

# Vented explosion of $H_2$ /air mixture : a comparison benchmark study

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E.Vyazmina/S.Jallais/L.Krumenacker/A.Tripathi/A.Mahon/J.Commanay/  
S.Kudriakov/E.Studer/Th.Vuillez/F.Rosset



# Vented explosions

- Vented explosions are widely studied, both experimentally and numerically
- Several analytical models exist for the overpressure inside the enclosure
- In complicated cases it is very difficult to find a proper analytical model:
  - presence of multiple vents
  - obstacles
  - flammable layer
  - gradient

Maximum internal and external overpressures, the length of the external flame etc. => definition of the safety distances requires an accurate and validated prediction based on CFD modeling

- comparison with experimental data
- several recommendations for CFD modeling of vented explosions

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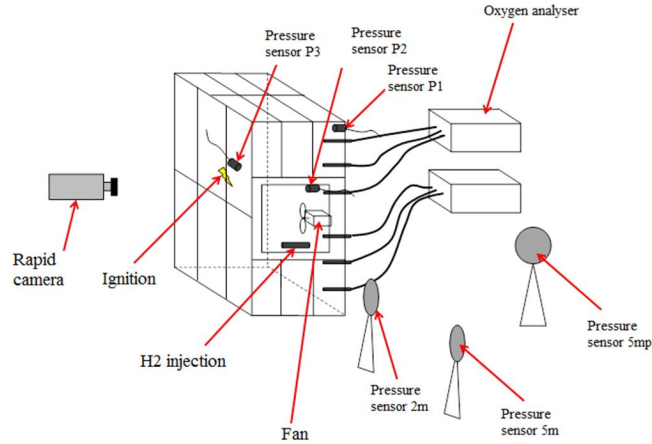
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# 1

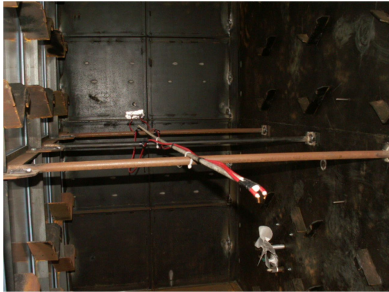
## Bench description

# Experimental chamber<sup>1</sup>



## Experimental set-up:

- Test chamber of 2m x 1m x 2m and square vent of 0.49m<sup>2</sup>
- Homogeneous H<sub>2</sub>/air mixture of 16.5% ( $\pm 0.4\%$ )
- BW ignition
- Fresh gas movement was visualized by adding particles of NH<sub>4</sub>Cl



## Measurements:

- 3 piezo-resistive sensors (0-10 bar) for overpressure inside
- 3 piezo-resistive sensors (0-2 bars ) for overpressure outside at 2m, 5m (at the axis of the vent) and 5 m away from the vent (on the axis perpendicular to the chamber)
- 100Hz low-pass filter is used for the pressure signal

<sup>1</sup> Daubech, J., Proust, Ch., Gentilhomme, O., Jamois, D., Mathieu, L., Hydrogen-air vented explosions: new experimental data, Proc. of 5th ICHE, 2013.

