ADVANCEMENT IN HEAT AND MASS TRANSFER MODELLING

RESULTS FROM BLEVE CFD SIMULATIONS

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Introduction

- This work continues the study published in:
  Ustolin, F., Tolias, I. C., Giannissi, S. G., Venetsanos, A. G., & Paltrinieri, N. (2022),
  ***A CFD analysis of liquefied gas vessel explosions**,*
  Process Safety and Environmental Protection, 159, 61-75

- In our previous work the **BMW tests** (Pehr, 1996) of LH2 tank explosion were studied using CFD simulations

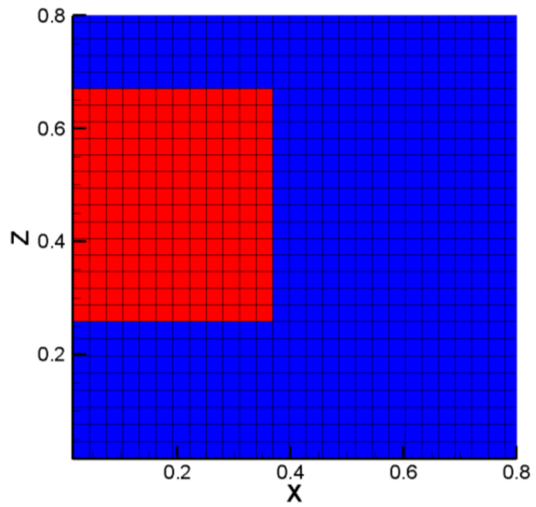
- BMW tests:
  - Liquid H2 is stored in a 120-liter cylindrical vessel
  - H2 mass varied between 1.8 and 5.4 kg
  - Various storage pressures: 2 – 15 bars
  - Unknown H2 mass and liquid fraction in each experimental case
  - Pressure was measured at 3 m distance

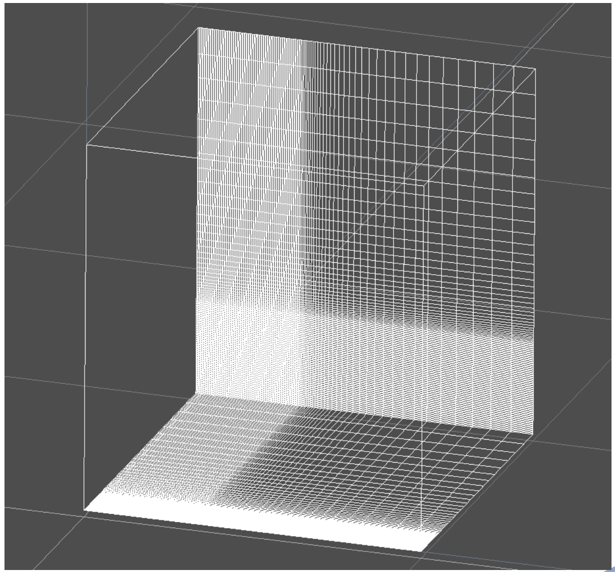
Case studies

- In our previous study the Cold BLEVE case was examined (no ignition)
- In this study:
  - Effect of physical and modelling parameters
    - Tank position – measuring point
    - Combustion (Hot BLEVE vs Cold BLEVE)
    - Air condensation
    - Turbulence modeling approach
    - Liquid fraction in the tank
  - We study the 11 bar storage pressure case
    - 1st scenario: 11bar / full vapor / Cold BLEVE
    - 2nd scenario: 11bar / full vapor / Hot BLEVE
    - 3rd scenario: 11bar / liquid fractions effect / Cold and Hot BLEVE

CFD parameters

- ADREA-HF code is used
- Tank model: rectangular parallelepiped
  - Height: 0.412 m
  - Base: 0.707 × 0.412 m
- Double symmetry (x & y axis)
- Cell size inside tank: 0.029 m
  - Number of cells in the quarter of the tank: 1176 (12×7×14)
  - Grid independence was achieved
- Domain size: 10 × 10 × 11 m





