# Delayed explosion of hydrogen high pressure jets in a highly obstructed geometry

Elena Vyazmina, Simon Jallais, Jérôme Daubech, Jérôme Hebrard, Audrey Duclos, L. Gastaldo, N. Daudey

# DELAYED EXPLOSION OF HYDROGEN HIGH PRESSURE JETS IN A HIGHLY OBSTRUCTED GEOMETRY

**Vyazmina, E.[1], Jallais S.[1], Daubech, J.[2], Hebrard, J.[2], Duclos, A.[3], Gastaldo, L.[4], and Daudey, N. [5]**
**[1] Centre de Recherche Paris-Saclay, AIR LIQUIDE Research & Development, BP 126, 78354, Jouy-en-Josas, France,**
**[2] INERIS, 60550 Verneuil en Halatte, France,**
**[3] Research Department, AREVA Stockage d'Energie, Domaine du Petit Arbois, BP71, 13545 Aix en Provence, France**
**[4] IRSN, 13115, Saint-Paul-Lez-Durance, France**
**[5] EDF – DIPNN – SEPTEN GS / IN, 12 - 14 Avenue Dutrievoz, 69628 Villeurbanne, France**

**Elena.Vyazmina@airliquide.com**

**ABSTRACT**

Delayed explosions of accidental high pressure hydrogen releases are an important risk scenario in safety studies of production plants, transportation pipelines and fuel cell vehicles charging stations. Such explosions were widely explored in multiple experimental and numerical investigations. Explosion of high pressure releases in highly obstructed geometries with high blockage ratio is a much more complicated phenomenon. This paper is dedicated to the experimental investigation of the influence of obstacles on a delayed deflagration of hydrogen jets. The computational fluid dynamics (CFD) code FLACS is used to reproduce experimental data. In the current study the computed overpressure signals are compared to the experimentally measured ones at different monitoring points. Simulations are in close agreement with experimental results and can be used to predict overpressure where experimental pressure detectors were saturated. For homogenous stationary clouds a new approach of equivalent mixture of $H_2$/air (~16.5%) to stoichiometric mixture of $CH_4$/air is suggested. This approach is validated versus experimental data from the literature in terms of overpressure maxima. A parametric study is performed using FLACS for various concentrations in the same geometry in order to identify a possible transition from deflagration to detonation.

## 1.0 INTRODUCTION

Recently, Jallais et al. [1] demonstrated that hazards associated with hydrogen jet explosions are comparable with other scenarios typically considered today in risk studies, such as jet fires and unconfined vapor cloud explosions (UVCE). It is, therefore, important that delayed ignition jet explosion is included as one of the scenarios to be considered when assessing the potential consequences of accidental hydrogen releases.

Delayed explosions of hydrogen jets from high pressure storages in free field were widely investigated experimentally [2-7] and numerically [1, 2, 3, 8]. A simple engineering method for computing of consequences based on TNO Multi-Energy method was suggested for blast propagations, Vyazmina et al. [8] and Jallais et al. [1]. However all these investigations were done for free jets without interaction with obstacles.

However in real scenarios considered in risk assessment studies for production plants, cylinder filling centers, transportation pipelines, charging stations of FCV etc., high pressure jets can impact obstacles (pipes, valves, etc), creating a large and powerful vapor cloud explosion (VCE).

In order to shed light on the effect of obstacles on the delayed explosion of hydrogen jets, a new study based on experimental and numerical investigations is performed. This study is done in the frame of a JIP project Exjet 2 bis, where INERIS, Air Liquide, Areva, IRSN and EDF are joint together.

## 2.0 EQUIVALENT CONCENTRATION FOR STEADY HOMOGENEOUS CLOUDS

For numerical investigations a commercial CFD code FLACS v10.5 [9] is used. For FLACS validation, simulation results are compared to experimental data of Sail et al. [10]. Then a validation approach is used to perform a parametric study.

### 2.1 Experimental Description

Sail et al. [10] carried out explosion experiments in a congestion module constituted by a 3D array of 20 mm diameter tubes with 140 mm intervals (figure 1). The size of module was 3 m x 1 m x 0.5 m. The module was surrounded by a steel frame covered by a plastic sheet. The steel frame was 20 cm larger and higher than the module. See Sail et al. [10] for more details.


Figure 1: Experimental module used by Sail et al. [10].

The experimental facility was equipped by 6 pressure sensors (there is no information about pressure sensor L2 in the publication [10]), see table 1 for their positions.

