DELAYED EXPLOSION OF HYDROGEN HIGH PRESSURE JETS: AN INTER COMPARISON BENCHMARK STUDY

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ABSTRACT

Delayed explosions of accidental high pressure hydrogen releases are an important risk scenario for safety studies of production plants, transportation pipelines and fuel cell vehicles charging stations. As a consequence, the assessment of the associated consequences requires accurate and validated prediction based on modeling and experimental approaches. In the frame of the French working group dedicated to the evaluation of computational fluid dynamics (CFD) codes for the modeling of explosion phenomena, this study is dedicated to delayed explosions of high pressure releases. Two participants using two different codes have evaluated the capacity of CFD codes to reproduce explosions of high pressure hydrogen releases. In the first step the jet dispersion is modeled and simulation results are compared with experimental data in terms of axial and radial concentration dilution, velocity decay, and turbulent characteristics of jets. In the second step a delayed explosion is modeled and compared to experimental data in terms of overpressure at different monitor points. Based on this investigation several recommendations for CFD modeling of high pressure jets explosions are suggested.

1.0 INTRODUCTION

Recent work on delayed explosions of high pressure jet of hydrogen showed their importance for risk assessment studies for production plants, cylinder filling centres, transportation pipelines, charging stations of FCEV etc, see e.g. Miller et al. [1], Daubech et al. [2], Jallais et al. [3].

It has been amply discussed that H_2 releases at high pressure create turbulent jets which in a case of a delayed ignition lead to a formation of vapour cloud explosion (VCE). The turbulence in the jets can significantly accelerate the flame, leading to a significant overpressure, see Jallais et al. [3].

Delayed explosion of high pressure H_2 releases investigated experimentally by multiple authors: Miller et al. [1], Daubech et al. [2], Grune et al. [4], Willoughby and Royle [5], Takeno et al. [6] and Chaineaux [7]. Recent works have also suggested the application of TNO Multi-Energy method for blast propagations (see Vyazmina et al. [8] and Jallais et al.[3]).

Studies of Daubech et al. [2], Vyazmina et al. [8], Jallais et al. [3] also demonstrated that computational fluid dynamics (CFD) FLACS code [9] can be used for modelling of H_2 jet explosions. Comparison of simulations to experimental results showed reasonable agreement for the overpressure magnitude [1, 2, 3, 9].

In order to obtain a more general conclusion on the application of a CFD tool for safety computations, two different codes have been compared to each other and to available experimental data from Daubech et al. [2]. This initiative is performed in the frame of the French working group dedicated to the evaluation of CFD codes for the modelling of explosion phenomena. The present paper describes this validation and gives several recommendations for the modelling of dispersion of high pressure releases and their delayed explosion.

2.0 BENCH DESCRIPTION

The original experimental campaign was performed at the INERIS Montlaville test site within the frame of a Joint Industrial Program EXJET together with Air Liquide, and AREVA Energy Storage in 2013. Experiments were dedicated to explosion of high pressure jets in a free field involving no interaction with obstacles. For a more detailed description of the test set-up and results, see Daubech et al [2].

2.1 Dispersion Tests

Experiments were performed in an abandoned rock quarry, where there is no perceptible wind. The set-up consists of a 5 m^3 gas storage connected to a release diameter of 12 mm through a 35 mm diameter flexible hose, see figure 1. A full crossing valve is used to limit the pressure drop. Hydrogen was released in the horizontal direction at an elevation of 1.5 m above the ground into a flat open area. Temperature and pressure were also measured at the release point. The mass flow was approximately 250g/s according to Daubech et al [2].

