VENTED EXPLOSION OF HYDROGEN / AIR MIXTURE: AN INTER COMPARISION BENCHMARK EXERCISE

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ABSTRACT

Explosion venting is widely using mitigation solution in the process industry to protect indoor equipment or buildings from excessive internal pressure caused by an accidental explosion. However, vented explosion is a very complicated phenomenon to model with computational fluid dynamics (CFD). In the framework, of a French working group, the main target of this investigation is to assess the predictive capabilities of five CFD codes used by five different organizations by means of comparison with the recent experimental data. On this basis several recommendations for the CFD modelling of vented explosions are suggested.

1.0 INTRODUCTION

Explosion vent is a mitigation solution commonly used in the process industry to an internal pressure occurred due to an accidental internal explosion. Explosion vent are used to protect both internal equipment and a building itself. Internal explosions with a presence of an explosion vent are so-called “vented explosions”. Explosion vents allow the pressure leave the closed domain, hence dropping the internal overpressure lower than it adiabatic limit. For several configurations explosion vents also assist to an inflammable mixture partly leave the enclosure and reducing the total explosion masse.

Vented explosions have been widely studied experimentally, numerically and analytically to estimate an overpressure corresponding to vented explosion in an enclosure. There are also several analytical models able to give an estimation of an overpressure corresponding to vented explosion in an enclosure. However analytical or engineering models could not give the full overpressure field evolution in time outside the enclosure, see for instance Jallais et al.[1]. Sometimes these engineering models give inconsistent results for hydrogen, due to a number of different fitting parameters, leading to a strong effect on the overpressure peak. In other more complicated cases, for instance in the presence of multiple vents, obstacles or flammable 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 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.

In order to use CFD codes for safety computations, first of all the codes must be validated versus various available experimental data. Inter-comparison exercises (CFD vs. experimental data) were already performed in the past, see for instance validation of by Baraldi et al. [2] and Vyazmina [3] for 0.95 m^3 vented vessel, Bauwens et al. [4], Keenan et al. [5] and Vyazmina et al. [6] for 64m^3 chamber.

Current study is dedicated to the evaluation of the ability of the CFD codes to reproduce experimental results obtained in a medium scale vented explosion chamber (4 m^3), Daubech et al., [7]. In order to obtain a more general conclusion on the application of a CFD tool for safety computations, 5 different codes are compared to each other and to available experimental data from Daubech et al. [7].

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 by Air Liquide, Fluidyn, Apsys, CEA and ODZ-Consultants. The present paper describes this validation and gives several recommendations for the modelling of vented explosions

2.0 BENCH DESCRIPTION

In the framework of an ANR project Dimitrhy, Daubech et al. [7] performed vented deflagrations of various homogeneous hydrogen-air mixtures in a 4 m^3 explosion test chamber with overall dimensions of 2 m x 1 m x 2 m. For considered here test case a square vents of 0.49 m^2 located on the front wall, see Figure 1. Overpressure was measured using 3 piezo-resistive sensors (0-10 bar). The measurement uncertainty is ± 0.1 % of the full measurement scale.