Table 1 Positions of pressure sensors in experiment of Sail et al. [10].

| | Ignition | L1 | L3 | L4 | L5 | L6 | L7 |
|---|---|---|---|---|---|---|---|
| Location | X=0m;<br>Y=0m;<br>Z=0.25m | X=-2.26m;<br>Y=0m;<br>Z=1.05m | X=0.37m;<br>Y=0m;<br>Z=0m | X=1.07m;<br>Y=0m;<br>Z=0m | X=2.05m;<br>Y=0m;<br>Z=0m | X=4.09m;<br>Y=0m;<br>Z=1.05m | X=1.07m;<br>Y=2.5m;<br>Z=1.05m |

The module and surrounding it tent were filled by a stoichiometric mixture of methane/air. Two experiments were performed for this configuration (experiments 3 and 3bis from table 8 of Sail et al. [10]).

**2.2 Numerical simulations**

2.2.1 Flame velocity estimation

The laminar flame velocity in the stoichiometric mixture of methane/air is $S_L$=0.366 m/s and the expansion ratio σ (the ratio of unburned to burned gas) is σ=7.52. Flame velocity is proportional to $S_L\,\sigma$ = 2.75.

The equivalent mixture of hydrogen/air in terms of flame velocity must be between 14% and 17% $H_2$/air, see table 2.

Table 2 Flame velocities for different concentrations of $H_2$/air mixture.

| Concentration $H_2$/air, % | $S_L$ m/s | σ | $S_L\,\sigma$ |
|---|---|---|---|
| 14 | 0.288 | 4.42 | 1.27 |
| 15 | 0.362 | 4.63 | 1.68 |
| 16 | 0.462 | 4.83 | 2.23 |
| 17 | 0.572 | 5.03 | 2.88 |

2.2.2 Numerical set-up

For numerical simulations a commercial CFD code FLACS v10.5 [9] 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 [11]. The SIMPLE pressure correction algorithm is used [12]. 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 burning velocity during the explosion varies from the laminar burning velocity to quasi-laminar burning velocity and it become turbulent eventually it reaches congested region [9]. The flame turbulent burning velocity is based on Bray's expression [13].

FLACS is commonly used for modelling of very complex geometries, such as process plant, which often involve complex arrangements of pipes and ducts that are too small to resolve with the mesh. To resolve such small-scale structures would produce a very fine mesh, hence distributed porosity approach is applied in FLACS. This approach involves assigning porosities to the individual mesh cells containing small "sub-grid" obstacles. A volume porosity value of zero corresponds to a completely solid obstruction whilst a volume porosity value of one corresponds to free space. Additionally, FLACS calculates area porosities on each of the control volume faces. The approach specifies a source term in the fluid momentum equations which applies a resistance to fluid flow according to the porosity values of the control volumes. Additional production terms are included in the transport equations for the turbulent kinetic energy and dissipation rate to account for the generation of turbulence by sub-grid obstacles, for more details see [9].

The simulation domain is chosen to be 20m in the stream-wise direction, 12m in the cross-stream and 6m in the vertical direction. The open boundary conditions ("pressure wave") are imposed on lateral, upstream, downstream and upward boundaries, no-slip (ground effect) is imposed at the ground boundary.

The grid resolution should be chosen to obtain a sufficiently accurate result within an acceptable time. In the zone of interest (within combustion zone) the grid is chosen to be homogeneous with a grid size of 4cm, outside the zone the grid is 25cm. Tubes in module are aligned with the mesh, to reduce the effect of turbulence generated by porosity . Solution independence on the spatial resolution was verified using a finer grid.

**2.3 Results**

2.3.1 Comparison with experiment

Unfortunately Sail et al. [10] did not give the full overpressure signal; only overpressure magnitudes are available in the publication. Simulation results are compared with experimental measurements at pressure sensor locations for overpressure magnitude, see fig 2. The comparison with experimental data at various pressure sensors shows that hydrogen/air mixture of 16% is in best agreement with the experimental data for the stoichiometric methane/air mixture. Hence 16% of $H_2$/air is equivalent in terms of reactivity to stoichiometric $CH_4$/air.

