

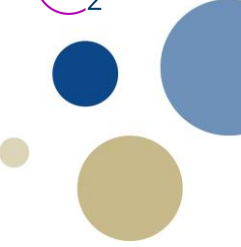
# A CFD Analysis of Liquid Hydrogen Vessel Explosions Using the ADREA-HF Code

9<sup>th</sup> International Conference on Hydrogen Safety (ICHS 2021)



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# Introduction

Collaboration with PRESLHY partner NCSR “Demokritos”

Aim of the work: provide critical indications on the Boiling Liquid Expanding Vapour Explosion (BLEVE) theory

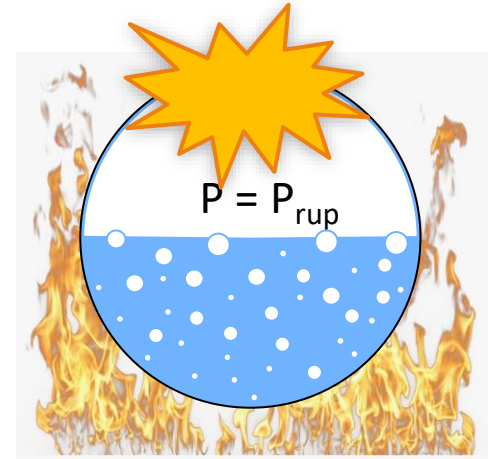
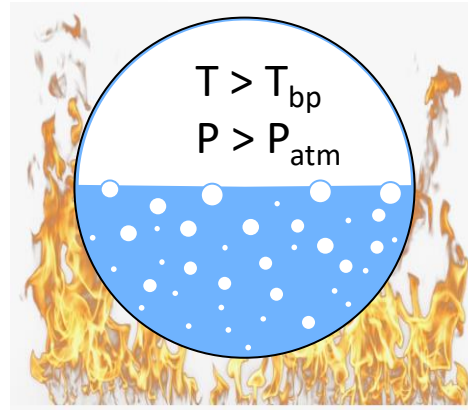
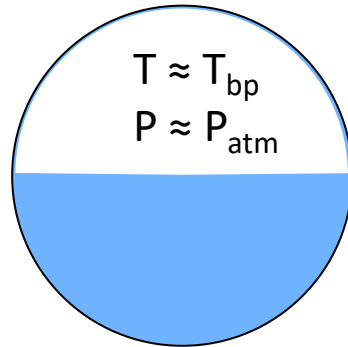
- CFD analysis of BLEVE for liquid  $\text{CO}_2$  ( $\text{LCO}_2$ ) and liquid hydrogen ( $\text{LH}_2$ ) tanks
- Study the dynamic of the blast wave (no combustion)

# BLEVE

Physical explosion might result from the catastrophic rupture of a tank containing a superheated liquid due to the rapid depressurization