# 2

## Simulations description

# Bench participants and code description

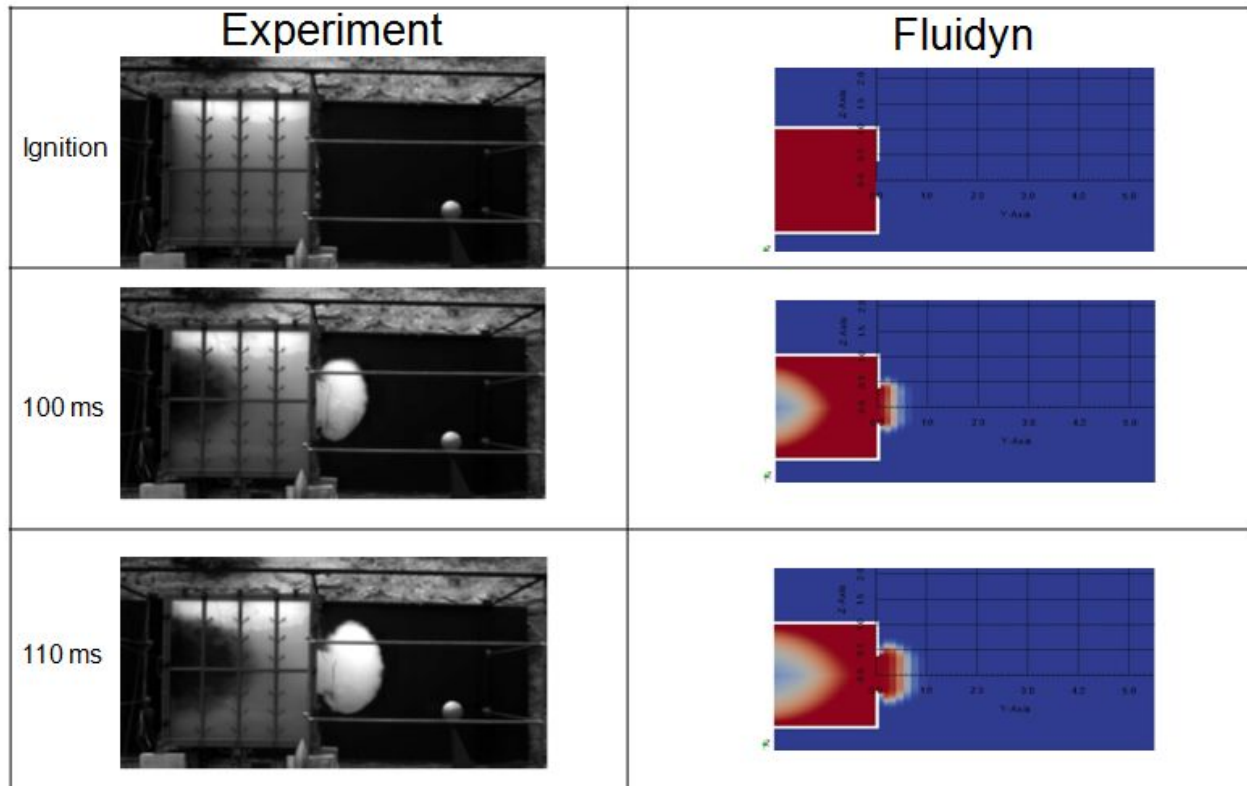
Participant / Code	Domain (LxWxH)	Mesh	Number of grid cells	Turbulence modelling	Boundary conditions
<b>Air Liquide / FLACS v10.4</b>	10m by 5.5m by 5.5m	inside the box and in the evacuated cloud: 2.5cm	~6 M	RANS, k-eps	open outlet “plane wave” & wall boundaries for obstacles
<b>APSYS / OpenFOAM 3.0.0</b>	7.5m by 7m by 3.5m	Grid size 1.5cm close to walls, inside the box 3.125cm, outside 6.25cm	~1.2 M	LES - k-equation eddy viscosity model	open outlet boundaries & wall boundaries for obstacles
<b>CEA / EUROPLEXUS</b>	7.5m by 2.5m by 3m	Uniform 5cm	~1 M	Euler	Absorbing boundary conditions
<b>Fluidyn / Fluidyn-VENTEX</b>	7.5m by 8.5m by 4.5m	inside the box: 3cm; Refined in the axes of the explosion	~750k	RANS, k-omega SST	Open boundaries
<b>ODZ-Consultants / FLACS v10.3</b>	8m by 7.5m by 3m	Uniform 3cm	~6.2 M	RANS, k-eps	open outlet “plane wave” & wall boundaries for obstacles