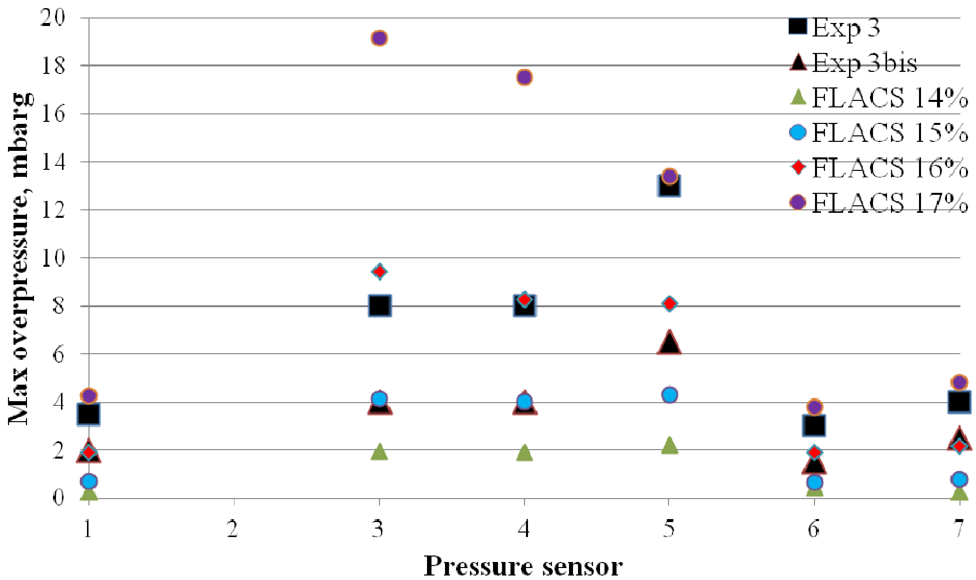


Figure 2: Overpressure magnitudes at various pressure sensors: simulations vs experiments.

This simulation not only validates the application of FLACS v10.5 for explosion in highly obstructed area, but also suggests a new approach of an equivalent mixture $H_2$/air in terms of reactivity for explosion simulations of other less reactive gases. However, to fully validate this approach a comprehensive comparison is required (in terms of the shape of overpressure signal, impulse etc.). Comparison with other experimental set-ups will is also necessary for the full validation of the equivalent approach.

The overpressures computed by FLACS using the concept of distributed porosity and the "equivalent reactivity" are in close agreement with the experimental results. Porosity concept used in FLACS for geometry representation increases the turbulence via the interactions of the flow and the flame with obstacle, which in its tern accelerates the flame.  This suggests that flame acceleration is mainly caused by turbulence generated by the obstacles.

### 2.3.2 Parametric study

A parametric study using FLACS v10.5 is performed to compute the explosion of various $H_2$/air concentrations in an obstructed volume, see figure 3. The concentration of the mixture is varied from 14% to stoichiometric mixture. Figure 3 appears that starting from 22%-24% of $H_2$/air the overpressure inside the module (L5 sensor) is saturated, suggesting the transition deflagration to detonation (DDT) occurs.

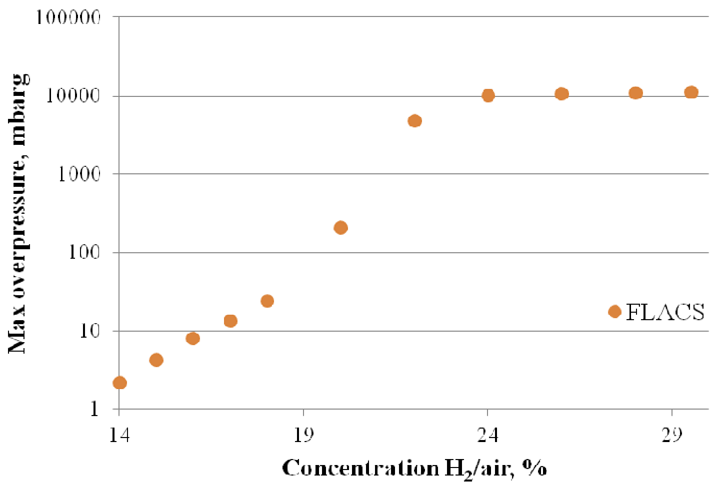


Figure 3: Overpressure magnitudes at pressure sensor L5 for various $H_2$/air mixtures.

