VALIDATION AND RECOMMENDATIONS FOR CFD AND ENGINEERING MODELING OF HYDROGEN VENTED EXPLOSIONS: EFFECTS OF CONCENTRATION, OBSTRUCTION AND VENT AREA

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ABSTRACT

Explosion venting is commonly used in the process industry as a prevention solution to protect equipment or buildings against excessive internal pressure caused by an explosion. This article is dedicated to the validation of FLACS CFD code for the modeling of vented explosions. Analytical engineering models fail when complex cases are considered, for instance in the presence of obstacles or H_2 stratified mixtures. CFD is an alternative solution but has to be carefully validated. In this study, FLACS simulations are compared to published experimental results and recommendations are suggested for their application.

1.0 INTRODUCTION

Explosion venting is commonly used in the process industry as a prevention solution to protect equipment or buildings against excessive internal pressure caused by an explosion. Vented explosions have been widely studied, both experimentally and numerically. There are also several analytical models able to give an estimation of the overpressure corresponding to the internal explosion. The evolution and validation of one of these models is described in ref. [1]. However, for hydrogen, these different engineering models show conflicting results due to the number of different factors that may influence the peak overpressure. In other more complicated cases, for instance in the presence of multiple vents, obstacles or in the presence of a H_2 layer or gradient, it is very difficult to find a proper analytical model giving reliable results in a wide spectrum of possible geometry configurations. Thus these specific configurations must be further addressed by experimental investigations. However since it is not always possible to carry out an experiment in realistic dimensions, CFD could 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.

In order to use a CFD code for safety computations, first of all the code must be validated versus various available experimental data. In the following, the ability of the CFD code FLACS [2] to reproduce experimental results obtained in a selection of three vented explosion chambers – with and without obstructions with mixtures of various concentrations – is addressed. The representation of the various mechanisms that result in the observed overpressure profiles is emphasized.

2.0 BRIEF DESCRIPTION OF THE EXPERIMENTAL FACILITIES

2.1 FM Global outdoor chamber

Bauwens et al. [3, 4] performed deflagrations of homogeneous hydrogen-air mixtures with approximately 18% (±0.3%) of hydrogen in a 63.4 m^3 explosion test chamber with overall dimensions of 4.6 x 4.6 x 3.0 m. Square vents of 5.4 m^2 and 2.7 m^2 were located on the front walls. Only the back wall ignition (BWI) position is considered here. For more details about the experimental set-up, see [3-8].

The results from measurements were pre-processed using an 80 Hz low-pass filter [3-7]. Due to uncertainties of ±0.3% in the concentration (18.3% and 17.9% of hydrogen/air mixture) two different pressure curves were measured in experiments ref[3, 4]. The measured overpressure inside the chamber varied from 0.125 barg up to 0.15 barg from one experiment to another (for 18.3% and 17.9% relatively). Fig 1 shows some differences in the overpressure signal, however the flame velocity remains approximately the same in both experiments.