CFD parameters

- **Main equations**
  - Continuity, Navier – Stokes, Energy (static enthalpy), Species
  - EoS: Peng-Robinson
- **Combustion modeling**
  - Eddy dissipation concept (EDC) (Magnussen & Hjertager, 1977)
    - The term in the model associated with products is omitted
    - No need for ignition:
      Combustion occurs as soon as hydrogen and air are mixed
    - Model constant used: 1.0

$$\overline{\dot{\omega}_F} = \rho \frac{1}{\tau_t} \min\left(Y_F, \frac{Y_O}{s}\right)$$

- **Phase change:** Raoul approximation is used
- **Numerical details**
  - High order convective scheme (MUSCL)
  - Small time-steps: CFL = 0.01

1^{st} scenario

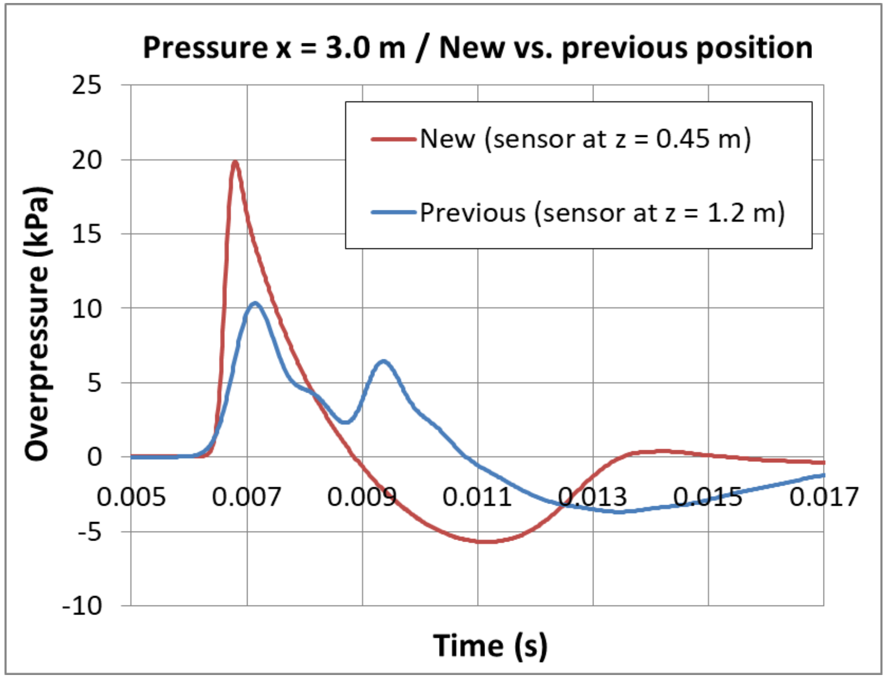
- **1^{st} scenario parameters:**
  - Storage pressure: 11 bar
  - Storage temperature: 32 K
  - Full vapor initial stage
    - Liquid is formed because of temperature decrease due to expansion
  - Cold BLEVE

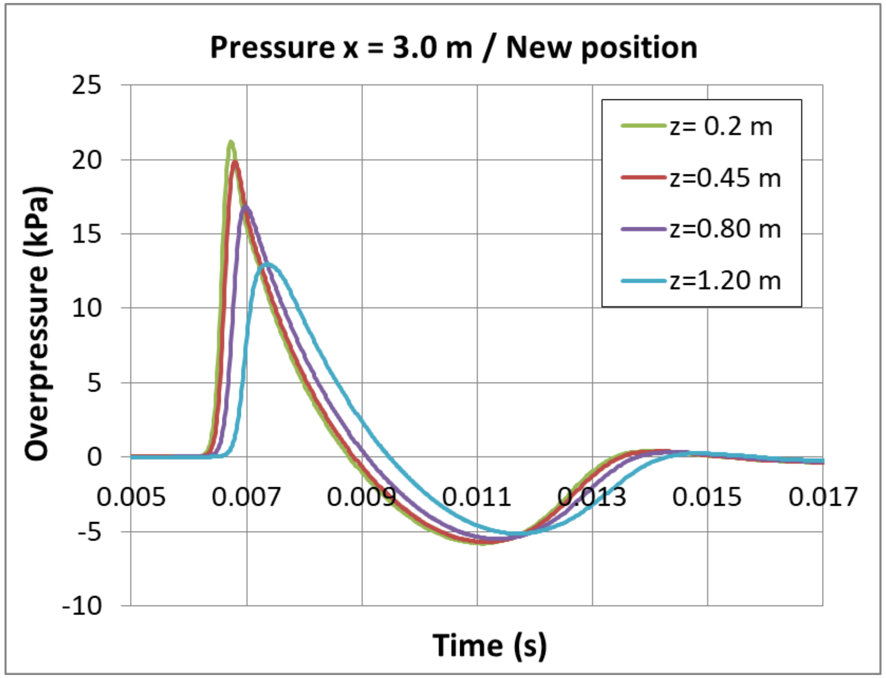
- **Studied the effect of:**
  1. Tank position
  2. Turbulence modelling approach
  3. Air condensation