Figure 4 shows the flame propagation velocity for mixture 20% (left frame) and 24% $H_2$/air (right frame). In the case of 20%, the flame velocity is much lower than the speed of sound in the burned gas, whereas for 24% $H_2$/air the flame velocity is higher than the speed of sound suggesting DDT. Thomas et al. [14] also experimentally observed DDT at 22% $H_2$/air in a congested rig. For DDT to occur, a flame needs to accelerate to beyond a certain critical flame speed. This speed is usually close to the choking flame speed. Dorofeev [15, 16] emphasised that for flame speed higher than 500 m/s speeds, transition to detonation might be possible.

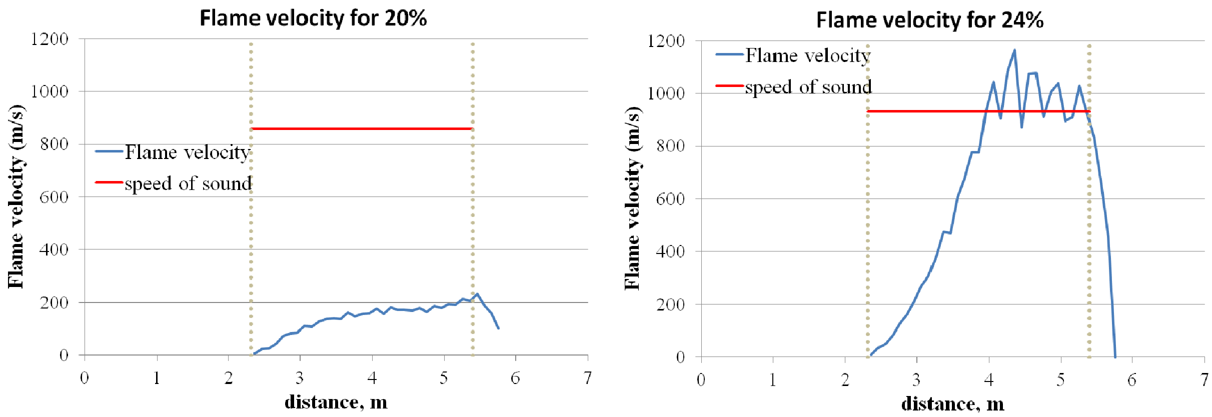


Figure 4: Flame velocity inside the module for 20% (left frame) and 24% (right frame) $H_2$/air mixtures. Vertical dotted lines correspond to the limits of the module.

## 3.0 DELAYED EXPLOSION OF HYDROGEN JET IN OBSTRUCTED MODULE

FLACS is validated for delayed explosions of hydrogen jets in a free field; see for instance [1-3, 9]. In the first part of the current paper FLACS showed good agreement with to experiments of methane-air UVCE in highly congested volumes. However to complete and extend its validations for delayed explosion of hydrogen jets in a congested module, it is needed to compare simulations results with corresponding experimental data.

### 3.1 Description of the experiment

The experimental set-up consists of a 5 $m^3$ gas storage connected to a release diameter of 12 mm located 1m above the ground; a congested module similar to the one on fig 1 is situated 1.4 m from the release point. Ignition is located on the axis of the jet at 0.8m from the release point, corresponding to approximately 50% $H_2$/air mixture in the jet. Pressure is measured by 6 pressure sensors: L1 is located close to the ignition; L2 and L3 are located outside the module and perpendicular to the jet axis; L4 is located inside the module on the jet axis, L5 and L6 are located downstream of the module on the jet axis, see table 3 for exact locations of pressure sensors. Experiment is duplicated. Pressure sensors L5 and L6 are saturated in both experiments. The saturation pressure for all sensors is approximately 1 barg.

Table 3: Positions of pressure sensors in the experiment.

| | Ignition | L1 | L2 | L3 | L4 | L5 | L6 |
|---|---|---|---|---|---|---|---|
| Location | X=0.8m;<br>Y=0m;<br>Z=1m | X=0.8m;<br>Y=0m;<br>Z=1m | X=1.6m;<br>Y=2m;<br>Z=1m | X=1.6m;<br>Y=4m;<br>Z=1m | X=2.3m;<br>Y=0m;<br>Z=1m | X=4.8m;<br>Y=0m;<br>Z=1m | X=6.8m;<br>Y=0m;<br>Z=1m |

### 3.2 Numerical simulations

3.2.1 Numerical set up

For simulations FLACS v10.5 [9] is used. Simulation set-up is very similar to the case of a stationary cloud. The simulation domain is 20m in the streamwise direction, 12m in the cross-stream and 7m in the vertical direction. The spatial resolution is 4cm, outside the zone of interest the grid cell is 25cm.