# 3

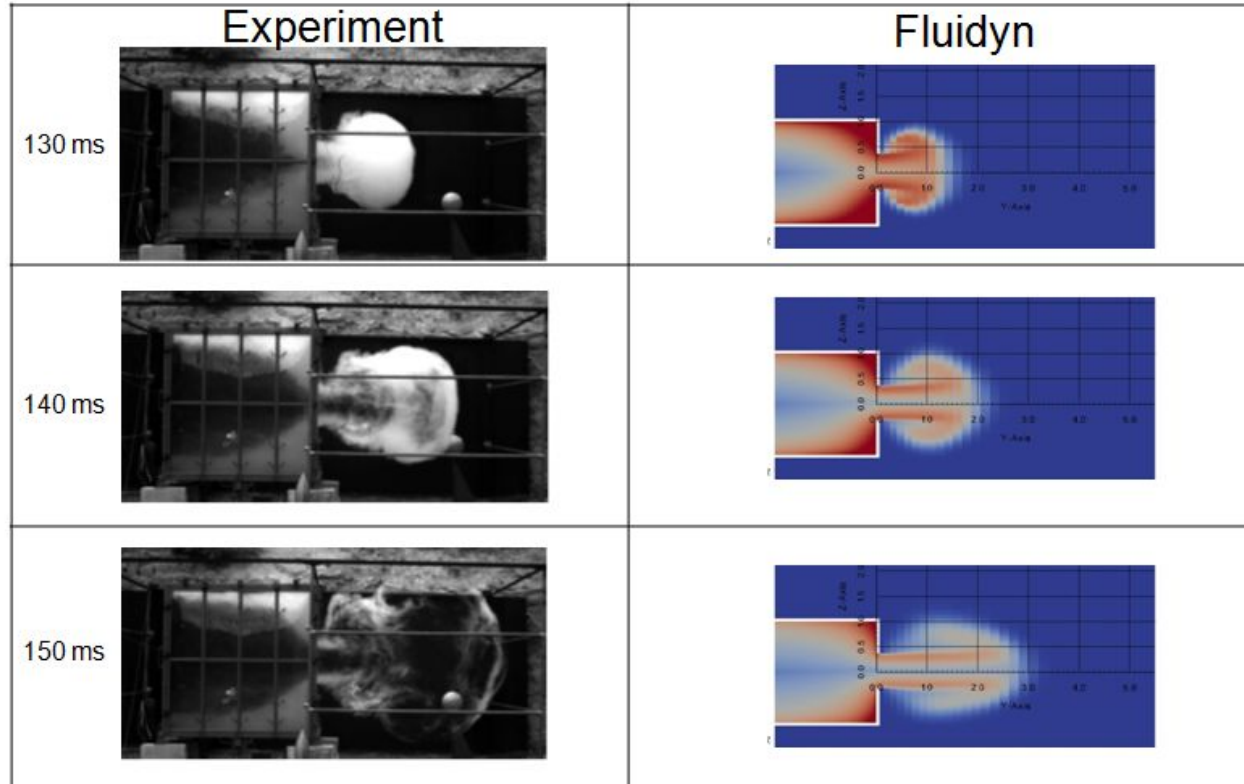
## Simulation results



# Results from numerical simulations: development of VEX

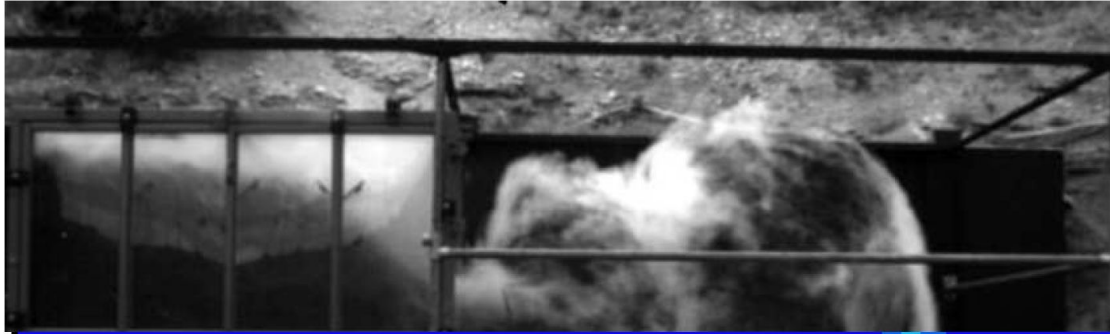


# Results from numerical simulations: development of VEX



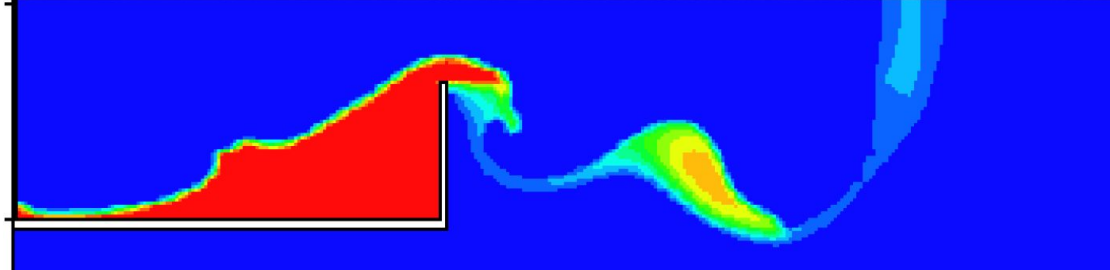
# The moment of the external explosion

EXP