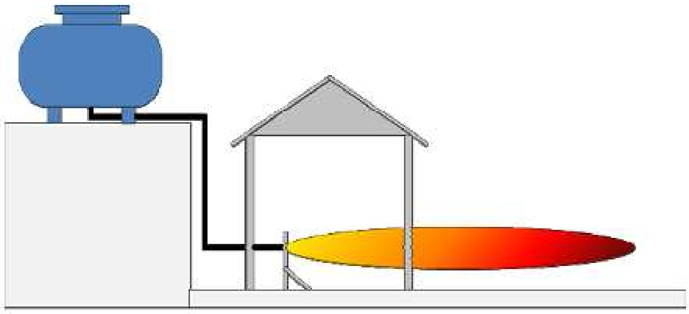

Figure 1: Global view of the setup

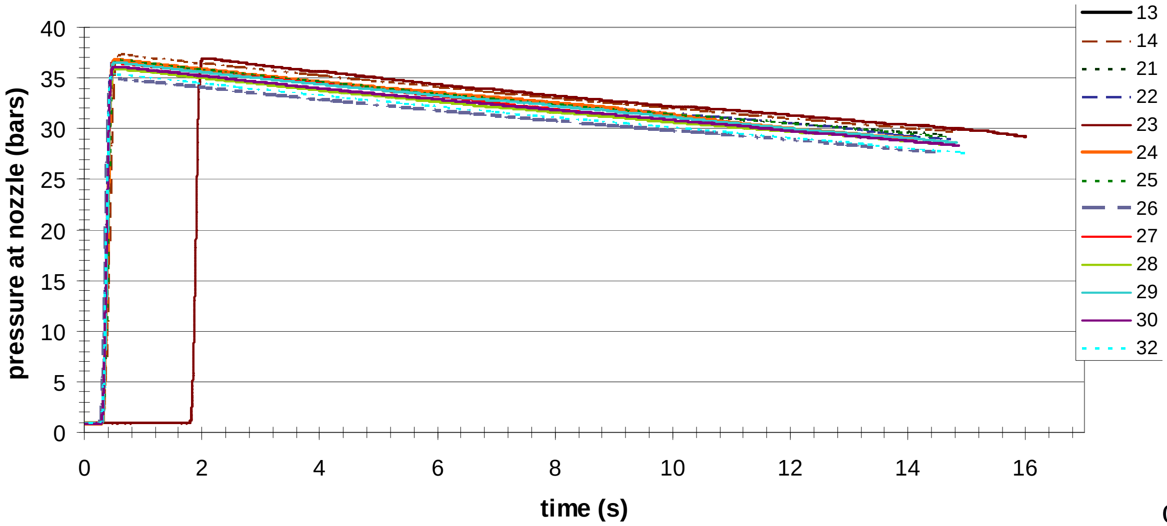

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Figure 2: The measured pressure at nozzle vs time for various experiments.

Figure 2 demonstrates the time evolution of the measured pressure at the nozzle. The pressure at the nozzle varied in time due to the reservoir depressurization; and the initial pressure slightly varied from one experiment to another.

The H_2 concentrations in the cloud, as well as radial and streamwise velocities, were measured at different axial positions (1.25, 2, 3, 4.5, 7.5 and 10 m from the release point). Concentrations in the cloud were measured using paramagnetic O_2 analyzers. Velocities were measured using Pitot probes (also called McCaffrey probe). These probes were equipped with rapid pressure sensors allowing the measurement of turbulence intensity.

Experiments were repeated 3 times, the release duration was 15 sec allowing for accurate measurements of concentrations and velocities in a stabilised cloud.

2.2 Explosion Tests

For explosion experiments, aerial overpressures were measured using 3 high speed piezo-resistive sensors placed in a lens allowing for measurements of the incident overpressure. The sensor L1 was placed 20 cm away from the release point. The sensors L2 was located on the axis of the jet 2 m downstream from the igniter and the sensor L3 was set perpendicularly to the jet axis, 2.5 m away from the igniter, see fig 3. All sensors were located 1.3 m above the ground.

For all experiments, the ignition occurred 5 seconds after the start of the release. All the experiments were duplicated under the same conditions.

Daubech et al [2] used a powerful ignition (8500 J) produced by the explosion of a stoichiometric H_2/O_2 mixture in a tube of 5.5 cm diameter and of 50 cm length, ignited by a pyrotechnical match (60 J). The ignition device produced a 40 cm long flame. To obtain the ignition on the release centreline, the extremity of the tube was placed 20 cm below the release axis. The ignition position was chosen at the location corresponding to a hydrogen concentration of 30% on the centerline (1.8 m downstream of the release point).

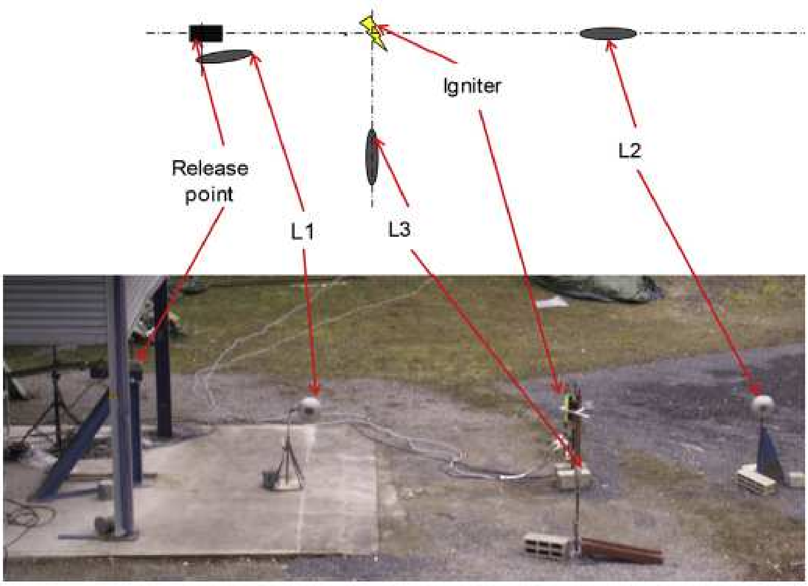


Figure 3: Positions of pressure sensors and ignition from the release point

3.0 SIMULATIONS DESCRIPTION

Two groups provided their computations for modelling the dispersion of hydrogen jet and then its explosion.