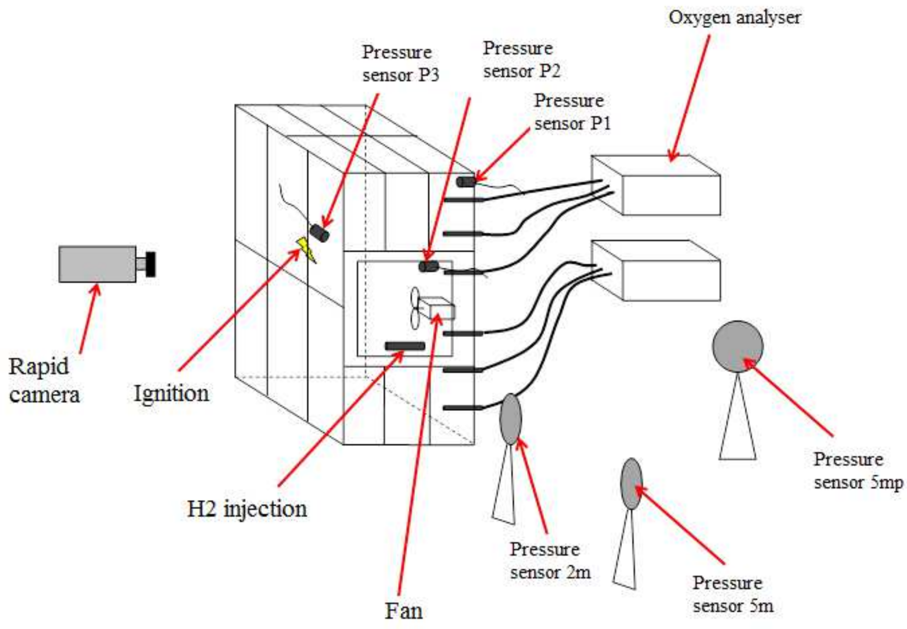


Figure 1. Instrumentation positions of the experimental set-up

The measurement of the outside chamber pressure is performed by 3 piezo-resistive sensors (0-2 bars), located above the ground on lenses allowing for non-perturbed overpressure at 2 m, 5 m away from the chamber (at the axis of the vent), Figure 1. The third sensor 5mp is located on the axis perpendicular to the chamber one, 5 m away from the vent. The measurement uncertainty for these sensors is ± 0.1 % of the full measurement scale. Current numerical investigation aims to reproduce a test-cases corresponding to the mixture of 16.5% (±0.4%) and vent area of 0.49 m^2. Ignition is supplied close to the wall opposite the vent (back wall ignition).

Prior to ignition and during mixing, the unburned mixture was contained within the chamber using a plastic sheet. Ignition was supplied close to the wall opposite the vent (back wall ignition), see [7] for more information.

The hydrogen injection into the chamber was performed by a tube of 1 mm located in the lower part of the chamber. For homogenization of the mixture inside the chamber a fan was used, when the homogenization was achieved the fan is turned off and the mixture was then in rest during 5-10 minutes. U' was not measured, however it was estimated to be U'=0.1 m/s.

Fresh gas movement and deflagration inside and outside the chamber was visualized by adding fine particles of NH4Cl, filmed by a fast camera [7]. The results from measurements were pre-processed using a 100 Hz low-pass filter Vyazmina et al. [6].

3.0 SIMULATION DESCRIPTIONS

Five organizations with strong skills in numerical modeling of gas explosions participated in the code benchmarking activities with four CFD codes (FLACS from GEXCON, EUROPLEXUS, OpenFOAM, Fluidyn-VENTEX) to simulate this experiment.

CFD code FLACS (Flame Acceleration Simulator) is a commercial code developed by GEXCON, [8]. FLACS is dedicated to explosions of gases and dusts. In current simulations FLACS versions 10.3 and 10.4 are used. These versions of FLACS solve the compressible Navier-Stokes equations on a 3-D Cartesian grid using a finite volume method. K-eps model equations are used for turbulence.

EUROPLEXUS is simulation software dedicated to the analysis of fast transient phenomena involving structures and fluid in interaction. The model used for validation is based on the RDEM (Reactive Discrete Equation Method) approach which requires the solution of the reactive Riemann problem between the burnt and un-burnt regions [9]. The system of equations is the reactive Euler equations plus a transport equation for the progress variable. The burning velocity is expressed as a product of several factors, similar to approach of [4], and each factor is represented by an algebraic equation [10].

OpenFOAM (Open source Field Operation And Manipulation) is a C++ toolbox of customized numerical solvers and pre/post processing utilities for the solution of continuum mechanics problem, including CFD. It includes a various range of solvers that are available for computation, either within structured / unstructured mesh, of simulation cases thanks to the finite volume method. In current simulations, XiFoam solver (solver for compressible premixed / partially-premixed combustion with turbulence modelling) is used [11] and [12]. K-equation eddy-viscosity model (compressible LES turbulence model) is used for turbulence.

Fluidyn-VENTEX is a dedicated software solution of explosion scenarios with 3D CFD in congested environments (buildings, process and industrials sites) with models and solvers for gaseous cloud deflagration, solid material detonation and pneumatic explosion. It contains an adds-on structural solver for the deformation and stress response of blast walls. For the detailed description of the combustion model see [13] and [14].

For mesh validation a protocol of SUSANA project is used [15]. According to gird sensitivity analysis (verifying CFD results independence on grid) it is found that one must use from 14 cells up to 30 cells in the vent area depending on the code and model.