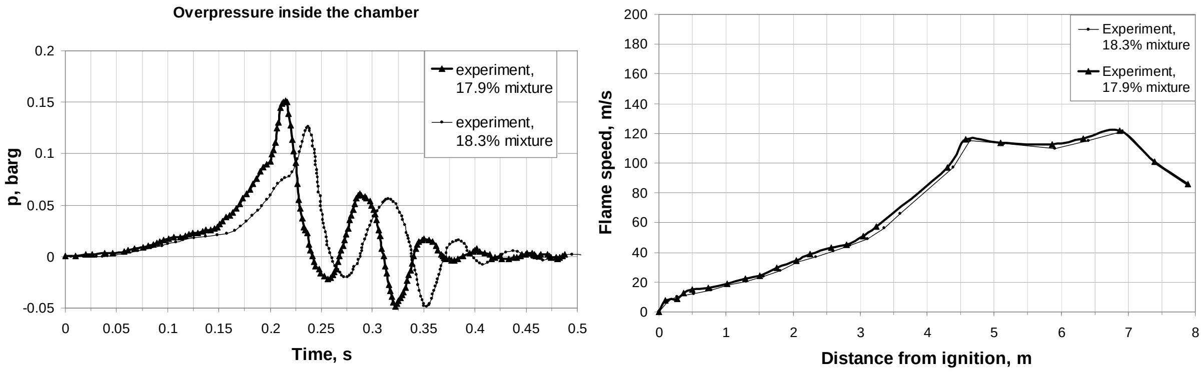

Figure 1. Experiments of 17.9% and 18.3% hydrogen/air explosion in a 63.4 m3 chamber (BWI, vent area 5.4 m2): on the left the overpressure inside the chamber, on the right the flame velocity.

2.2 KIT indoor chamber

The combustion chamber itself is almost cubic with inner dimensions of 1 x 0.96 x 0.98 m^3 (H x W x D). The vent area is 0.25 m^2 (0.5m by 0.5m). The vent is located in the centre of the enclosure wall. The experimental facility volume containing the combustion chamber is approximately 160 m^3, see ref [9]. Homogeneous hydrogen-air mixtures are considered in current paper.

The overpressure history is recorded using a set of 8 fast pressure transducers. The results from measurements were pre-processed using an 200 Hz low-pass filter. The18% hydrogen-air mixture is ignited by a spark in the centre of the rear plate co-called back wall ignition.

2.3 INERIS outdoor 4m^3 chamber

INERIS performed vented deflagrations of various homogeneous hydrogen-air mixtures in a 4 m^3 explosion test chamber with overall dimensions of 2m x 1m x 2 m ref. [10]. For considered here test-cases a square vent of 0.25 m^2 and 0.49 m^2were located on the front walls.

Overpressure was measured using 3 piezoresistive sensors. The measurement uncertainty is ± 0.1 % of the full measurement scale (16.5% and 15.5% of hydrogen/air mixture). The measurement of the outside chamber pressure is performed by 3 piezoresistive sensors, located above the ground on lenses allowing for non-perturbed overpressure at 2m, 5m away from the chamber (at the axis of the vent). The third sensor 5mp is located on the axis perpendicular to the chamber one, 5 m away from the vent. The results from measurements were pre-processed using an 100 Hz low-pass filter.

Ignition is supplied close to the wall opposite the vent (back wall ignition).

3.0 NUMERICAL SIMULATIONS SETTINGS

FLACS is a commercial code developed by GexCon to simulate gas explosions in offshore oil and gas production platforms. FLACS is a computational fluid dynamics (CFD) code that solves the compressible Navier-Stokes equations on a 3-D Cartesian grid using a finite volume method.

The RANS (Reynolds-Averaged Navier-Stokes) k-ε model equations are solved in FLACS for turbulence ref [2, 13]. The SIMPLE pressure correction algorithm is used ref [14].

In FLACS combustion model the flame 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 Brey's expression [15]. The reaction zone in a premixed flame is thin compared to practical grid resolutions. In FLACS, the flame zone is thickened by increasing the diffusion by a factor β and simultaneously reducing the reaction rate by a factor $1/\beta$. β is chosen such that the flame thickness becomes 3-5 grid cells.

3.1 FM Global outdoor chamber

The computational domain was chosen to be 35m long in the streamwise direction (from -5m up to 30m), 20 m in the cross-stream direction and 15 m in the vertical direction. The geometry is represented on the grid (with the volume and area blockage ratios equal to either 0 or 1). The centre of the chamber was chosen at coordinates (0, 0, 1.5m). At the open outlet boundaries a "plane wave" boundary condition was used, see ref. [2] for more information about the choice of boundary conditions. The vent position was chosen to be at the centre of the wall. The gravity is activated and is parallel to the vertical Z axis. Turbulent velocity fluctuation of 0.1 m/s and an initial turbulence length scale of 0.01 m were imposed as initial conditions on the hydrogen-air mixture inside the chamber.