1st scenario: 11bar / full vapor / Cold
Effect of tank position

- Change compared to **previous study** *(Ustolin et al. 2022)*:
  1. **Tank position moved** from 1.2 m to 0.45 m (center point)
     (due to closer examination of experimental photos)
  2. **Sensor point moved also** from 1.2 m to 0.45 m
     (because in the experiments pressure measured 3 m away from the middle of the tank)

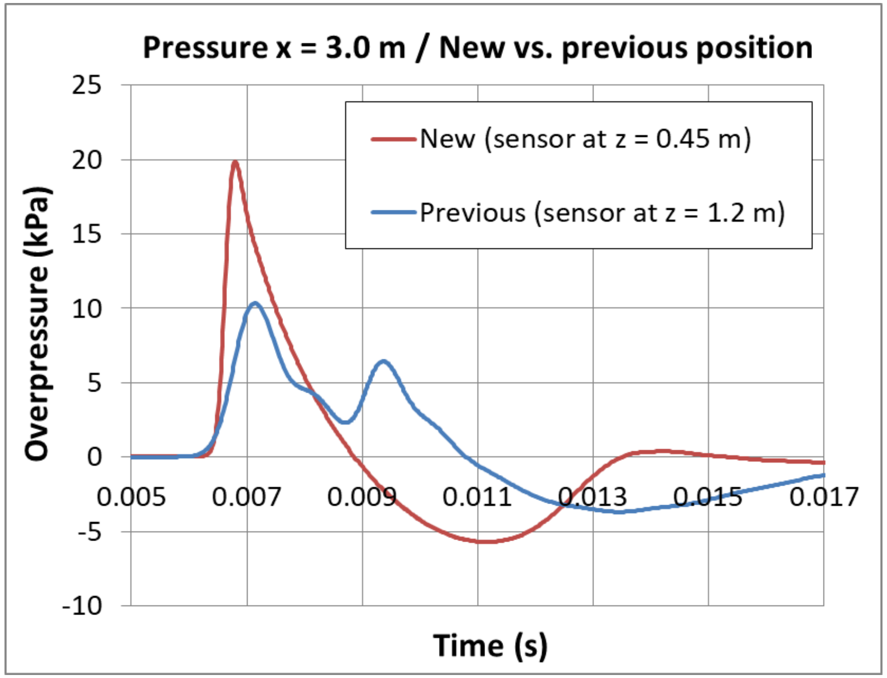
1^{st} scenario: 11bar / full vapor / Cold
Effect of tank position