Table 1. Simulation setup used for the benchmark

Participant/ Code	Computation domain	Mesh	Total number of grid cells	Turbulence modelling	Boundary conditions	Initial conditions
Air Liquide / FLACS v10.4	Streamwise 10 m, crosstream 5.5 m, vertical 5.5 m	2.5 cm, inside the chamber and in the region of evacuated cloud, outside this region stretching parameter 1.1	~6 M	RANS, k-eps	open outlet boundaries "plane wave"	velocity fluctuation of 0.1 m/s and an initial turbulence length scale of 0.005 m, T= 20°C
APSYS / OpenFOAM 3.0.0	Streamwise 7.5 m, crosstream 7m, vertical 3.5 m	Grid size 1.5 cm close to walls, inside the chamber 3.125 cm, outside the chamber 6.25 cm	~1.2 M	LES - k-equation eddy viscosity model	Open outlet boundaries & wall boundaries for obstacles	T=20°C
CEA / EUROPLEXUS	Streamwise 7.5 m, crosstream 2.5 m, vertical 3 m	Uniform 5 cm	~1 M	Euler	Absorbing boundary conditions	T=20°C
Fluidyn / Fluidyn-VENTEX	Streamwise 7.5 m, crosstream 8.5 m, vertical 4.5 m	3cm inside the box; Refined in the axes of the explosion	~750k	RANS, k- omega SST	Open boundaries	T=20°C
ODZ-Consultants / FLACS v10.3	Streamwise 8 m, crosstream 7.5 m, vertical 3 m	Uniform 3 cm	~6.2 M	RANS, k-eps	open outlet boundaries "plane wave"	T=20°C

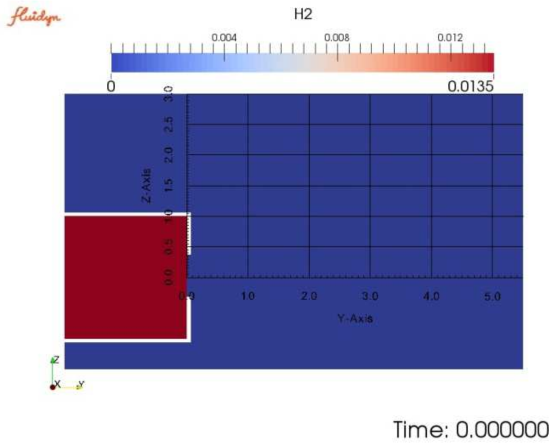
4.0 RESULTS FROM NUMERICAL SIMULATIONS

Simulations results compared with experimental measurements inside and outside the test chamber in terms of concentration evolution in time, overpressure magnitude and the shape of the pressure signal.

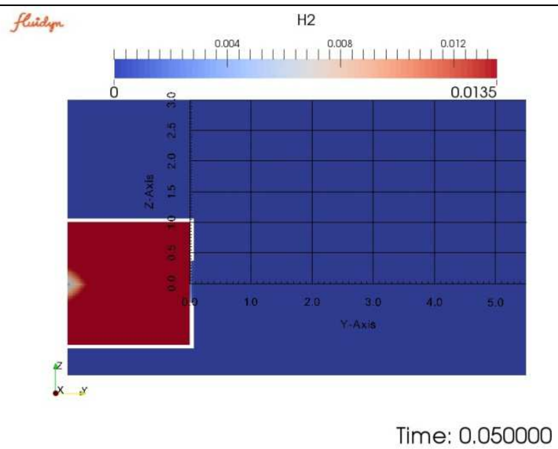
Figure 2 demonstrates the development of vented explosion from the ignition to the final state (explosion of the evacuated outside mixture cloud). Snapshots demonstrate the concentration evolution in time:

experiments on the left vs. simulations of Fluidyn on the right. Snapshots from simulations correctly describe the vented explosion phenomenon and give a good estimation of time dynamics of the flame development. Frame at from 100ms to 120ms show the cloud formation outside the enclosure at 130ms the internal flame approaches the vent, giving almost full combustion at 150ms. According to experimental snapshots (at 130ms -150ms) and pressure history curve (fig 3), the overpressure maximum corresponds to the explosion of the evacuated cloud (external explosion) for both experiments and simulations.