A constant size-grid of 10 cm is sufficient to correctly reproduce the flow dynamics (results from size-grid of 10 cm and 7.5 cm matches close). Ref [8] underlines that even a constant grid size of 20 cm is accurate enough for similar geometry to correctly reproduce the explosion of propane. In our investigation however we use a constant grid of 10 cm size. A non-stretched mesh was chosen to correctly reproduce the pressure wave propagation outside the combustion chamber.

We model the explosion of 18.3% and of 17.9% H_2-air mixture.

3.2 KIT indoor chamber

The computational domain is the same size as the experimental facility. In the simulations the centre of coordinates was chosen in the same way as in the experiment. The gravity is activated and it is parallel to the vertical Z axis. A constant size-grid of 4cm is sufficient to correctly reproduce the flow dynamics (results from size-grid of 4 cm and 2 cm match close). No initial turbulence is imposed in the simulations. The concentration of hydrogen/air mixture is the same as in the experiment and is18%.

Since the experimental enclosure was located inside a specific explosion chamber (160 m^3), three different boundary conditions are tested for modelling: "Plane Wave", "Euler" and "Nozzle". "Plane Wave" boundary condition represents the open boundary such that the pressure wave can go through the boundary with no reflection. However simulations show, even in the case of the reflection, that this does not affect the overpressure peak corresponding to the vented explosion.

3.3 INERIS outdoor 4m^3 chamber

The computational domain was chosen to be 10m long in the streamwise direction, 10 m in the cross-stream direction and 5.5 m in the vertical direction. It was verified that this computational domain is large enough and that the effect of boundary conditions on the pressure wave propagation is negligible. The centre of the chamber was chosen at coordinates (0m, 0m, 1m). Similarly to FM Global experiment, at the open outlet boundaries a "plane wave" boundary condition was used. The vent was located at the centre of the wall. The gravity is activated and is parallel to the vertical Z axis.

Due to the presence of the fan a turbulent velocity fluctuation of 0.1 m/s and an initial turbulence length scale of 0.01 m were imposed as initial conditions on the hydrogen-air mixture inside the chamber, T=20°C.

The grid size was kept constant in the region ([-1m, 3.5m] in the streamwise direction, [-1.55m, 1.55m] in the cross-stream direction and [0m, 2.5m] in the vertical direction), then the grid is stretched in all three directions with a stretching factor 1.1.

The grid convergence is verified and obtained for the grid size of 2.5 cm. In the case of back wall ignition, the ignition point was chosen to be 1cm away from the back wall.

4.0 RESULTS FROM NUMERICAL SIMULATIONS FOR FM GLOBAL OUTDOOR CHAMBER

4.1 Overpressure

Fig. 2 shows the evolution of the overpressure in time as obtained from numerical simulations vs. experimental results at 6 sensors inside the chamber. Since the experimental overpressure varied from one experiment to another, in fig 2 we present both experimental curves corresponding to the maximum overpressure of 0.15 barg (on the left) and 0.125 barg (on the right).