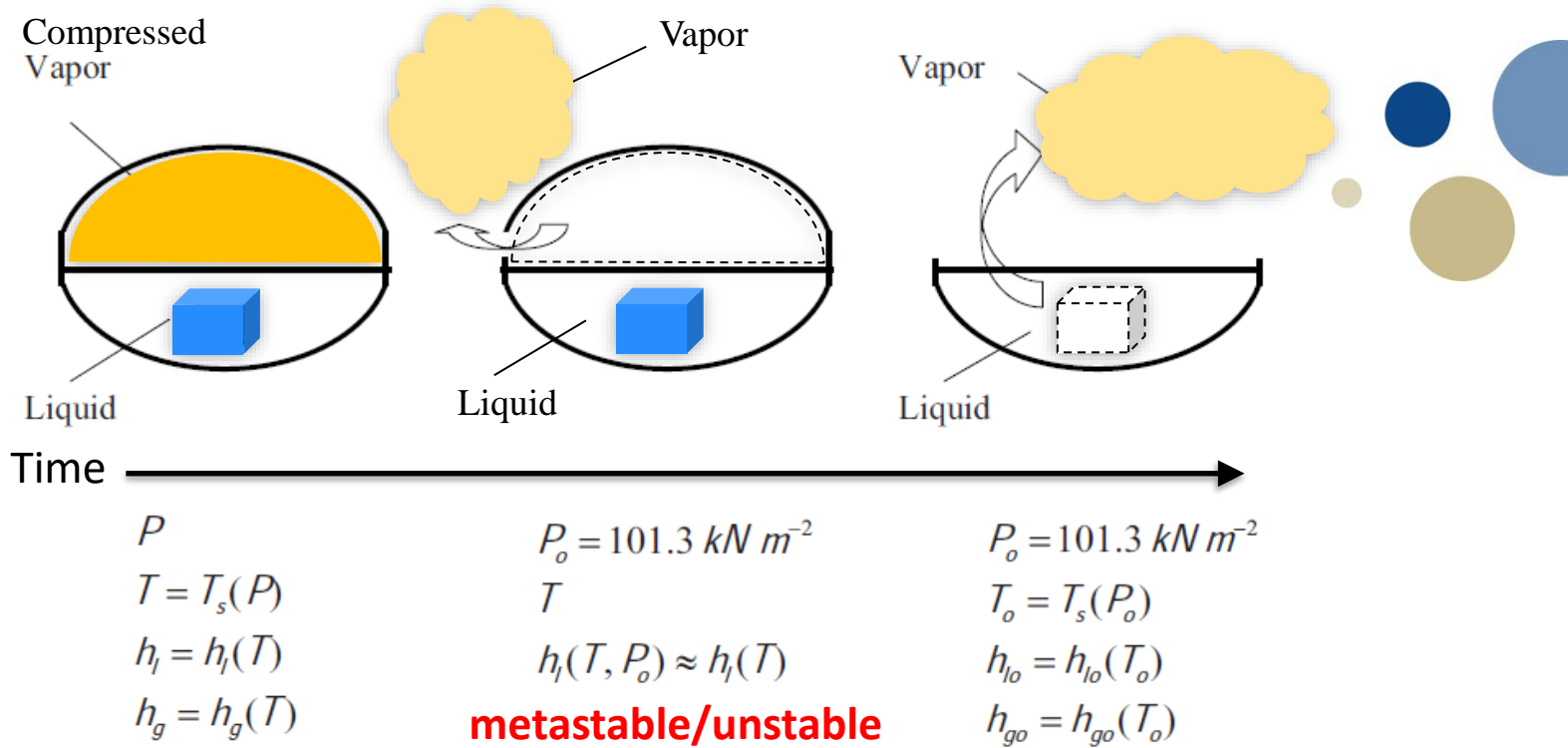
## Chain of events leading to the tank rupture

Valid for  
cryogenic  
substances



Time

# BLEVE



Hot liquid undergoing sudden depressurization in a tank (adapted from [Casal, 2008])

Consequences: pressure wave, missiles and fireball (flammable substances)

# Liquid CO<sub>2</sub> explosion tests

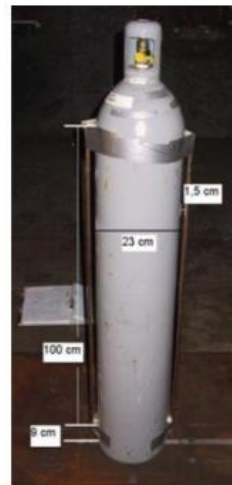
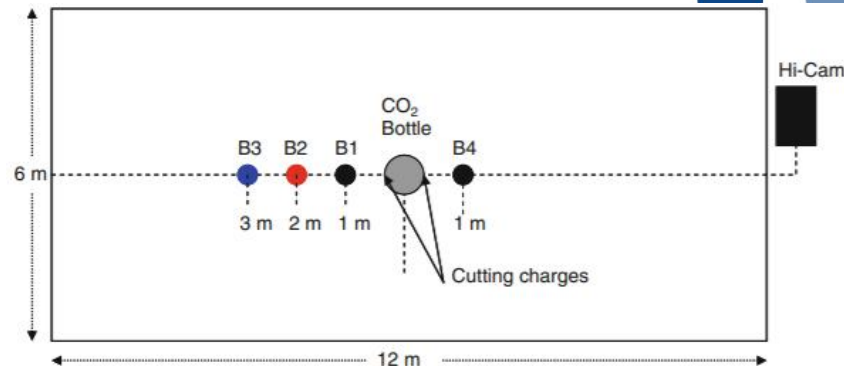
Laboratory for Ballistic Research (TNO  
Defence, Security and Safety)