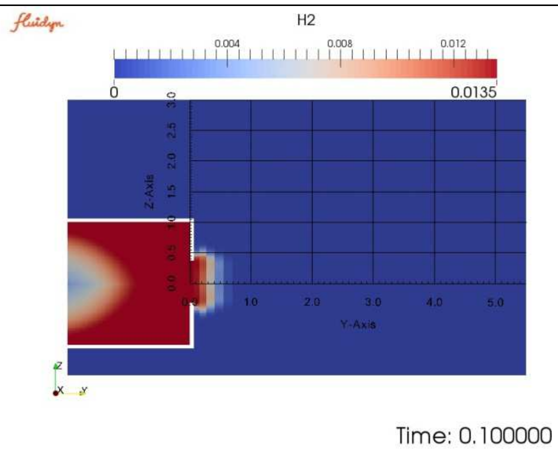
Ignition

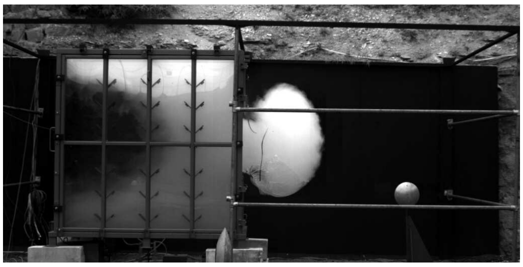
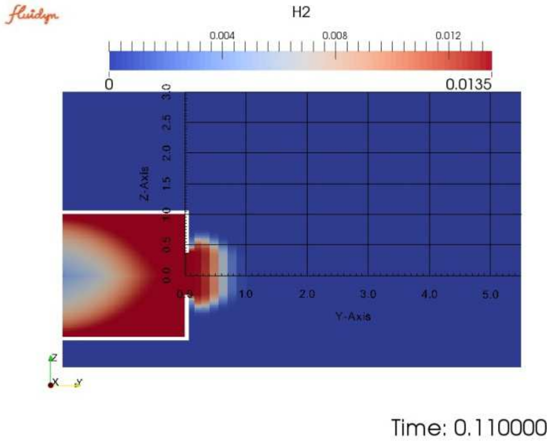
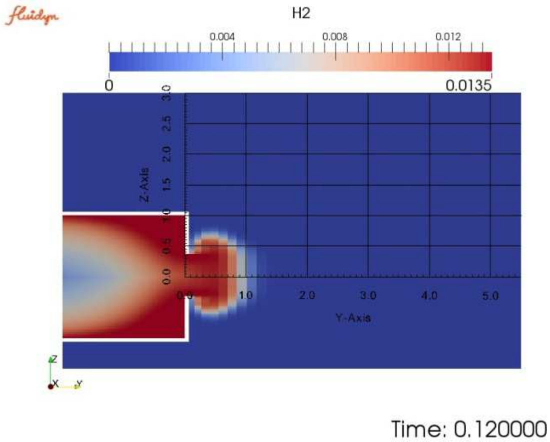
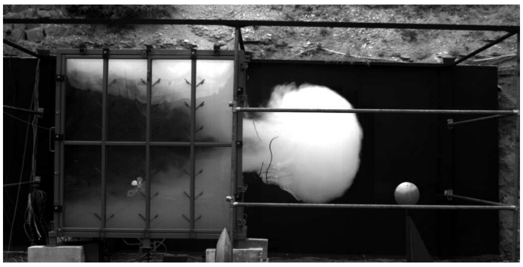
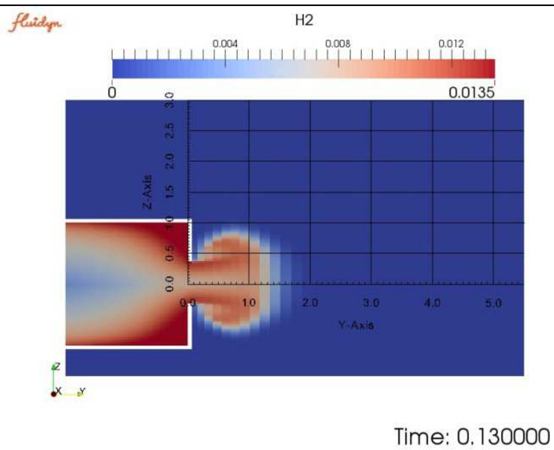