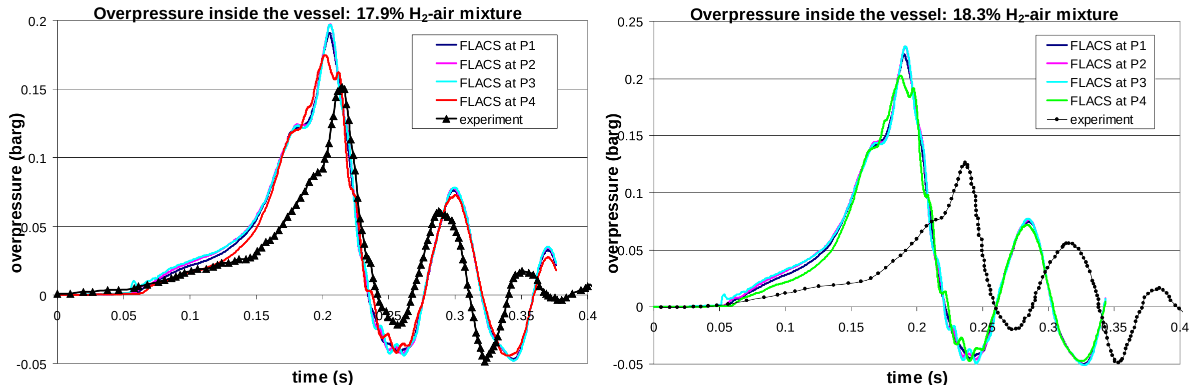

Figure 2. The overpressure as a function of time at various pressure sensors inside the combustion chamber: simulations vs. experimental results (in black).

Experimental overpressure signals have two main maxima, the first one corresponds to the pressure from the external explosion and the second overpressure corresponds to the vibration of the flame surface from the combustion of the rest of the mixture inside the chamber. In the case of numerical simulations only the first overpressure peak (external explosion, see fig. 3) can be computed. For the correct modelling of the second peak, the simulation mesh must be very fine (the order of mm) to represent the flame thickness and flame wrinkling due to the acoustic flame instabilities, see [8] for more details. However FLACS simulations reveal the second overpressure spike. The detailed investigation showed that its origin is purely numerical, and can be explained by the pressure reflection from the simulation domain boundary. The larger computational domain the later the second spike arrives.

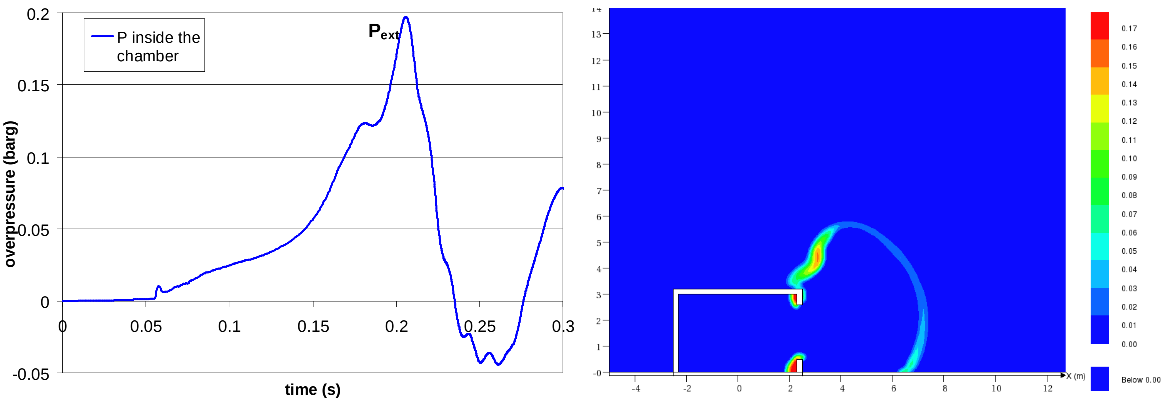

Figure 3. The evolution of the overpressure inside the chamber in time (on the left), snapshots of the mixture concentration (on the right) at the moment corresponding to the external explosion P_{ext} (first overpressure spike t=0.207sec).

Fig. 2 shows that the first overpressure spike computed by FLACS is in quite good agreement with experimental data for the for 17.9% mixture, with a slight overestimation of the overpressure maximum. Simulations also tend to anticipate the spike. The results of FLACS simulations performed with lower concentration are in better agreement with experimental.

4.2 Flame propagation

The dynamics of the flame velocity at the centreline of the combustion chamber with the distance from the ignition position including both experimental and FLACS simulation results are illustrated in Fig. 4. In spite of the difference in experimental overpressures, the flame velocity is approximately the same in both experiments. FLACS flame dynamics is closer to the experimental data for a lower concentration mixture (17.9% H_2/air mixture).

