
12.2	no	33	34
11.95	5mm (SS)	38	42

5.0 CONCLUSION

The experiments are devoted to study effects of vent mixture non-uniformity and vent cover on maximum overpressure inside the vented test chamber. General results of the experiments are analyzed in terms of maximum overpressure:

1. Vented deflagration of a stratified hydrogen-air mixture leads to several times higher maximum overpressure compared to the uniform hydrogen-air composition with the same hydrogen inventory. The maximum combustion overpressure and dynamics of combustion are governed by the maximum hydrogen concentration but not by the average concentration or hydrogen inventory.

2. A vent cover leads to greater combustion pressure increase during vented deflagration. Enormous negative pressure phase is occurred.

The comparison of results from 3D FLACS simulations to experimental data for vented explosion of various stratified concentrations shows that FLACS overestimates the overpressure: by ~30% for 20% and by a factor of 2 for 25%. Since FLACS is in the situations investigated always conservative, it could be safely used in industrial situations.

Both simulations and experiments demonstrated that the approach of the average concentration for a stratified mixture is wrong. The explosion is governed by the maximum concentration in the upper layer at the beginning during the flame acceleration inside the enclosure and by average concentration in the evacuated outside the enclosure cloud.

6.0 ACKNOWLEDGMENT

The authors thank Air Liquide for sponsoring this work and for permission to publish this paper. This work is performed in the frame of a FCH JU project HyIndoor.

7.0 REFERENCE

1. Jallais, S. and Kudriakov, S., An inter-comparison exercise on engineering models capabilities to simulate hydrogen vented explosions, Proceedings of the 5th ICHS, September 2013, Brussels.

2. Daubech, J., Proust, Ch., Gentilhomme, O., Jamois, D., Mathieu, L., Hydrogen-air vented explosions: new experimental data, Proceedings of the 5th ICHS, September 2013, Brussels.
3. Vyazmina, E. and Jallais, S., Validation and recommendations for CFD and engineering modeling of hydrogen vented explosions: effects of concentration, stratification, obstruction and vent area, *International Journal of Hydrogen Energy*, **41**, 2016, pp. 15101-15109.
4. Bauwens, C.R, Chaffee, J., Dorofeev, S.B. Effect of ignition location, vent size and obstacles on vented explosion overpressures in propane-air mixture, *Combust Sci Tech,* **182**, 2010, pp. 1915-1932.
5. Cooper, M.G, Fairweathe, M. and Titre, J.P., On the mechanisms of pressure generation in vented explosions, *Combust Flame*, ;**65**,1986, pp.1-14.
6. Bauwens, C.R., Chao, J., Dorofeev, S.B., Effect of hydrogen concentration on vented explosion overpressures from lean hydrogen air deflagrations. *Int J Hydrogen Energy,* **37,** No.22, 2012, pp. 17599-17605.
7. Kuznetsov, M., Friedrich, A., Stern, G., Kotchourko, N., Jallais, S. and L'Hostis, B., Medium-scale experiments on vented hydrogen deflagration. *JLPPI,* **36,** 2015, pp.416-428.
8. Rocourt, X., Awamat, S., Sochet, I. and Jallais, S., Vented hydrogen - air deflagration in a small enclosed volume, *IJHE*, **39**, 2014, pp.20462-20466.
9. Bauwens, C.R., Chao, J. Dorofeev, S.B., Evaluation of a multi peak explosion vent sizing methodology, Proceedings of the IX ISHPMIE, July 2012. Cracow, Poland.
10. Bauwens, C.R., Chao, J. Dorofeev, S.B., Effect of hydrogen concentration on vented explosion overpressure from lean hydrogen-air deflagration, Proceedings of the 4th ICHS, September 2011, San Francisco.
11. Chao, J., Bauwens, C. and Dorofeev, S., An analysis of peak overpressures in vented gaseous explosions, *Proceedings of the Combustion Institute*, **33**, 2, 2011, pp.2367-2374
12. Pedersen, H., Middha, P., Modelling of vented gas explosions in the CFD tool FLACS, *Chem Eng Trans*, **26**, 2012, pp 357-362.
13. FLACS User’s Manual, GexCon, Bergen, 2016
14. Harlow, F. H. & Nakayama, P. I., Turbulence transport equations. *Physics of Fluids*, **10**, 1967, pp.2323–2332.
15. Patankar, S. V. (1980). Numerical Heat Transfer and Fluid Flow. Taylor & Francis.
16. Bray, K. N. C., Studies of the turbulent burning velocity, *Proceedings of the Royal Society of London*, Series A, 431, 1990, pp. 315-335.
17. Kuznetsov, M., J. Grune, A. Friedrich, K. Sempert, W. Breitung and T. Jordan, (2011) Hydrogen-Air Deflagrations and Detonations in a Semi-Confined Flat Layer, In: Fire and Explosion Hazards, Proceedings of the Sixth International Seminar (Edited by D. Bradley, G. Makhviladze and V. Molkov), pp. 125-136
18. Kuznetsov, M., J. Yanez, J. Grune, A. Friedrich, T. Jordan, Hydrogen Combustion in a Flat Semi-Confined Layer with Respect to the Fukushima Daiichi Accident, *Nuclear Engineering and Design*, **286**, 2015, pp.36-48