50 ms



100 ms



 110 ms	
 120ms	
 130 ms	

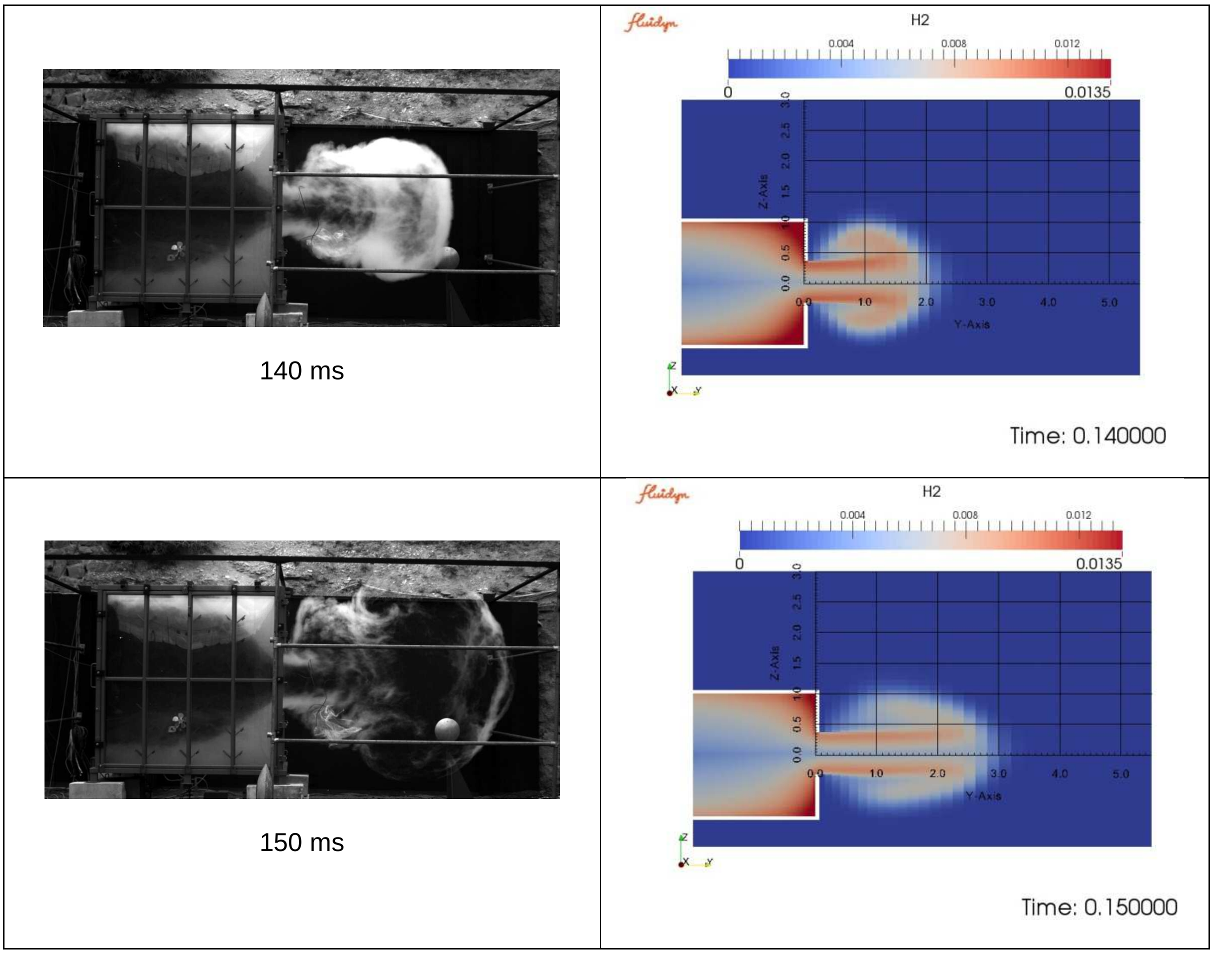


Figure 2. Development of vented explosion: experiment (on the left) vs. simulations of Fluidyn (on the right)

The pressure evolution inside the combustion chamber is displayed on figure 3 (detector P1). All CFD codes are in good agreement with experimental measurements: giving overestimation of the overpressure magnitude by 25% (Fluidyn), 23% (APSYS), 21% (ODZ), 20% (AL) and 8% (CEA). Figure 3 also demonstrates that all codes except Fluidyn predict the appearance of the overpressure pike slightly in advance compare to experiment, whereas Fluidyn overpressure maximum is delayed in time.

For the back wall ignition and large vent area overpressure signals show one maxim. It corresponds to the pressure from the external explosion: rapid combustion of the evacuated outside turbulent combustion mixture. Figure 4 shows the moment of vented explosion, on top experimental results and on the bottom numerical simulations (concentration of the hydrogen/air mixture). One can see that experimental and numerical snapshots perfectly match.

CEA, APSYS and Air Liquide also compared the flame propagation found experimentally with simulations of Europlexus, OPENFOM and FLACS v10.4, figure 5, 6 and 7 correspondingly. Simulated flame shows the same tendency as in the experiment: at the beginning it slightly accelerates approaching to the vent (flame velocity is approximately 30 m/s), when one observe a violent flame acceleration up to 185 m/s due to the rapid burning of the evacuated outside the enclosure cloud of fresh gas. A deceleration of the flame both numerical and experimental is observed at the end. This is due the slow burning of the rest of the mixture (less reactive and less turbulent) in the evacuated cloud