Bunker: 6 × 12 × 4 m

40-l LCO<sub>2</sub> bottle wrecked by explosive:

- D = 0.23 m
- h = 1.37 m
- fd = 95%
- T = 290 K
- P = 5.2 MPa

[van der Voort, M.M., van den Berg, A.C., Roekaerts, D.J.E.M. et al. Blast from explosive evaporation of carbon dioxide: experiment, modeling and physics. Shock Waves 22, 129–140 (2012)]



# BMW safety tests

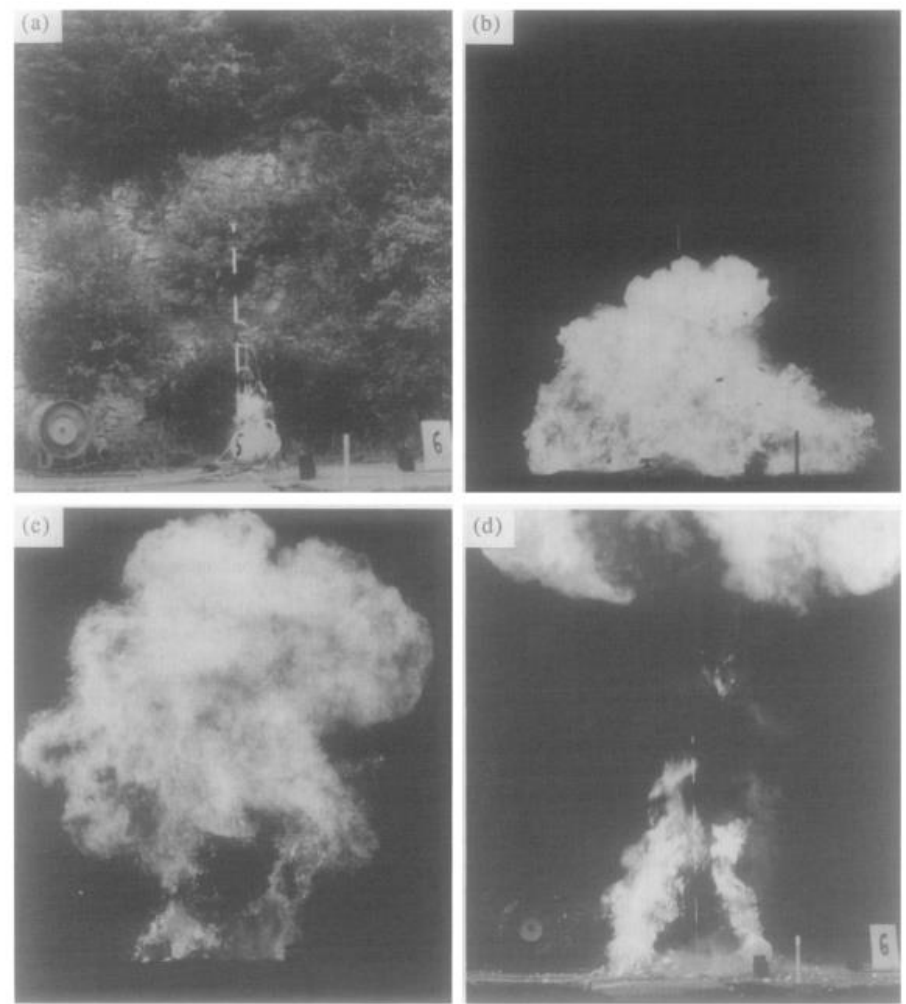
## Bursting tank scenario test

Ten single wall vessels insulated with foam and ruptured with explosives:

- $V = 120\text{-l}$
- $P = 0.2 \div 1.5 \text{ MPa}$
- $m_{\text{LH}_2} = 1.8 \div 5.4 \text{ kg}$

Many uncertainties (e.g. filling level, initial temperature, tank dimensions)

[Pehr, K., 1996. Aspects of safety and acceptance of LH2 tank systems in passenger cars. Int. J. Hydrogen Energy 21, 387–395]



g. 3. Development of a fireball. (a) Ignition; (b) 250 ms after ignition; (c) 1250 ms after ignition; and (d) 1800 ms after ignition.

# CFD analysis methodology

- ❑ CFD code: ADREA-HF
- ❑ Homogeneous Equilibrium Model (HEM)
- ❑ Raoult's law for ideal mixture
- ❑ k-epsilon turbulence model with wall function
- ❑ Peng-Robinson and Redlich-Kwong-Mathias-Copeman EoS were tested

The code was validated with the LCO<sub>2</sub> experiments and then employed for the simulation of the LH<sub>2</sub> BMW explosion tests.



# CFD analysis methodology

The Navier-Stokes equations, continuity equation, energy equation of the mixture and conservation equation of species. The Favre-averaged equations are (Einstein summation convention is used):

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i}{\partial x_i} = 0,$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{u}_i}{\partial x_j} = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \mu_{eff} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \right) + \bar{\rho} g_i,$$

$$\frac{\partial \bar{\rho} \tilde{H}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{H}}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{Pr_t} \frac{\partial \tilde{H}}{\partial x_j} \right) + \frac{D\bar{p}}{Dt},$$

$$\frac{\partial \bar{\rho} \tilde{q}_k}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{q}_k}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{Sc_t} \frac{\partial \tilde{q}_k}{\partial x_j} \right) + \bar{R}_k, \quad k = 1, \dots, N_{subs},$$

Assumption: instantaneous and uniform rupture of tanks in all directions

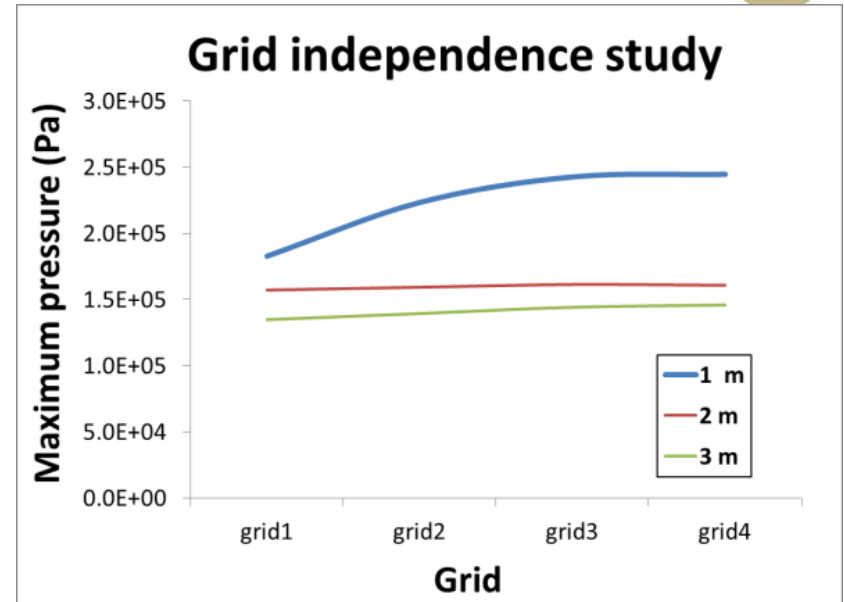
# LCO<sub>2</sub> simulation configuration

Initial conditions of the LCO<sub>2</sub> BLEVE simulation (assumption: 100% LCO<sub>2</sub>)