#### 3.2.2 Simulation results

The comparison of simulation results with experimental measurements at 6 overpressure monitoring points is shown on Fig.5 : L1 sensor is located near the ignition point, sensors L2 and L3 are perpendicular to the jet axis, the sensor L4 is located inside the module and sensors L5 and L6 are located on the axis of the jet 4.8 m and 6.8m downstream from the release point. Both experimental and numerical signals are shifted in time by -0.0094 sec and + 0.02 sec respectively to obtain the maximum signal at the same instant.

Fig.5 demonstrates good agreement between simulations and experimental data for overpressure magnitudes at L1, L2 and L3. At the sensor L2 simulations reproduce the double peak structure of the overpressure signal observed also experimentally. Here the first peak corresponds to the accidental overpressure wave, and the second one is its reflection by the ground.

At the sensor L4 (inside the module) FLACS v10.5 gives a much higher overpressure than experimentally measured. Computed overpressure is 3.62 barg, whereas the experimental one is l.064barg. This significant difference can be explained by the fact that the experimental sensor is probably saturated (the saturation pressure is approximately 1 barg for all sensors). However, it is uncertain the level of agreement that can be reached with a more appropriate sensor. Hence, this would need verification with additional experiments in the future. It is also possible that the simulated flame accelerates slightly earlier than in the experiment (at shorter distances), leading to a higher overpressure earlier than in the experiment. That is why at the sensor L5 and L6 FLACS gives lower overpressure.

At L5 the computed overpressure (~950mbarg) is still the same order as the experimental one > 1 barg (the sensor is saturated). At L6 FLACS significantly underestimates the experimental overpressure.

Pressure signals at sensors L4, L5 and L6 are very steep for experiments and numerical simulations; this pressure signal suggests a possibility of DDT. However FLACS can only suggest a possibility for DDT, which is the case here. It is not completely adapted to perform precise simulations of DDT, this is rather why the computed overpressure at the sensor L6 is underestimated compare to the experimental measurements.

Basically, for delayed explosions of hydrogen releases from high pressure reservoir in a congested module FLACS v10.5 shows reasonable agreement with experimentally measured overpressure in the deflagration regime, correctly representing the overpressure magnitude. FLACS gives a very high overpressure inside the module 3.62 bars (the experimental pressure signal is saturated here). Both experiments and simulations suggests a DDT or a strong flame acceleration in the module (experimental pressure signals are very steep and sensors are saturated).