Table 1. Participants and their CFD codes.

Bench participant	Air Liquide	IRSN
CFD code	FLACS v10.4 [9, 10]	P²REMICS [11, 12]

Before starting the modelling procedure the experimental conditions must be correctly evaluated and reproduced, for instance one must know the initial pressure at the nozzle. Fig 2 shows that the average pressure, P_{mean}, at the orifice is 36.412 bars, the maximum pressure, P_{max}, is 37.371 bars and the minimum pressure P_{min} is 34.954 bars. Since during the measurements the pressure slowly decreases, for simulations it is decided to take the pressure which is the minimum P_{min}, see table.

Table 2: Description of the jet

Reservoir pressure (barg) and temperature (°C)	34 / 25
Ambient pressure (barg) and temperature (°C)	0 / 10
Nozzle temperature (°C)	10
Nozzle diameter D (mm)	12
Mass flow rate (kg/s)	0.259
Turbulence intensity	10%
Turbulence scale (mm)	0.1 D

The objective of this study is to compute jet dispersion and explosion in the region located more than 10 diameters from the orifice, hence for the modelling of releases from the high pressure reservoirs an equivalent source approach can be used. The parameters of the equivalent sources used by participants are listed in Table 3.

Table 3: Description of the equivalent sources

Equivalent source	FLACS	P²REMICS
Model of the equivalent source	FLACS Jet Program [10] models the expansion between the nozzle and the shock as an adiabatic process for a compressible gas (conservation of mass, momentum, and energy). The thermodynamic change across the shock front is not isentropic; here the Rankine–Hugoniot relations are employed. The pressure downstream of the shock front is	The Ewan and Moodie approach is used [15]. The hydrogen gas expansion from the reservoir to the nozzle is assumed isentropic. The equivalent source temperature and velocity are set to the nozzle temperature and velocity respectively.

	equal to the ambient one. This model is adapted from Birch et al. [13], and [14].	The notional nozzle pressure is set to the ambient one.
Equivalent source diameter (mm)	74	51
Equivalent source temperature (°C)	7.5	-25.15
Equivalent source velocity (m/s)	704.59	1197.78

Table 4 summarizes the modelling approaches used by participants. For CFD contributions, several strategies are adopted by considering axisymmetric 2D (P²REMICS) or full 3D volume (FLACS).

Table 4: Description of applied models

	FLACS	P²REMICS
Modeling approach	Fully 3D, no symmetry assumptions. Cartesian grid, compressible flow	2D, axisymmetric
Turbulence model	RANS, k-eps	RANS, k-eps with Kato and Launder modification [17] for combustion computations.
Combustion model	The flame turbulent burning velocity is based on Bray's expression [16]. The reaction zone in a premixed flame is thin compared to practical grid resolutions. The flame zone is thickened by increasing the diffusion by a factor β and simultaneously reducing the reaction rate by a factor 1/β. β is chosen such that the flame thickness becomes 3-5 grid cells. See for more details [10, 16]	The model is based on the turbulent flame-speed approach. The location of the flame brush is explicitly tracked by a phase-field technique (G-equation), the flame front being followed by an instantaneous combustion, thanks to an *ad-hoc* modification of the reactive term in the species mass balance equations [12]. The model is closed by the Peters turbulent flame speed correlation [18, 19]. The Iijima's correlation is used in order to compute the laminar flame speed [20].
Specifications, applied		A Low Mach number incompressible solver is used for the simulation of the dispersion phase, whereas for the combustion phase, a fully compressible formulation is used.

FLACS [10] does not recommend applying symmetry conditions for explosion simulations (boundaries must be moved apart to avoid the pressure reflection from the boundary conditions), hence it is decided to use full 3D approach with a large simulation domain even for dispersion simulations.