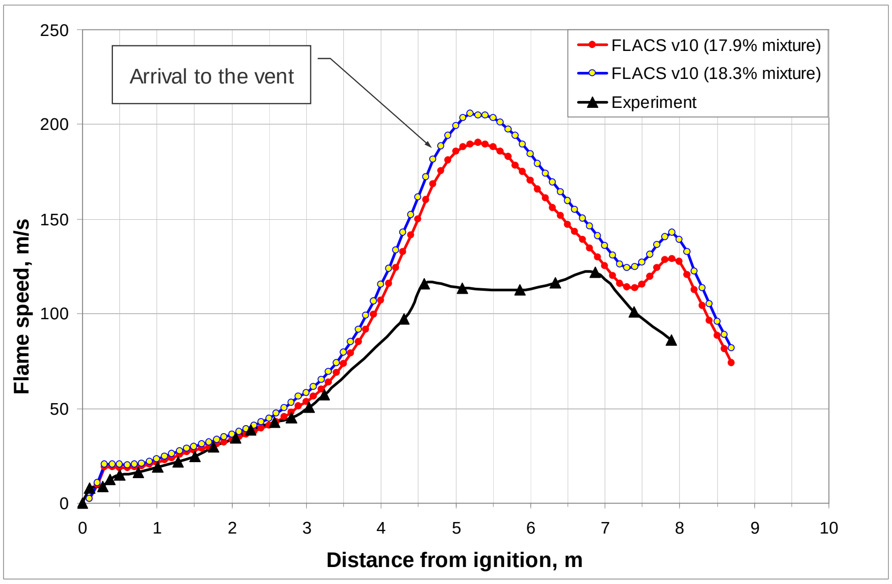

Figure 4. Averaged flame velocity versus distance from the ignition: FLACS v10 simulations vs. experiment.

One can see that the flame velocity is approximately the same, showing a close match with experimental measurements until 3m. However at distances larger than 3.5 m FLACS the flame velocity is significantly higher than the ones from experiments. The largest difference in the flame speed is observed outside the combustion chamber in the region corresponding to the evacuated outside mixture cloud.

For the same mixture FLACS gives slightly higher laminar flame velocity ($0.71 m.s^{-1}$) than the one found from the experimental data ($0.68 m.s^{-1}$). The flame propagation weakly depends on the initial laminar velocity (on short distances all simulations results and experimental data match closely) but it rather depends on the turbulence intensity, which leads to the strong flame acceleration, especially in the region of the vented outside the chamber cloud of a fresh mixture.

4.3 Effect of obstacles and vent area on the overpressure

FM Global experiments are also performed in the presence of eight $0.40 \times 0.40\ m^2$ square obstacles of full height of the chamber. Table 1 shows the comparison of experimental and numerical data for with back wall ignition (BWI) in terms of the maximum overpressure corresponding to the vented explosion.

Table 1: Initial conditions for a vessel burst problem.

Vent area m^2	Concentration of H_2,%	Obstacles	Experimental overpressure (barg)	FLACS overpressure (barg)
5.4	~17.9	0	0.15	0.18
5.4	~18.1	8	0.43	0.69
2.7	~18	0	0.32	0.53

The presence of obstacles has a significant effect on the flame acceleration and hence on the overpressure. The wake behind the obstacles enforces very high turbulence intensity, thus high flame velocity propagation is observed, which leads to high overpressure. FLACS is conservative for the vented explosion without obstacles, with an overestimation of the overpressure by 30%. In the presence of obstacles the overpressure is overestimated by a factor of ~1.5. Simulations are still conservative.

FLACS uses concept of distributed porosity for geometry representation, where large represented on-grid and smaller objects represented on sub-grid. The porosity is a simplified local congestion and confinement allowing contribution of small objects to the flow drag, turbulence generation and folding of the flame. Effect of porosity geometry representation (with 0< blockage ratio<1) is also investigated. It is found that when the geometry is represented using the porosity model, the overpressure corresponding to the external explosion is overestimated in average by a factor of 2.2 for an empty chamber and even higher for the geometry with obstacles.