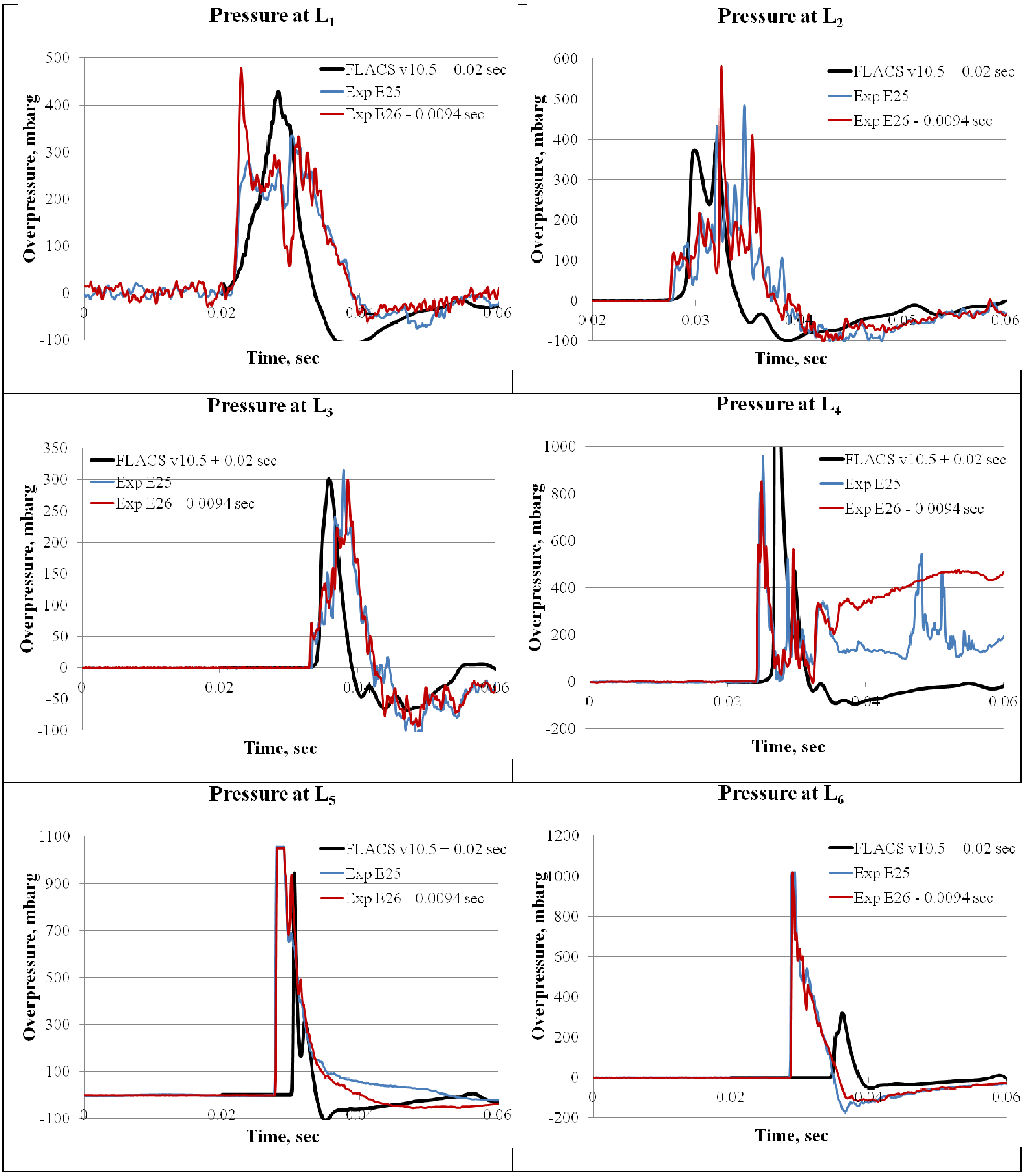


Figure 5: Overpressure at various positions: simulations (black curve) vs experiment (red and blue curves).

## 4.0 DISSCUSION AND CONCLUSION

Delayed explosion of accidental high pressure hydrogen releases in congested regions is an important risk scenario for safety studies. As a consequence, the assessment of the associated consequences requires an accurate and validated prediction based on modelling and experimental approaches. The target of this study is to give a synthesis of the outcomes of JIP project EXJET funded by INERIS/ AIR LIQUIDE/ AREVA/EDF and IRSN. The project is dedicated to an investigation of delayed explosion of high pressure releases of hydrogen in highly congested volume. It aims to understand the physical phenomenon and to validate CFD code FLACS v 10.5.

There are two types of VCE under investigation in this paper : VCE of a steady methane-air cloud in a highly congested module and a delayed explosion in of a high pressure hydrogen release filling a highly obstructed region.

For steady UVCE a new approach of an equivalent concentration for homogeneous clouds is suggested:

- A new approach is to use an equivalent mixture of $H_2$/air (~16.5%) to stoichiometric mixture of $CH_4$/air for explosions at rest (homogeneous clouds) by FLACS v10.5. This approach showed good agreement with experimental data in terms of overpressure maxima.

- Parametric study performed by FLACS v10.5 varying concentrations showed that at more than 22%$H_2$, the DDT (deflagration to detonation transition) is possible. However this conclusion must be validated experimentally.

For delayed ignition of high pressure hydrogen releases in highly obstructed regions :

- Simulation results are in reasonable agreement with experimental measurements in the deflagration regime, correctly representing the overpressure magnitude at 4 sensors out of 6. Numerical simulations are able to correctly represent not only the accidental overpressure wave, but also its reflection by the ground, leading to a double peak structure for the overpressure, also observed experimentally.

- Pressure sensor inside highly obstructed module is probably saturated approximately at 1barg, whereas at the same sensor FLACS v10.5 simulations give 3.6 barg.

- It is likely that in FLACSv10.5 flame accelerates slightly earlier compare to the experiment (at shorter distances), leading to a higher overpressure earlier than in the experiment; however the order of overpressure magnitude is comparable with experimental measurements.

- Both simulations and experiments suggest DDT inside the modules, however experiment must be repeated and the flame velocity must be measured to derive the final conclusion.

At the next step, delayed explosions of high pressure releases will be performed in another configuration with larger obstacles.

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