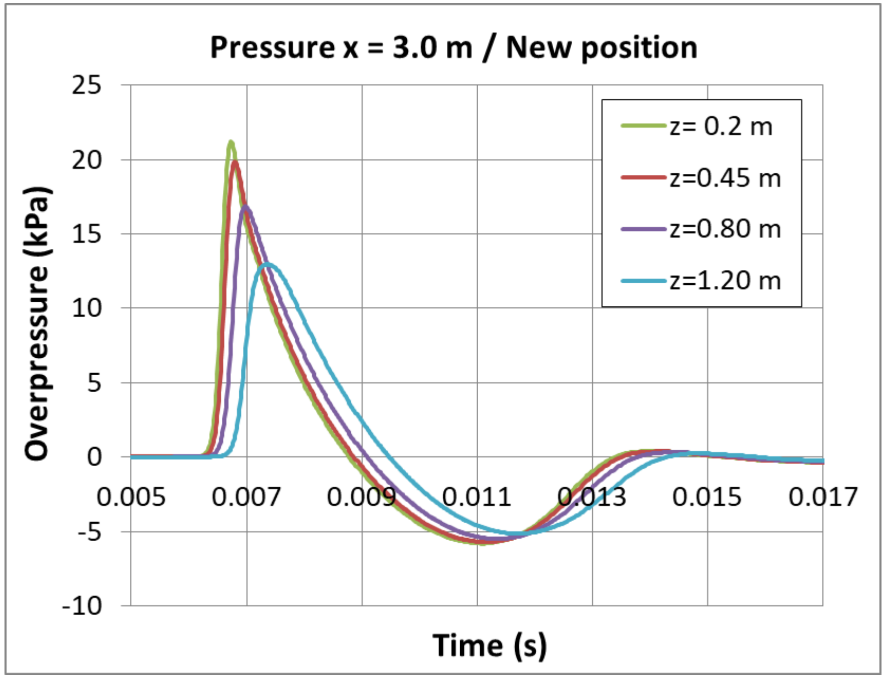




- Left figure: Comparison of previous and new tank position
- Right figure (new tank position):
  - Pressure decreases with height (at x = 3 m)
  - No double peak structure. Reflection of pressure wave due to the larger distance from the ground was responsible in the previous case

1st scenario: 11bar / full vapor / Cold
Effect of tank position





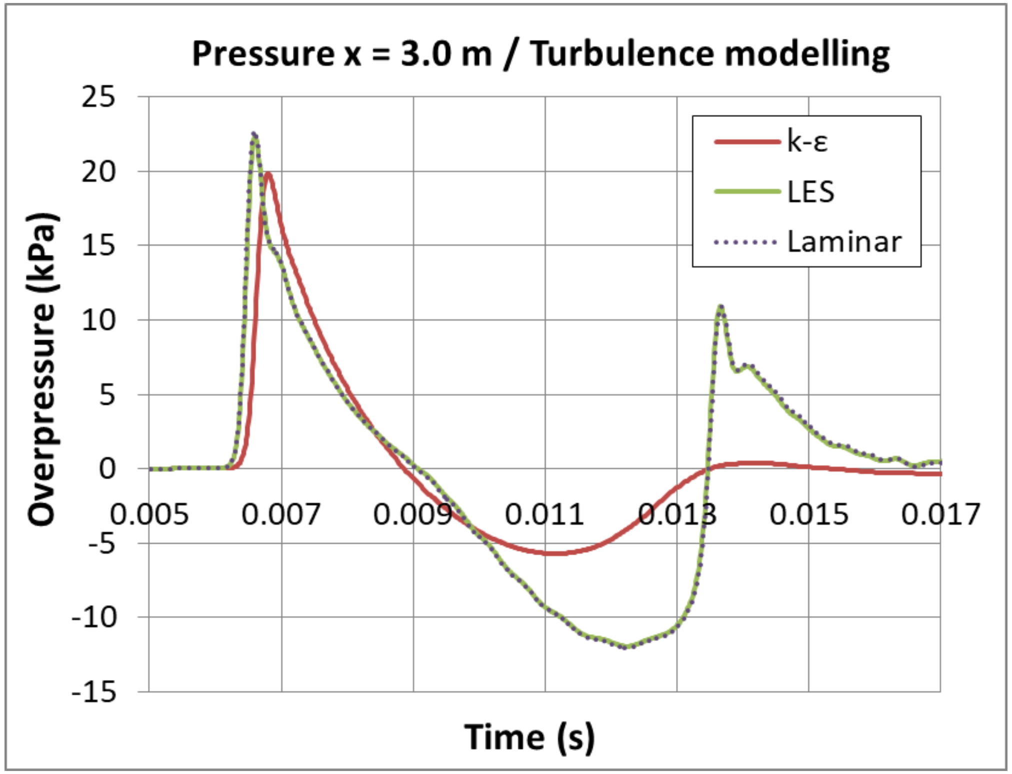
- **Conclusion**: The exact position of tank and pressure measurement is very important for model validation
- The exact shape of the tank perhaps has a non negligible effect on the results (future work)