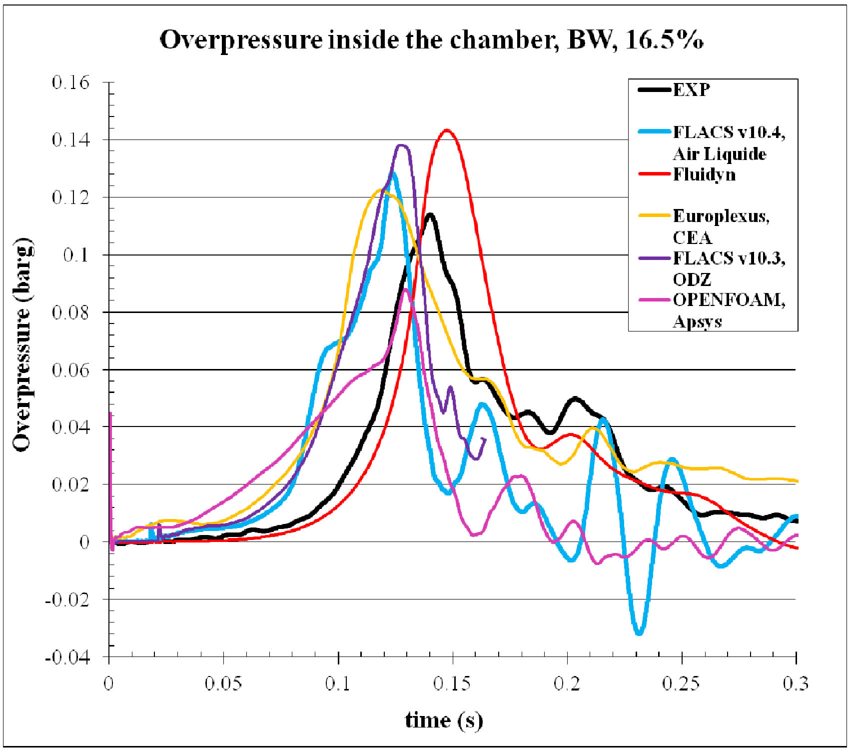


Figure 3. Pressure evolution inside the chamber (simulations vs. experiments)

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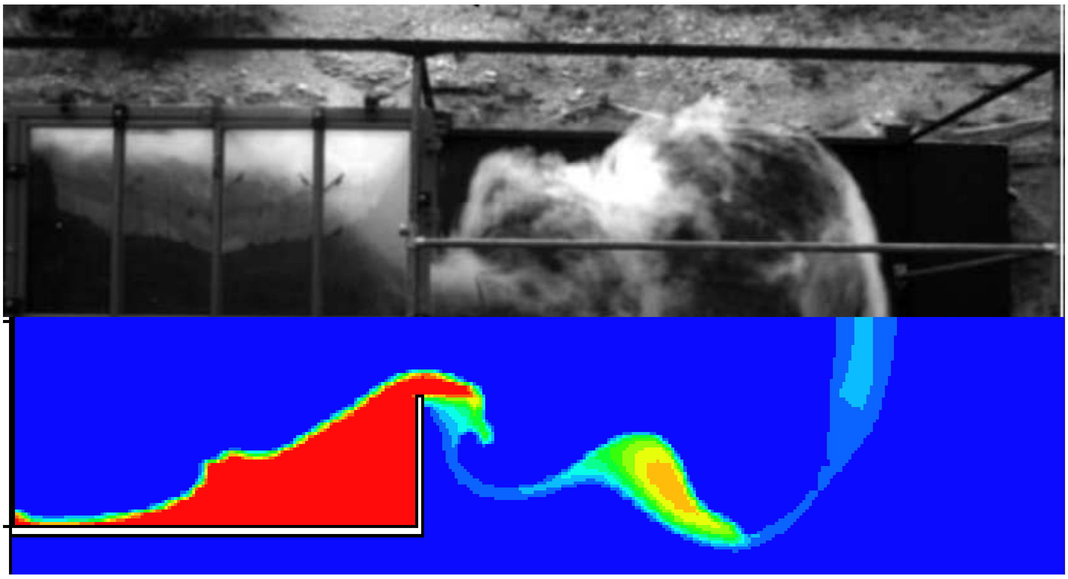


Figure 4. Moment of the external explosion: concentration of hydrogen. Experimental snapshot (on the top at time 143ms), simulations performed with FLACS v10.4 by Air Liquide (on the bottom at time 123ms).