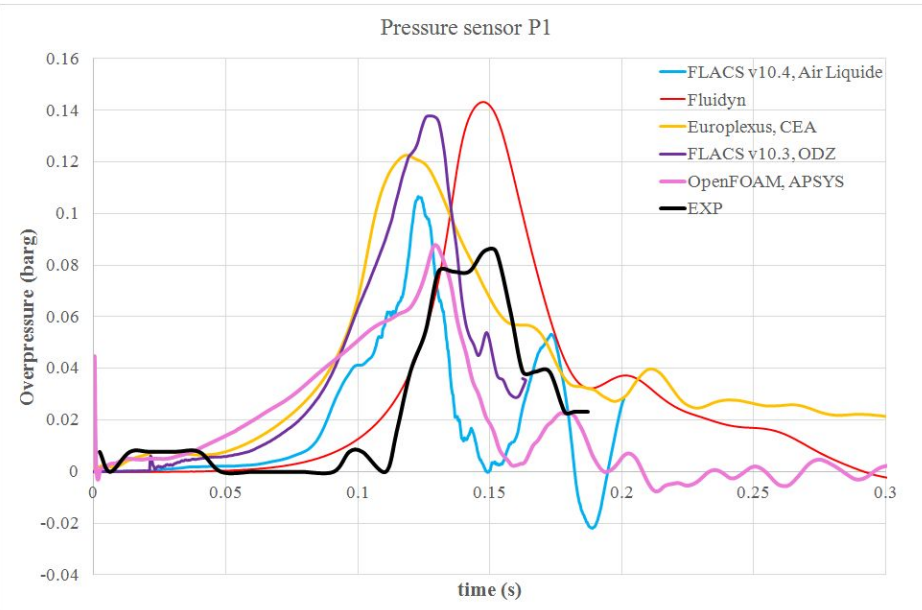
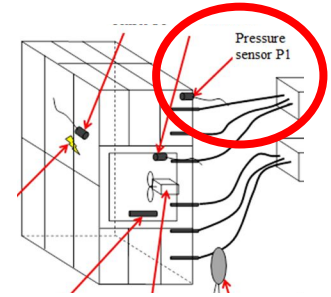


Experimental and  
numerical  
snapshots closely  
match

AL  
FLACS  
10.4



# Pressure evolution inside the chamber : P1

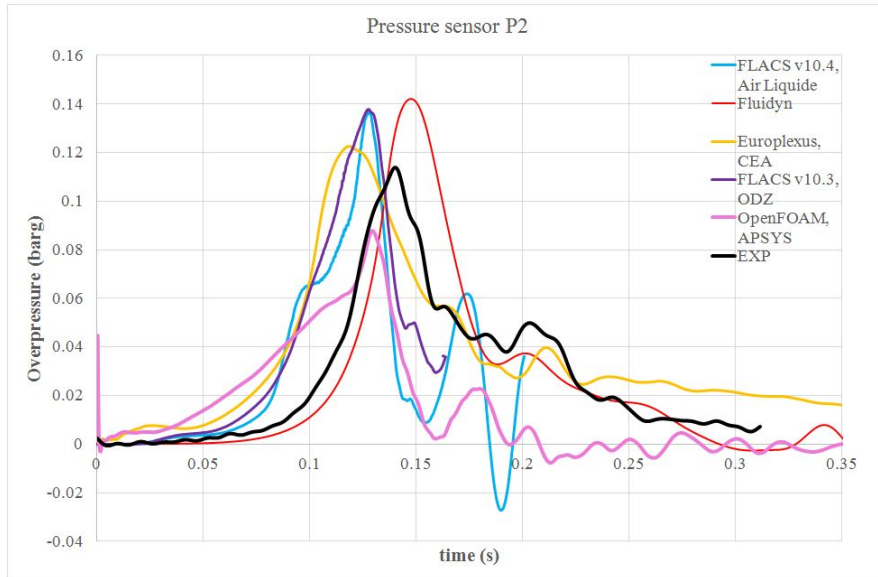
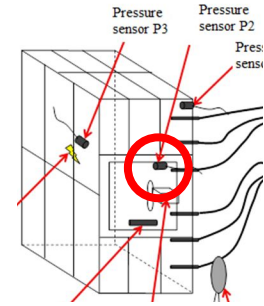