Pressure (Pa)	Temperature (K)	Density (kg/m <sup>3</sup> )	Mass (kg)
5,200,000	289.03	772.54	30.90

Computational meshes (double symmetry along y- and x-axis):

- × Grid 1: 33,792 cells
- × Grid 2: 113,960 cells
- × Grid 3: 265,832 cells
- × Grid 4: 469,560 cells



Relative error between grid 3 and 4  $\leq 1\%$  for all three sensors

# LH<sub>2</sub> simulation configuration

Characteristics of the simulated LH<sub>2</sub> tank and dimensions of the domain (double symmetry along y- and x-axis → ¼ tank)

Tank	Volume (litres)	Area (m <sup>2</sup> )	Height (m)	Orientation	Height from the ground (m)	Domain dimensions (m)
LH <sub>2</sub>	120	0.177	0.706	Horizontal	1	10 × 10 × 11

Initial conditions of the LH<sub>2</sub> BLEVE parametric analysis

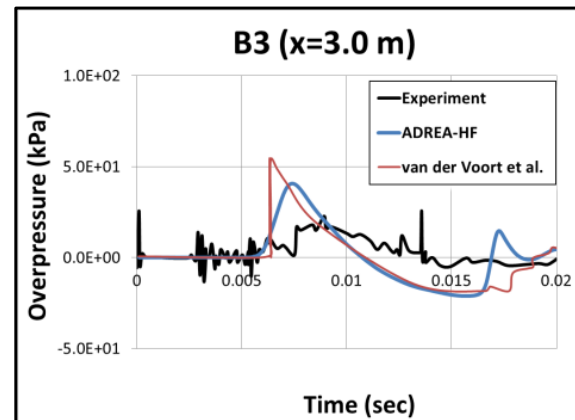
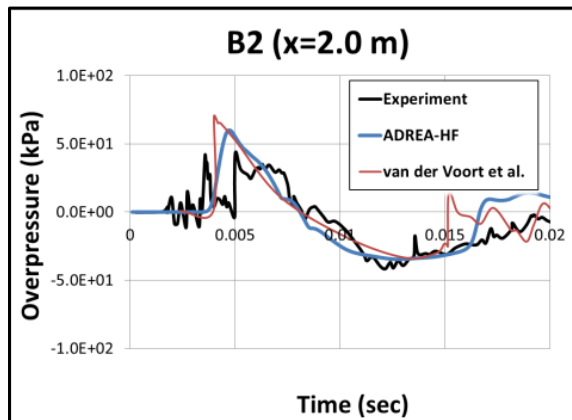
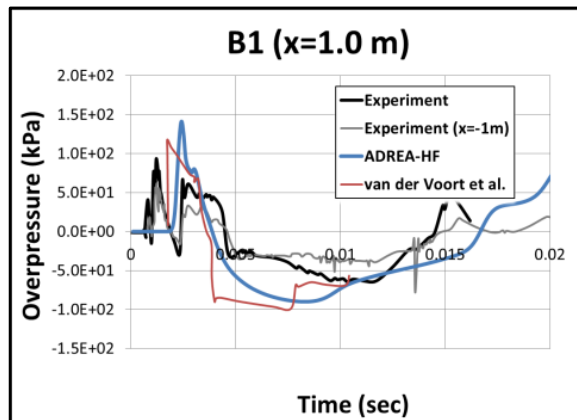
Simulation	Phase and status	Pressure (Pa)	Temperature (K)	Density (kg/m <sup>3</sup> )	Mass (kg)
LH2	Saturated L	1,101,325	32.10	42.42	1.27
GH2	Superheated V	1,101,325	32.93	15.00	0.45
LH2-GH2	L and V	1,101,325	32.10, 32.50	42.42 (L), 16.30 (V)	0.77