Table 5 gives an overview on the discretization in time and space used by participants

	Air Liquide (FLACS v10.4)	IRSN (P²REMICS)
Scheme in time:	first order backward Euler scheme	Semi-implicit scheme with fractional steps. First-order time discretization
Convection scheme:	Second-order ''kappa'' scheme (hybrid scheme with weighting between 2nd order upwind and 2nd	MUSCL for the scalars transport for the calculation of combustion and hybrid scheme for dispersion calculation,

	order central differences, with limiters for some equations)	centered scheme for Navier Stokes
Diffusion scheme	Second-order	Usual two-points flux finite volume approximation

Finally table 6 summarizes the main characteristics of the mesh used by the participants. Solution independence on the size of the computational domain and on spatial resolution is verified by all participants.

Table 6: Grid description

	Air Liquide (FLACS v10.4)		IRSN (P²REMICS)
	Dispersion	Explosion	
Size of the simulation domain (Length by Width by Height)	65m by 30m by 17m		15m in axial direction and 8m in the radial direction
Type of grid	structured, Cartesian		structured
Min and max size of grids	min 0.085m; max 0.25m	min 0.085m; max 0.25m	min 4.e-4m, max 2.6 e-3 m
Number of grid points	coarse: 2 381 060; average:4 129 125; fine: 4 179 175	average: 5 034 300 fine : 5 240 862	fine 446 566
Local refinement	Close to the release point	Refined in the explosion region and up to the pressure sensors locations	Refined in the explosion region and close to the orifice

4.0 RESULTS

4.1 Dispersion

Concentration plays an important role in the flame acceleration; hence its correct distribution in space and time is an important parameter for explosion modelling.

Experimental results of Daubech et al.[2] for dispersion are compared with CFD simulation. As shown in Fig. 4 experiments and FLACS v10.4 (Air Liquide) simulations are in good agreement for the hydrogen concentration decay vs. the streamwise direction. P²REMICS (IRSN) slightly overestimates the concentration, probably due to a different model for the equivalent source. For the radial concentration decay, FLACS v10.4 (Air Liquide) is in good agreement with experimental results, see fig 5, whereas simulation results of IRSN demonstrate a narrower radial concentration profile than the experimental one. This behaviour can be explained by the axisymmetry assumption, which does not take into account buoyant effect of hydrogen, hence limits the air entrainment in the jet. However axisymmetric results can be considered as more conservative compared to 3D. Another reason could be the use of a different correlation for the equivalent source. Indeed, IRSN performed the same computations presented here with the Birch [13] correlation instead of the Ewan and Moodie [15] approach. The results showed that the use of the Birch [13] correlation gives a better approximation of the concentration in the axial and radial directions, even with a 2D axisymmetric assumption.