1^{st} scenario: 11bar / full vapor / Cold
Turbulence modelling approach

- The new tank position is used in the rest of the work
- The effect of turbulence modelling approach was studied next
  - Standard k-ε model
  - LES approach
    - Smagorinsky-Lilly with C_s=0.1
  - Laminar approach

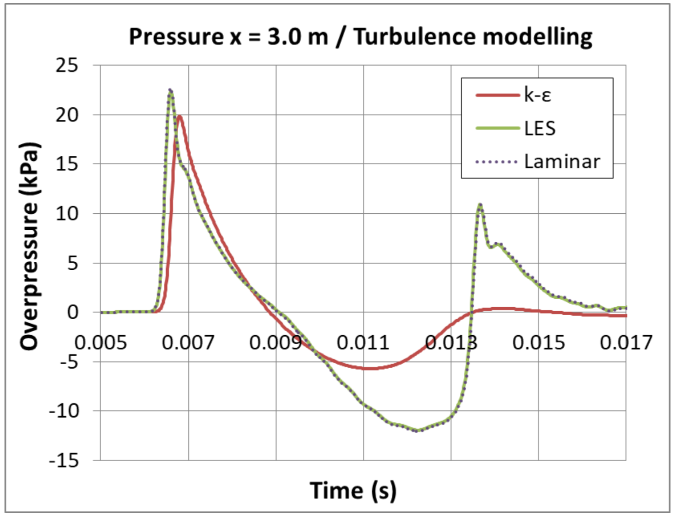
1^{st} scenario: 11bar / full vapor / Cold
Turbulence modelling approach

- LES and Laminar approach predicts the same overpressure
  - No resolved turbulence in LES
  - Much denser grids are required and proper initial perturbations to trigger turbulence
- Low mixing in LES and Laminar approach (due to low turbulence) results in:
  1. Small increase in maximum overpressure
  2. Large decrease of negative overpressure
  3. Creation of a second overpressure peak



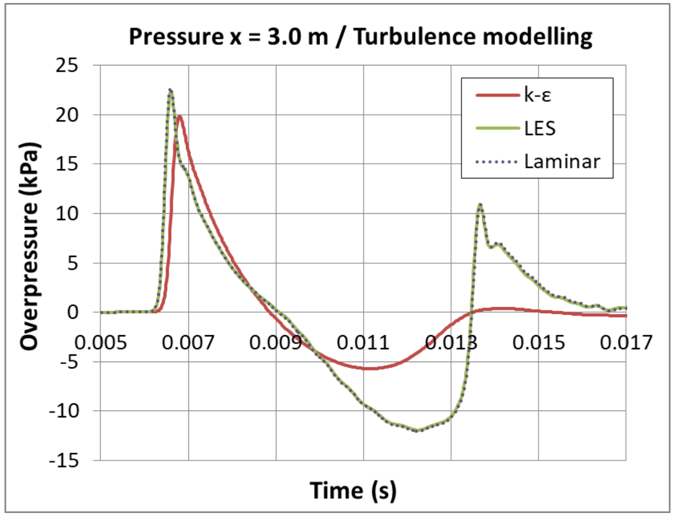
1^{st} scenario: 11bar / full vapor / Cold
Turbulence modelling approach

- **Second overpressure peak**
  - Minimum temperature
    - LES/Laminar: 12.5 K
    - k-ε: 17.3 K
  - Liquid hydrogen is formed at the center of the tank because of temperature decrease due to expansion
  - This volume evaporates rapidly resulting the second overpressure peak
  - The large turbulence predicted in k-ε model enhance mixing hindering temperature to decrease to very low values. Smaller volume of LH2 is formed