All CFD codes are in reasonable agreement with exp:

- the magnitude is overestimated by ~60% (**Fluidyn** and **ODZ**), 40% (**CEA**), 25% (**AL**), ~3% (**APSYS**)
- all codes except Fluidyn predict the appearance of the spike in advance compare to experiment
- whereas Fluidyn overpressure maximum is slightly delayed in time

# Pressure evolution inside the chamber : P2

P2 (114 mbarg) is larger than P1 (85 mbarg)  $\Rightarrow$  more important to obtain a better agreement on P2



All CFD codes are in reasonable agreement with exp:

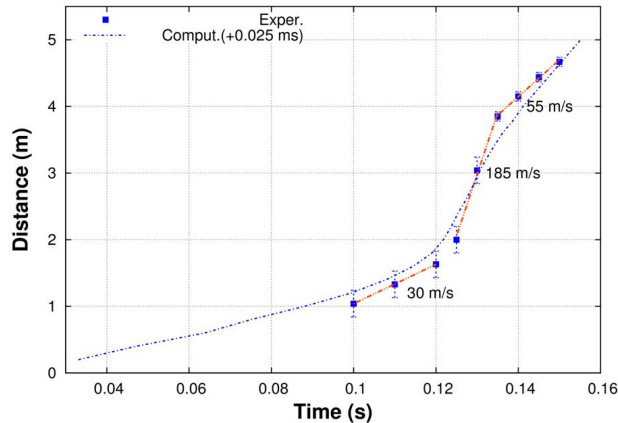
- the magnitude is overestimated by 25% (**Fluidyn**), 20% (**ODZ** and **AL**), and 7% (**CEA**)
- **APSYS** underestimates by 23%
- all codes except Fluidyn predict the appearance of the spike in advance compare to experiment
- whereas Fluidyn overpressure maximum is slightly delayed in time

# Flame propagation distance vs. time

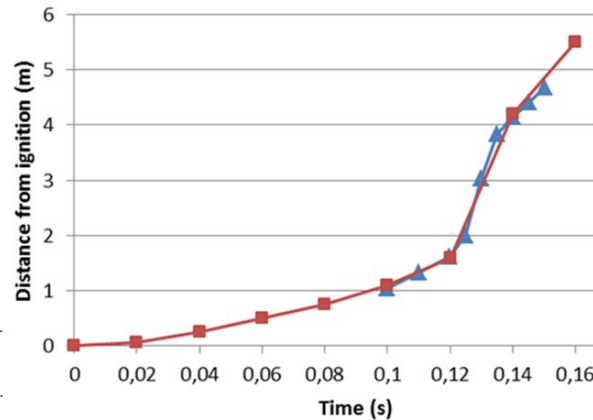
Simulated flame shows the same tendency as the experiment:

- slight acceleration approaching the vent (flame velocity is approximately 30 m/s),
- a violent acceleration up to 185 m/s due to the rapid burning of the evacuated cloud of fresh gas
- a deceleration of the flame at the end due to a slow burning of the rest of the mixture (less reactive and less turbulent)