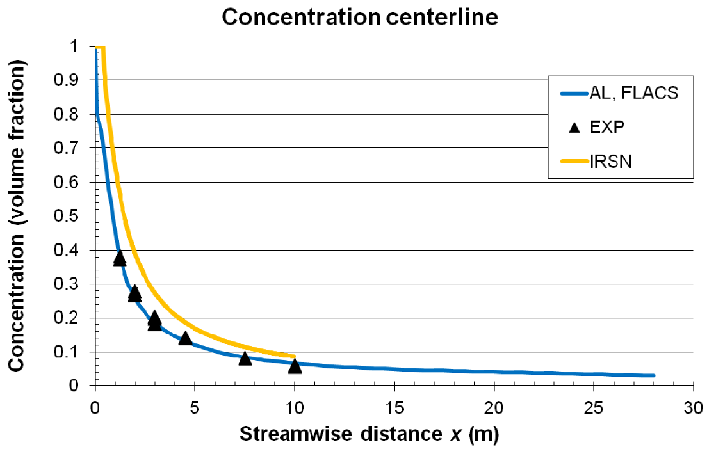
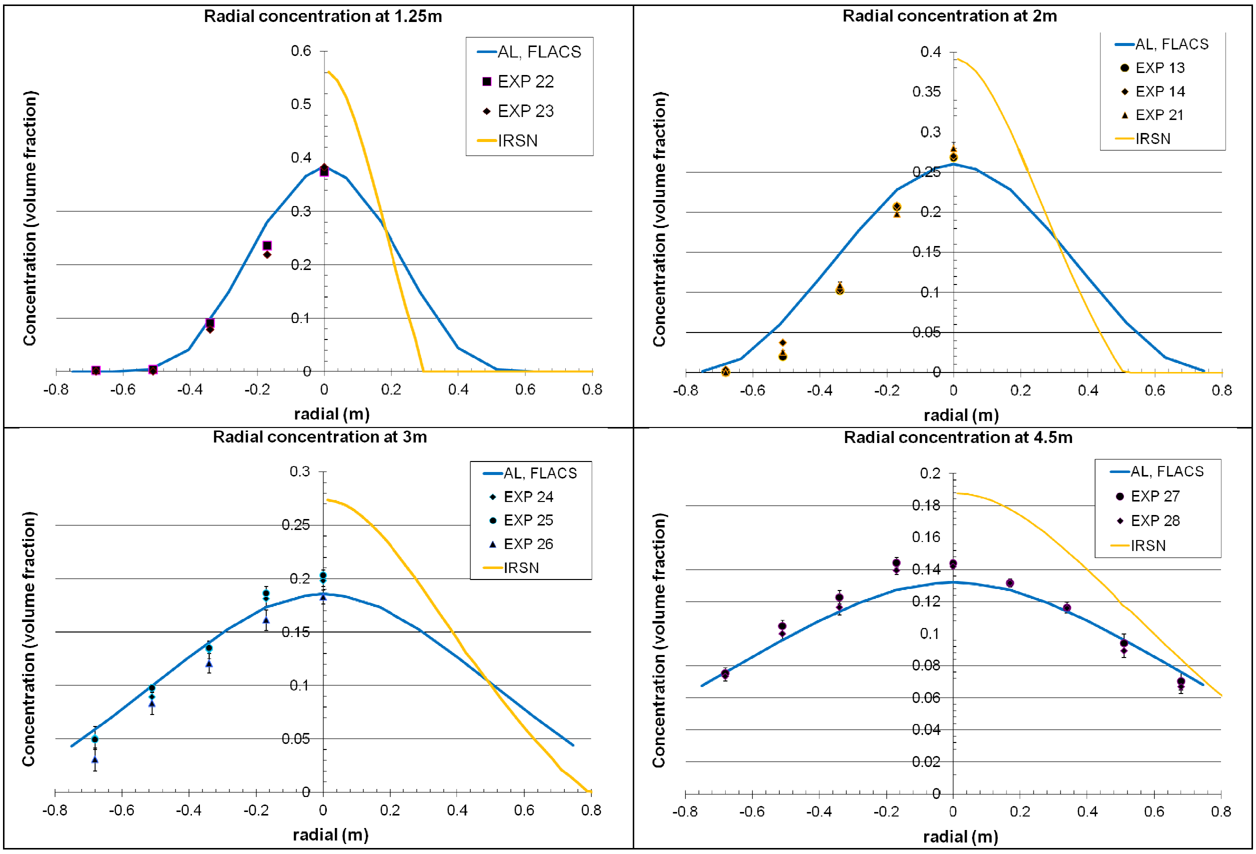


Figure 4: Concentration decay on the centreline – experiments vs. CFD: exp data are represented by markers, blue line – FLACS simulations (Air Liquide) and orange line - P²REMICS (IRSN).

In order to correctly represent the explosion in the highly turbulent jet it is requested to correctly reproduce not only the concentration distribution in axial and radial direction, but also the velocity field and the associated turbulence intensity.



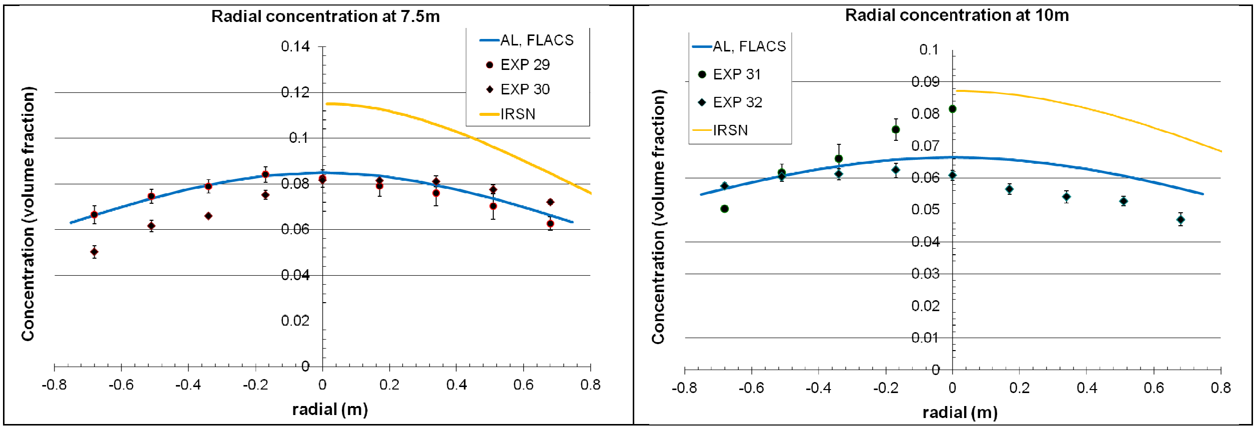


Figure 5: Concentration decay in the radial direction on various distances from the release point – experiments vs. CFD: exp data are represented by markers, blue line – FLACS simulations and orange line - P²REMICS.