1st scenario: 11bar / full vapor / Cold

Turbulence modelling approach



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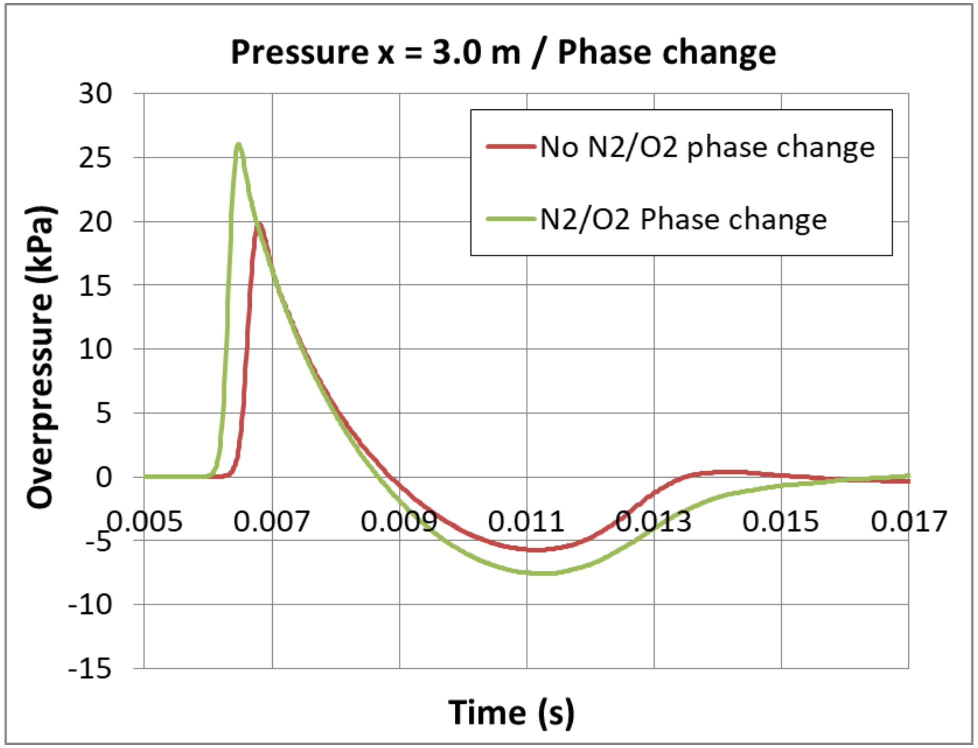
  - The large turbulence predicted in k-ε model enhance mixing hindering temperature to decrease to very low values. Smaller volume of LH2 is formed
- **Conclusion**
  - High levels of turbulence are expected due to the nature of the phenomenon
  - k-ε is more suitable for such simulations
  - Proper LES would require very large computational resources and very accurate representation of the experimental setup

1st scenario: 11bar / full vapor / Cold
Air phase change

- In the previous simulations air was not allowed to change phase
- The phase change of air substances (N_2-O_2) due to the low hydrogen temperature is examined next

1st scenario: 11bar / full vapor / Cold
Air phase change

- In the previous simulations air was not allowed to change phase
- The phase change of air substances (N2-O2) due to the low hydrogen temperature is examined next
- Maximum overpressure increases from 20 kPa to 26 kPa
- N2 and O2 turns into liquid or even solid.
- Heat release from phase change is probably the reason for pressure increase.