Combustion was not simulated

fd = 37%

# ADREA-HF code validation

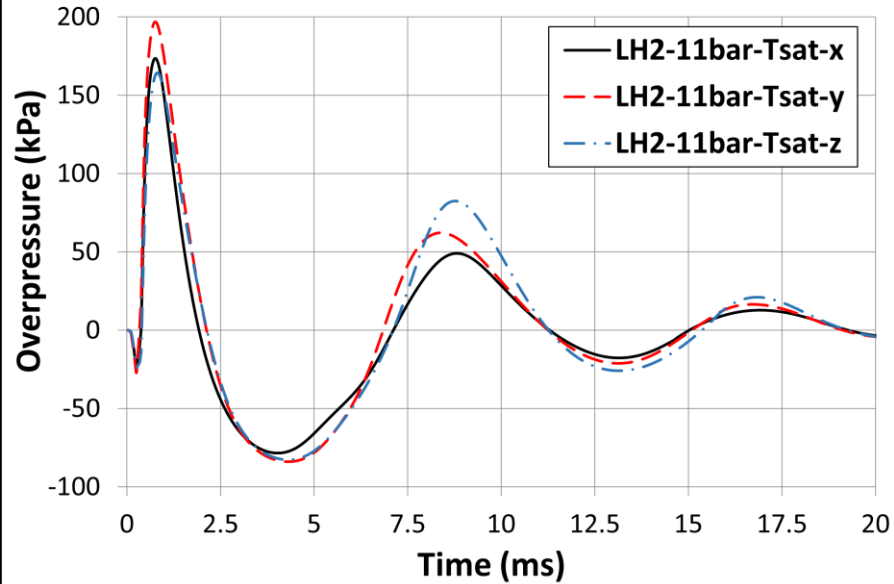
Results of the LCO<sub>2</sub> BLEVE simulations: peak overpressure of the blast wave in three different positions



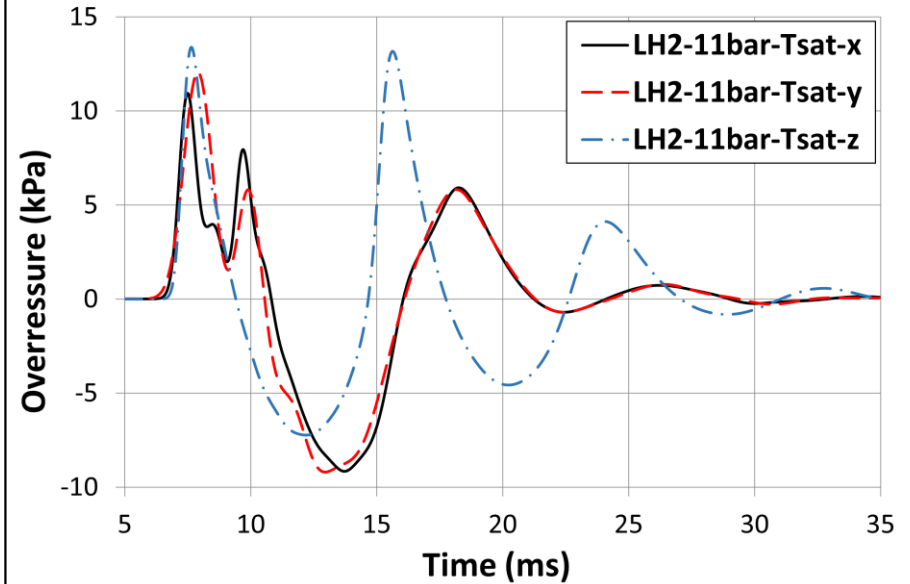
Experimental results are disturbed by the blast wave reflection on the bunker walls