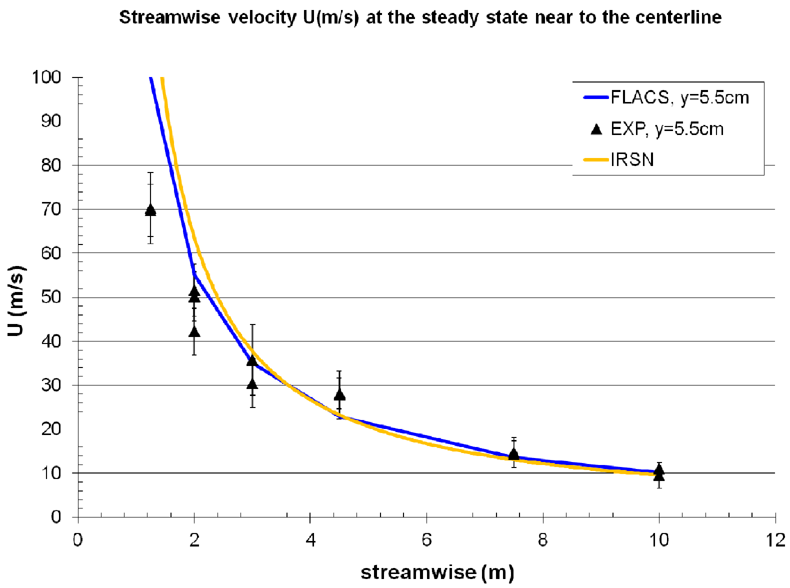


Figure 6: Velocity decay on the centreline – experiments vs. CFD: exp data are represented by markers, blue line – FLACS simulations and orange line - P²REMICS.

Figures 6 and 7 show the centreline velocity decay with the distance from the source in the streamwise and radial directions: CFD simulations vs. experimental measurements.

One can note a high error bar for experimental data for velocity decay on the centerline; however the comparison with simulations results showed that CFD results are in reasonable agreement with experimental data: Air Liquide and IRSN show a tendency to overestimate the velocity, the radial distribution is in acceptable agreement.

Figure 8 shows the fluctuation velocity distribution in the radial direction for various distances from the release point. At short distances (< 3 m) away from the source, the experimental detectors were saturated for some reasons, hence here for comparison with simulations only experimental data for x > 3 m are considered.

Figure 8 demonstrates that Air Liquide simulations (FLACS v10.4) and IRSN results are in reasonable agreement with measurements and with each other (both cases k-eps model).

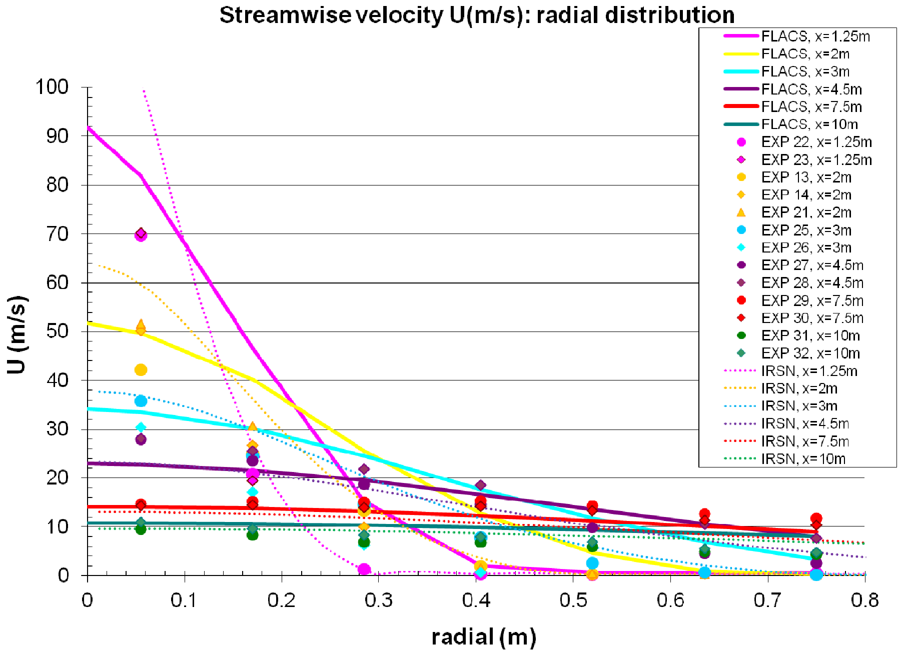


Figure 7: Velocity decay in the radial direction – experiments vs. CFD: exp data are represented by markers, solid line – FLACS simulations and dotted line - P²REMICS.