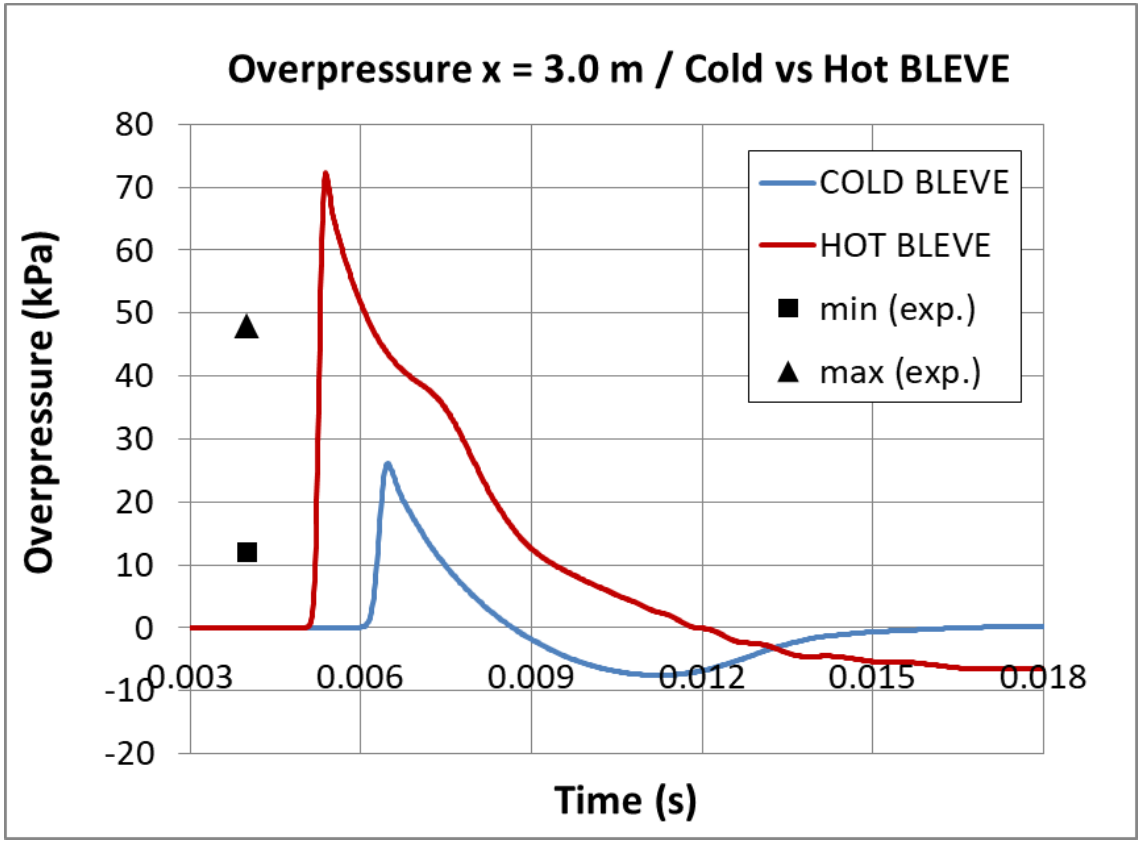


2^{nd} scenario: 11bar / full vapor / Hot

- The case of **HOT BLEVE** is studied next
- The effect of explosives used in the experiments is modelled by allowing H_2 to ignite automatically as soon as it mixes with the surrounding air
- Simulation parameters
  - New tank position (0.45 m above the ground)
  - k-ε turbulence model
  - N_2-O_2 is allowed to change phase