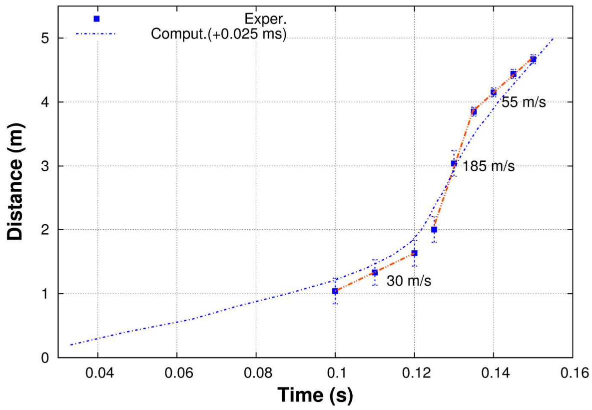


Figure 5. Flame propagation distance vs. time: comparison experimental measurements with simulations of Europlexus of CEA

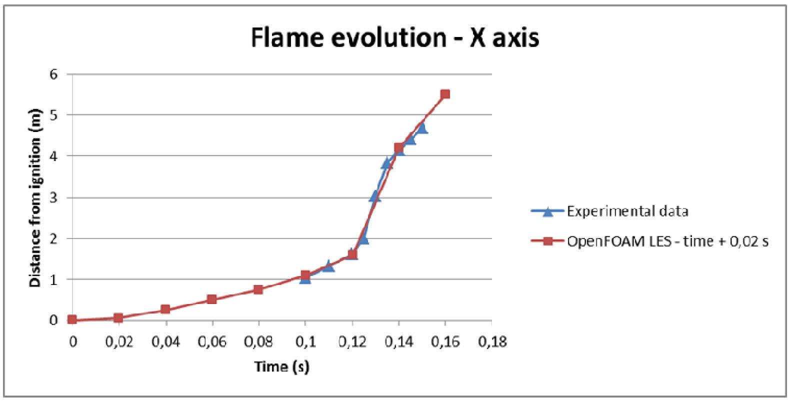


Figure 6. Flame propagation distance vs. time: comparison experimental measurements with simulations of OPENFOAM of APSYS

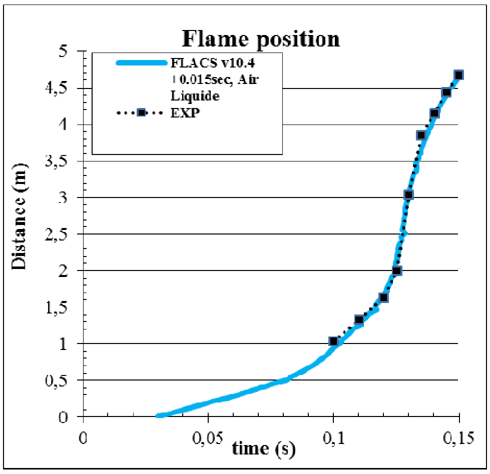
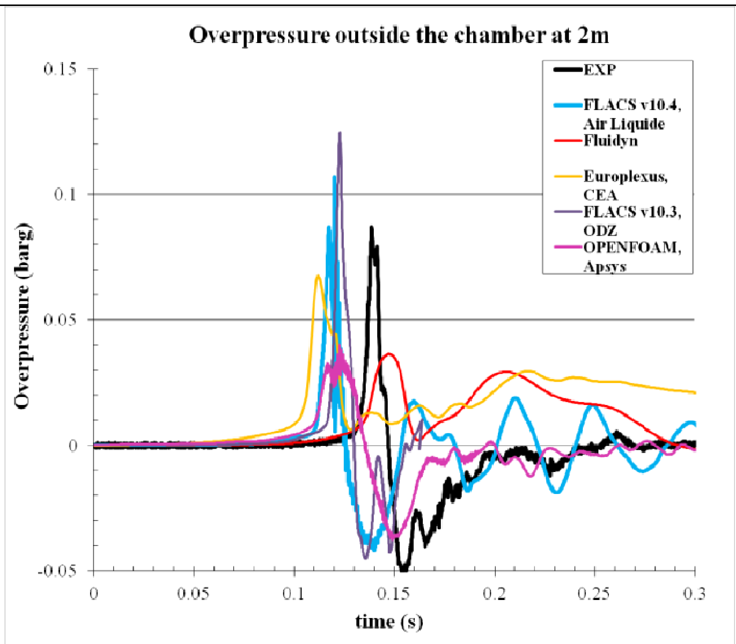


Figure 7. Flame propagation distance vs. time: comparison experimental measurements with simulations of FLACS v10.4 of Air Liquide

The pressure evolution outside the combustion chamber is shown in Figure 8. The overpressure magnitude at 2m from the enclosure is overestimated by 58% (Fluidyn), 54% (APSYS), 51% (CEA), 43% (ODZ), and by 12% (AL). At 5m from the enclosure the maximum overpressure is overestimated by 97% (ODZ), 46% (AL), 29% (Fluidyn), and by 24% (APSYS and CEA).