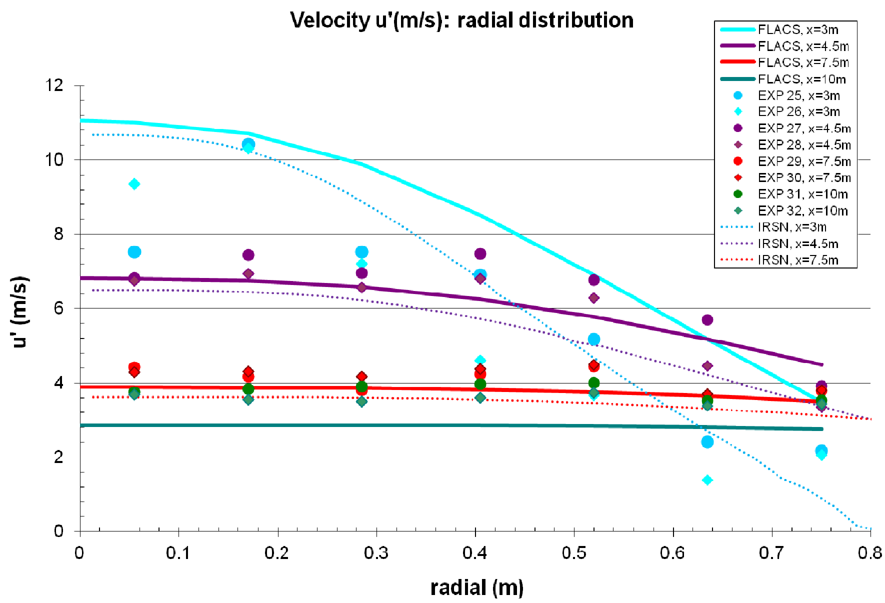


Figure 8: Fluctuation velocity u' in the radial direction for various distances from the release point – experiments vs. CFD: exp data are represented by markers, solid line – FLACS simulations and dotted line - P²REMICS.

In general all CFD simulations considered here give reasonable agreement with experimental data, hence it can be concluded that simulations correctly reproduce the physical phenomenon of jet dilution.

4.2 Explosion

The comparison of simulation results at 3 overpressure monitoring points is shown on Fig.9: L1 sensor is located near the release point (20 cm), the L2 sensor is located on the axis of the jet, 2 m downstream from the ignition, and the L3 sensor is located at 2.5 m from the ignition perpendicularly to the jet axis.