In the case of a smaller vent, the overpressure computed by FLACS significantly higher than the experimentally measured one (by a factor of ~1.5), the time of the detection of the maximum is 0.2 sec in FLACS simulations and is approximately 0.225 sec in experiments. This means the flame propagates faster by FLACS, and this leads to a higher overpressure.

In the presence of obstacles, for BWI the second overpressure peak corresponding to the vibration of the flame surface from the combustion of the rest of the mixture inside the chamber disappears. This leads to a better global agreement between simulations and experimental data in terms of the shape of the overpressure curve.

5.0 RESULTS FROM NUMERICAL SIMULATIONS FOR KIT INDOOR CHAMBER

The comparison of simulation results to the experimental measurements shows good agreement in terms of overpressure and of the time of its detection:

Table 2: The overpressure maximum inside the enclosure and the time of its appearance (FLACS results vs experimental data).

Vent area m^2	Concentration of H_2,%	Experimental overpressure (barg)	Experimental time of the max overpressure (sec)	FLACS overpressure (barg)	FLACS time of the max overpressure (sec)
0.25	~18	0.126	0.086	0. 136	0.061

The computed overpressure maximum matches closely the experimental ones, whereas the time of the appearance of the maximum overpressure is earlier in simulations than in the experiment.

Similar to FM Global in KIT experiment the first overpressure spike corresponds to the overpressure resulted from the external explosion, see fig 5.

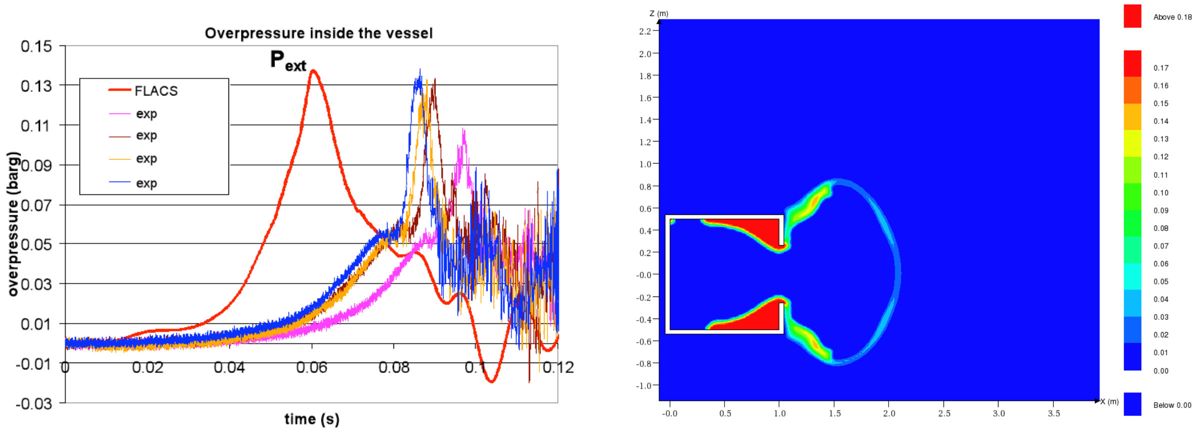

Figure 5. The evolution of the overpressure inside the chamber versus time (on the left), snapshot of the mixture (on the right) at the moment corresponding to the external explosion t=0.061sec (first overpressure spike).

The overpressure decay computed by FLACS outside the combustion chamber at inside the chamber (at 2 sensors) remains in close agreement with experimental data with a slight overestimation. Similarly to the overpressure inside the enclosure, the overpressure computed by FLACS appears approximately 25 ms earlier than in the experiment.

6.0 RESULTS FROM NUMERICAL SIMULATIONS FOR INERIS OUTDOOR 4M^3 CHAMBER

Consider the simulations of test cases corresponding to vent area of 0.49m^2 and of 0.25 m^2. In both case the ignition was performed at the back wall. The pressure evolution inside the combustion chamber for both test cases is shown in Fig. 6, where the comparison of experimental and computed overpressure is displayed.