It is worth to mention that initially AL used a starched grid just outside the enclosure to reduce CPU, therefore results at overpressure time curve at inside the chamber and outside it were too diffusive. Use of a uniform grid in the region of combustion zone (inside the chamber and in the region of the evacuated cloud) vanish this problem. In case of the pressure wave propagation in a far field GexCon [9] also recommends to use a uniform cubic mesh to minimise the artificial numerical dispersion of the overpressure wave.



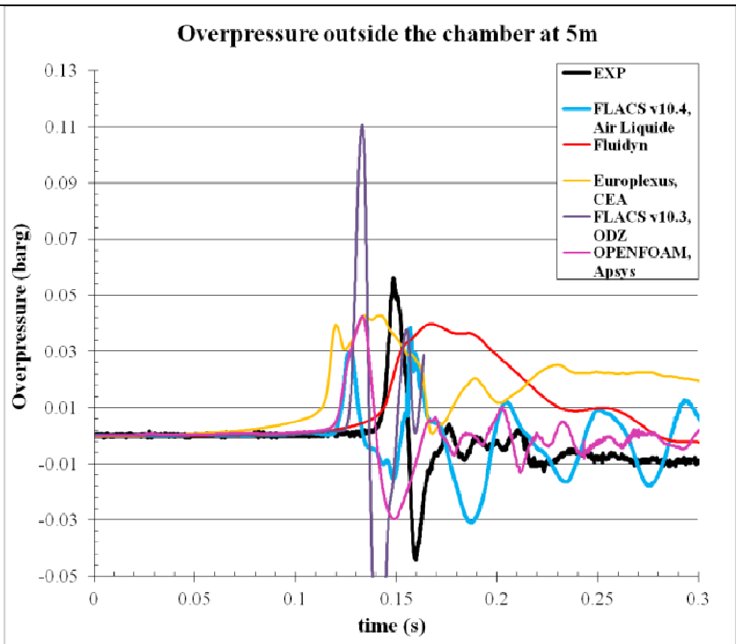


Figure 8. Pressure evolution outside the chamber (simulations vs. experiments)

The comparison of simulations and experimental results suggests that modeling results match closely experimental data inside the combustion chamber. However outside the combustion chamber it seems that the computed overpressure is slightly underestimated. This can be explained by two facts:

1. All participants (except ODZ-Consultants) of the benchmark considered that the combustion chamber is installed in a free field, without any flame or pressure interaction with any outside structure. However the detailed discussion with experimentalist shed light on the fact that the chamber is confined by two walls: one in the streamwise direction (50 cm away from the detector at 5 m) and another all along the lateral direction (just 50 cm away of the chamber wall). These walls create an extra confinement, leading to an interaction of the pressure waves. These multiple pressure reflections from the walls and from the ground increase the overpressure outside the chamber, but do not affect the pressure inside the chamber (in the absence of flame-structure interaction).
2. Simulations were performed on a stretched grid outside the combustion chamber (to reduce the CPU time), however this leads to extra numerical diffusion affecting the results and giving slightly lower overpressure.

5.0 DISSCUSION AND CONCLUSION

In order to use CFD codes for safety computations, first of all the codes must be validated versus various available experimental data. Current study is dedicated to the evaluation of the ability of 4 CFD codes, OpenFOAM, EUROPLEXUS, Fluidyn-VENTEX and FLACS (v10.3 and v10.4), to reproduce experimental results obtained in a medium scale vented explosion chamber (4 m^3). The representation of the various mechanisms that result in the observed overpressure profiles has been studied.

Based on this comparison several best practice recommendations can be done:

1. CFD can be used for large vent area and back wall ignition.

2. One must use from 14 cells up to 30 cells in the vent area depending on the code and model (solution independence on grid must be validated)
3. The grid must be uniform inside the chamber and in the region of the evacuated cloud.
4. For the correct estimation of the overpressure outside the enclosure, all confinements and external rigid structures located near the vent and in the region of interest must be taken into account (represented in CFD simulations or a correction factor must be suggested).
5. The grid must be uniform in the region of interest without any stretching.

These results must be validated for a larger concentration range, including gradient mixtures, central ignition location and a presence of obstacles inside the combustion chamber.

6.0 REFERENCE

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