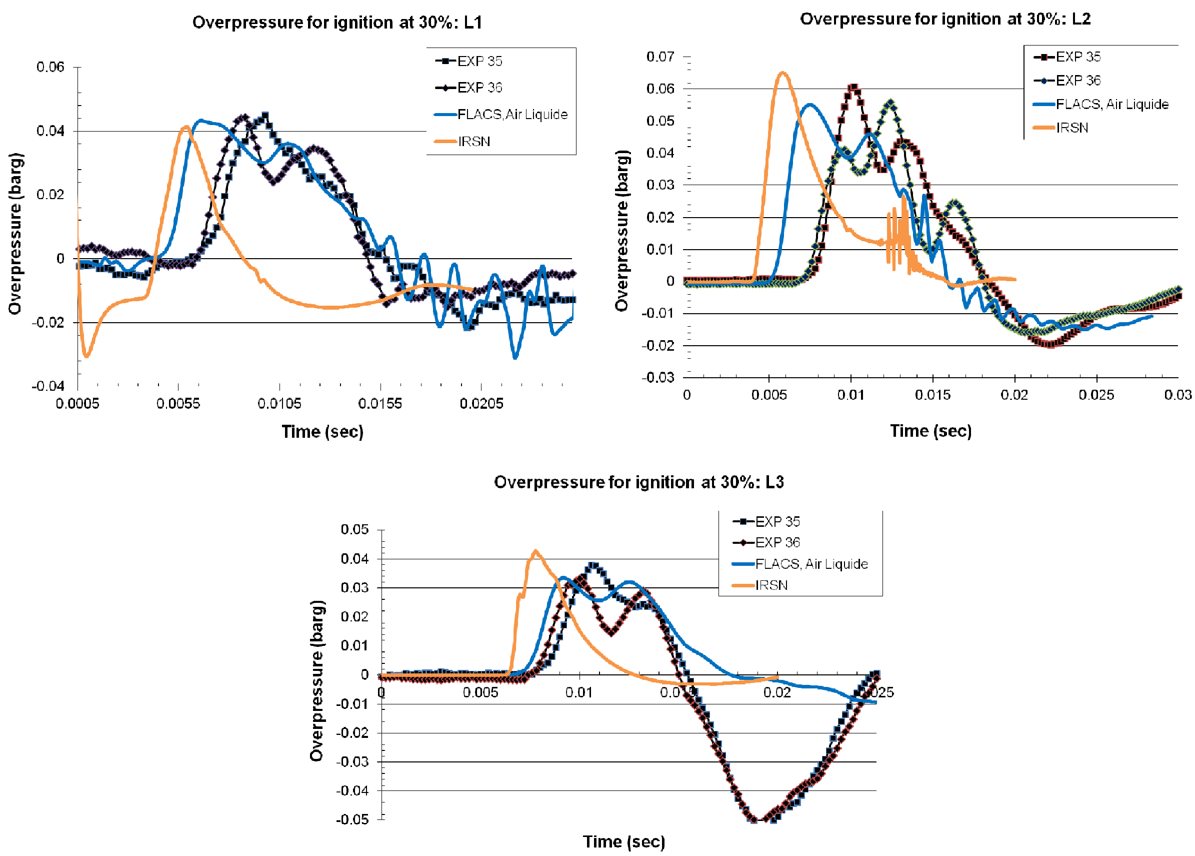


Figure 9: Comparison of simulated overpressure with experimental data at 3 monitor positions: exp data are represented by markers, blue line – FLACS simulations (Air Liquide) and orange line - P²REMICS (IRSN).

Fig. 9 demonstrates good agreement between simulations of both participants and experimental data for overpressure magnitude. IRSN overpressure on L2 and L3 sensors is slightly higher than the experimental one (probably due to the overestimation of the concentration on the centreline). The associated positive impulse is also correctly estimated by Air Liquide (FLACS v10.4), whereas IRSN (P²REMICS) gives a narrower overpressure peak.

Simulations of Air Liquide (FLACS v10.4) 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. Since IRSN considered the axisymmetric case there is no ground and thus the overpressure signal has only one peak.

Experimental overpressure signal on L3 shows an important negative phase of the signal due to a thermal divergence of the pressure sensor. This explains why numerical simulations do not reproduce this strong negative phase.

Basically, for explosions the computed overpressure signals reasonably match experimental data for both participants where the computed overpressure magnitude closely matches experimental measurements for both participants.

5.0 DISSCUSION AND CONCLUSION

Hazards associated with hydrogen jet explosions are important scenarios considered today in risk studies [2]. It is therefore important that delayed ignition jet explosion can be correctly reproduced by CFD tools when assessing the potential consequences of accidental hydrogen releases. For this purpose two groups performed a bench using two different CFD codes in the frame of the French working group dedicated to the evaluation of computational fluid dynamics (CFD) codes for the modeling of explosion phenomena. Simulation results were compared to each other and to experimental measurements performed by Daubech et al. [2], first for dispersion modeling and then for the explosion.

For dispersion both participants' CFD codes give reasonable agreement with experimental data, showing that simulations correctly reproduce the physical phenomenon of jet dilution. However 2D axisymmetric simulation overestimates the concentration on the centreline and in the radial direction. This could be due to the absence of buoyancy which leads to smaller air entrainment in the jet, giving a narrower concentration profile compared to experiments and 3D simulations. Another reason could be the use of a different correlation for the equivalent source. Indeed, IRSN performed the same computations presented here by changing only the notional nozzle approach. The results showed that the use of the Birch [13] correlation gives a good approximation of the concentration in the axial and radial directions, but is less accurate for the velocity decay.

For explosion simulations the computed overpressure signals reasonably match experimental data for both participants whereas the computed overpressure magnitude closely matches experimental measurements. In the case of the 2D axisymmetric approach the overpressure on sensors L2 and L3 is slightly overestimated, probably due to the overestimation of the concentration at the centreline. 2D simulations also give a narrower overpressure peak compared to 3D CFD and experiments, leading to an underestimation of the positive impulse.

3D 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 found in the experiments.

Based on this bench several recommendations can be given for CFD modelling of delayed explosion of high pressure jets of hydrogen.

- In dispersion simulations, a full 3D approach allows bench participants to avoid too conservative results for concentration distribution, since it takes into account buoyancy effects driven by space variations in the hydrogen concentration. This leads to a correct computation of the air entrainment into the jet, giving an appropriate concentration distribution in the radial direction

- For explosion simulations, in order to reproduce the pressure reflection by the ground a full 3D CFD approach must be used. In the 3D case the positive overpressure impulse is correctly estimated, whereas for 2D the positive impulse is underestimated.

6.0 REFERENCE

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