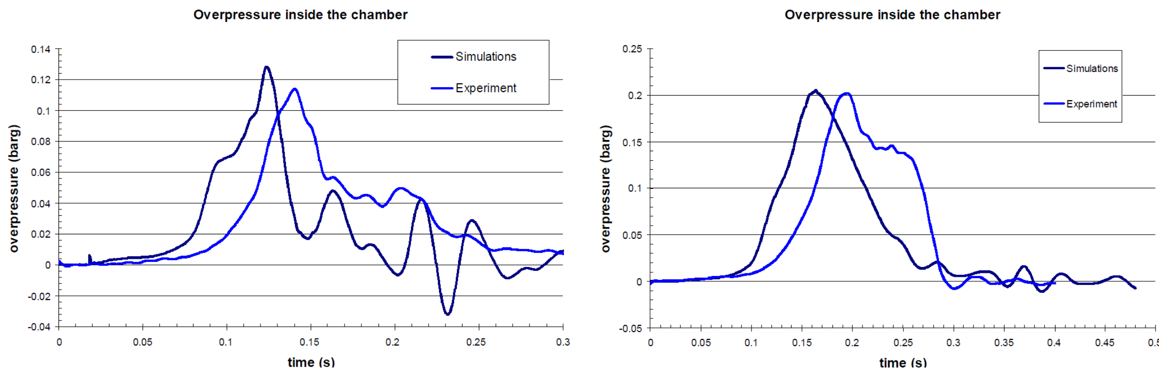

Figure 6. Pressure evolution inside the chamber for the back wall ignition (simulations vs. experiments): on the left the vent area is 0.49 m^2 and concentration 16.5% and on the right for the vent area of 0.25 m^2 and concentration 15.5%.

Results from this comparison show that in both cases simulations match quite closely experimental results for the overpressure.

Table 3: The overpressure maximum inside the enclosure and the time of its appearance (FLACS results vs experimental data).

	t of the flame exit (sec)	Pext (barg)	time (sec) correspond. to Pexp appearance (tPexp)	P (barg) at 2m	P (barg) at 5m	P (barg) at 2mp
16.5% H_2 mixture (vent area of 0.49 m^2)						
Experiment	0.128	0.114	0.14	0.087	0.056	0.029
FLACS	0.106	0.128	0.125	0.107	0.029	0.021
15.5% H_2 mixture (vent area of 0.25 m^2)						
Experiment	0.166	0.202	0.195	0.0767	0.0836	0.0245
FLACS	0.137	0.210	0.164	0.072	0.034	0.010

The comparison of simulations and experimental results (Table 3) suggests that the results from both modelling approaches match closely experimental data inside the combustion chamber. However outside the combustion chamber it seems that the computed overpressure is underestimated. This can be explained by the stretching of the computational grid outside the combustion chamber which leads to extra numerical diffusion affecting the results.

7.0 RESULTS FROM NUMERICAL SIMULATIONS OF OTHER CASES FROM LITERATURE

FLACS simulations are also performed for modeling of other experimental data known from literature such as [11]-[12]. All these experiments performed in cylindrical vessels of ~1m^3 [11, 12] and 10m^3 [12]. Table 4 gives a brief description of experimental facilities:

Table 4: The brief description of experiments from literature [11, 12].

Experiment	Volume of the chamber (m^3)	Vent area (m^2)	Hydrogen concentration, vol %
Pasman	0.95	0.2	30%
		0.3	
INERIS 1m^3	1	0.15	10%
			15%
			20%
			27%
INERIS 10m^3	10	2	14%
			23%

The comparison of simulation results to experimental data are summarized in fig 7.