# BLEVE blast wave overpressure

0.1 m from tank wall



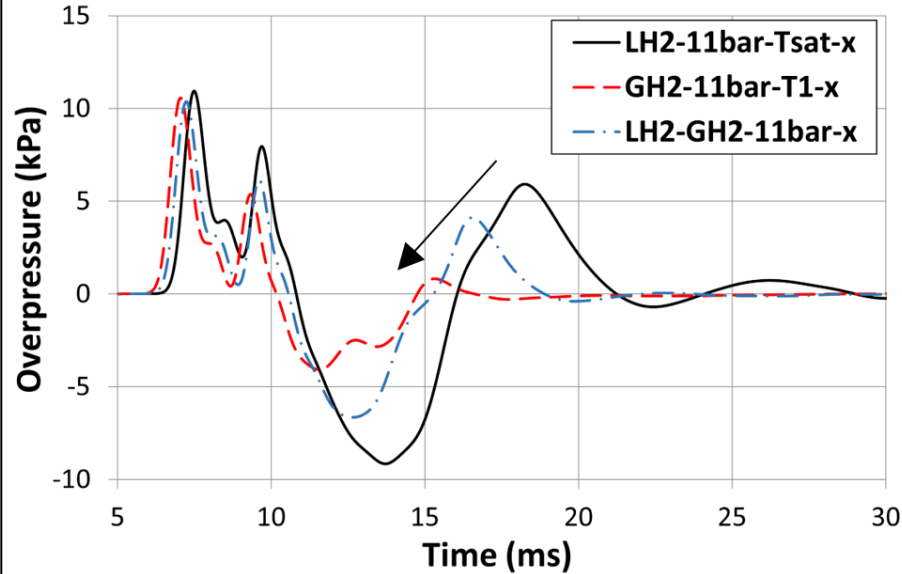
3.0 m from tank centre



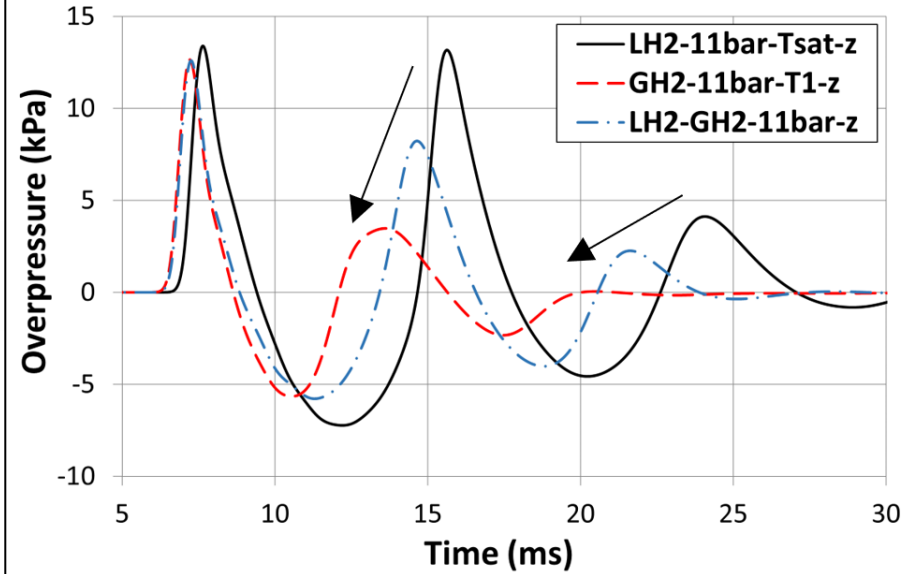
Second pressure peak at vertical axis as high as the first one at 3 m from the tank centre

# BLEVE blast wave overpressure

3.0 m from tank centre - x



3.0 m from tank centre - z



- second pressure peak at horizontal axis decreases with GH2,
- third press peak manifests only along vertical axis when LH2 is initially present
- no large differences in max overpressure yet in explosion duration

# Conclusions

- ✿ Differences in the overpressure of the pressure wave along vertical and horizontal axes
- ✿ Both LH<sub>2</sub> or GH<sub>2</sub> contribute to the explosion yield (similar maximum overpressure values)
- ✿ GH<sub>2</sub> simulation produces the shortest explosion, thus the smallest impulse
- ✿ Two pressure peaks for 100% GH<sub>2</sub>, while three peaks for the 100% LH<sub>2</sub>
- ✿ Maximum overpressure was not mainly affected by the hydrogen mass, while this parameter affects the blast wave impulse.

# Thank you for your attention



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