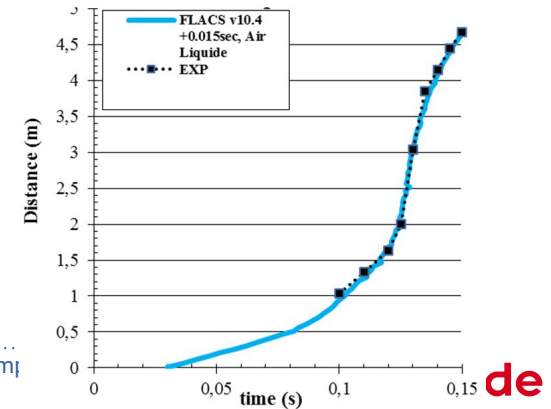
CEA



APSYS



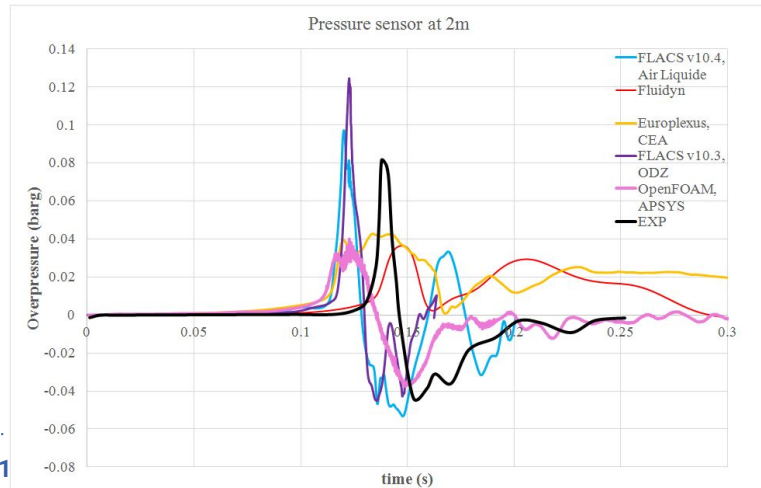
Air Liquide



# Pressure evolution outside the chamber at 2m and 5m

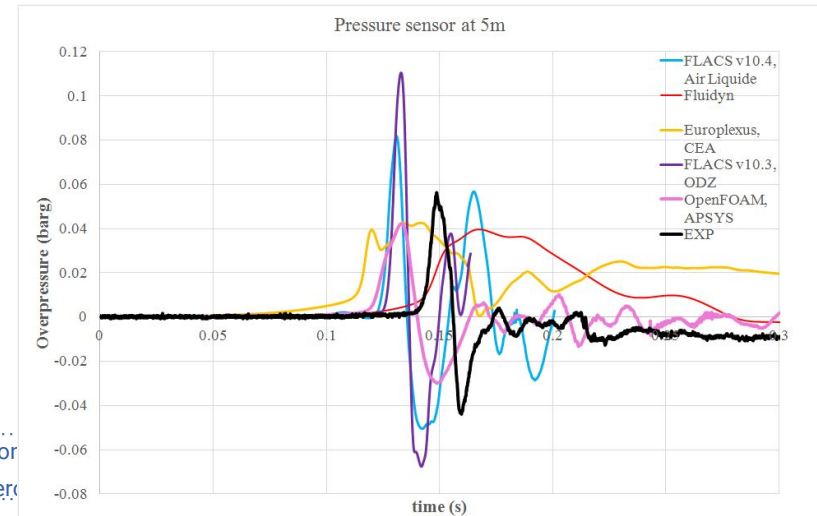
A 2m P is:

- overestimated by 50% (**ODZ**), 20% (**AL**)  $\Leftarrow$  presence of external walls
- underestimated by 50% (**Fluidyn** and **CEA**)  $\Leftarrow$  absence of external walls
- **APSYS** underestimates by 50%  $\Leftarrow$  mesh stretching in the this region  $\Rightarrow$  too diffusive



A 5m (close to the wall) P is:

- overestimated by 90% (**ODZ**), 50% (**AL**)  $\Leftarrow$  presence of external walls  $\Rightarrow$  increase of the P
- underestimated by 30% (**Fluidyn** and **CEA**)  $\Leftarrow$  absence of external walls
- **APSYS** underestimates by 25%  $\Leftarrow$  mesh stretching in the this region  $\Rightarrow$  too diffusive



# 4

## Conclusion and Discussion



# Conclusion

- Inside the combustion chamber CFD matches closely experiment
- Outside the overpressure is underestimated:
  - CEA and Fluidyn considered that the combustion chamber is installed in a free field, without any interaction with outside structure. But the experimental facility is confined by two walls:
    - one in the streamwise direction (50 cm away from the detector at 5 m)
    - another all along the lateral direction (50 cm away of the chamber wall)
  - ⇒ **extra confinement leads to the increase the overpressure outside the chamber**
  - ⇒ **no effect on the pressure inside the chamber (in the absence of flame-structure interaction)**
  - Simulations performed with a stretched grid (APSYS) in the region of pressure detectors lead to an extra numerical diffusion and giving lower overpressure

# Recommendations for CFD modelling of VEX

Based on the comparison sim/exp several **best practice recommendations** can be given :

- CFD can be used for large vent area and BWI
- The grid must be uniform inside the chamber and in the region of the evacuated cloud
- For the correct estimation of the overpressure outside the enclosure, all confinements and external rigid structures must be taken into account (represented in CFD simulations or a correction factor must be suggested)
- The grid must be uniform without any stretching in the region of interest (the region of monitoring points)

Results must be verified for other concentrations, gradient mixtures, CI and a presence of obstacles in the chamber



Thank you  
for your  
attention!!!