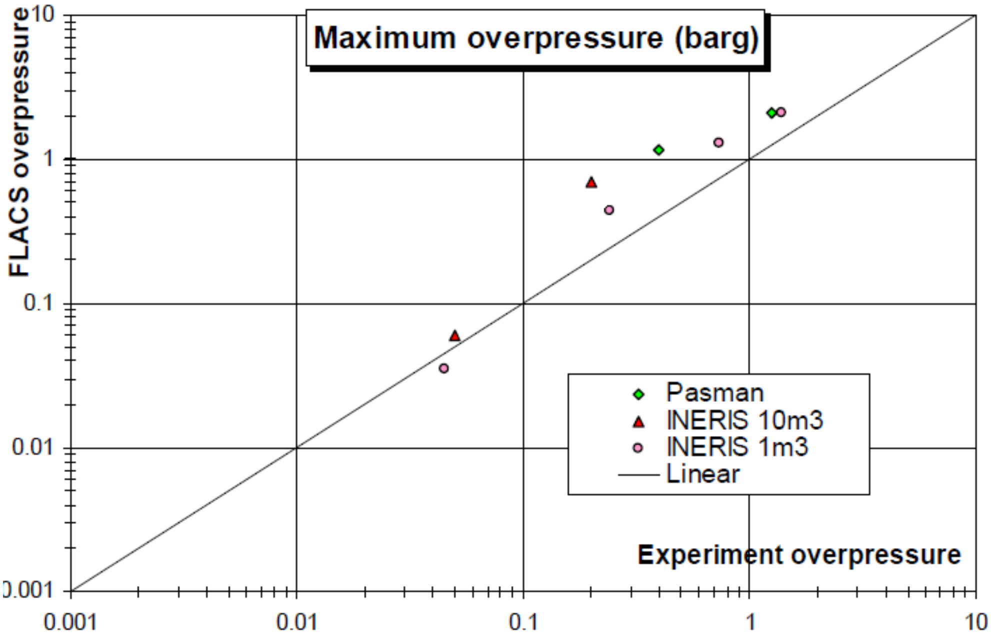

Figure 7. Summary of FLACS overpressure peak prediction capability compared to experiments from the literature ref [11]-[12]: on the horizontal axis the maximum overpressure spikes obtained from experiments, on the vertical axis are corresponding FLACS overpressure spikes values.

Fig 7 illustrates the ratio between the calculated value and the experimental data in terms of the maximum overpressure for all experiments presented here. The horizontal axis corresponds to the overpressure obtained from the experiment; the vertical one represents FLACS results. The straight line corresponds to the perfect match experimental-computed overpressure. The points below the line correspond to cases where FLACS underestimates the overpressure, points above the line to cases where FLACS overestimates the overpressure. One can see that FLACS overestimates the maximum experimental overpressure.

8.0 CONCLUSION

In the case of central ignition (CI) and forward ignition (FI) (close to the vent) the second peak (corresponding to the vibration of the flame surface of the rest of the mixture inside the chamber) can be dominant compare to the first one (originating from the vented explosion). The analysis of the simulations, for instance from ref [8], shows that FLACS is not able to compute the second overpressure spike. Thus for CI and FI ignitions FLACS simulations can lead to misleading conclusions. Currently there is no a CFD tool, which is able properly capture the second overpressure peak. Hence it is not recommended to use CFD tools for CI and FI.

In general for back wall ignition FLACS slightly overestimates the overpressure inside the chamber in the cases without obstacles. In the presence of obstacles inside the chamber, FLACS overestimates the overpressure by ~60%. Also in the presence of obstacles for BWI the second overpressure peak disappears, leading to a better general match between simulations and experimental data.

For a correct pressure wave representation outside of the combustion chamber (in a far field) it is recommended to use square grid (no-stretched). Use of the grid stretching can create an artificial numerical diffusion, leading to an underestimation of the overpressure magnitude in a far field.

Simulation results show that the turbulent subgrid model (used when the geometry is represented by means of porosity) overestimates the turbulence, hence the flame velocity is overestimated too, which leads to higher overpressure. Hence in the cases of not high obstruction it is recommended to represent geometry directly on grid (with the volume and area blockage ratios equal to either 0 or 1).

9.0 REFERENCES

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