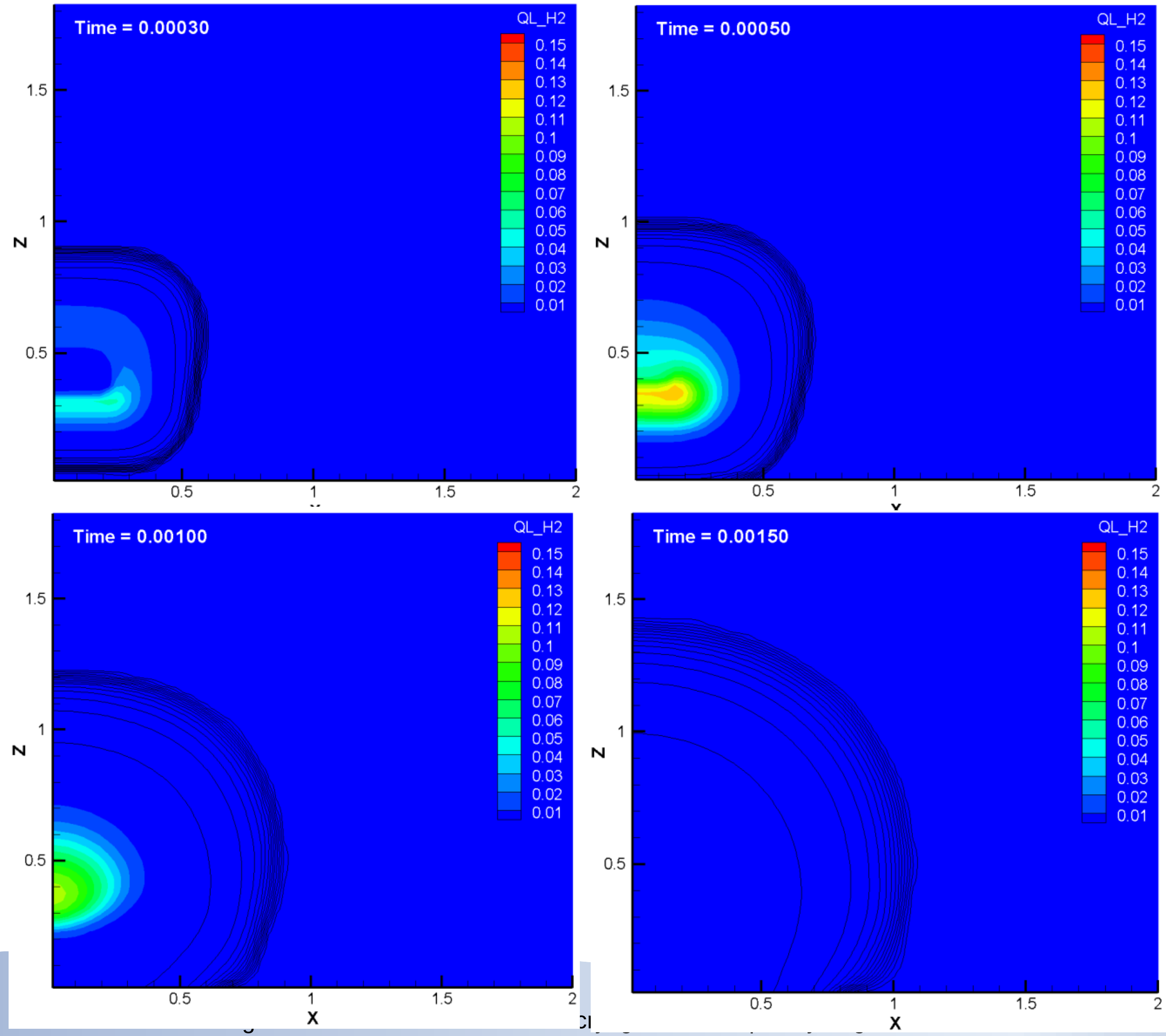
2nd scenario: 11bar / full vapor / Hot

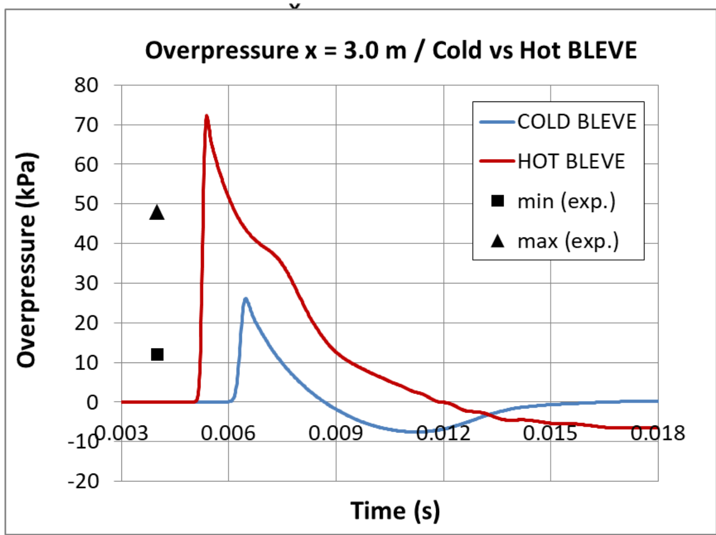
- Pressure increases significantly compared to the Cold BLEVE case
- Experiments:
  - Measured max. overpressure around 12 and 48 kPa (unknown max. time)
  - Unknown liquid fraction in tank
  - Mixture always ignited



2^{nd} scenario: 11bar / full vapor / Hot

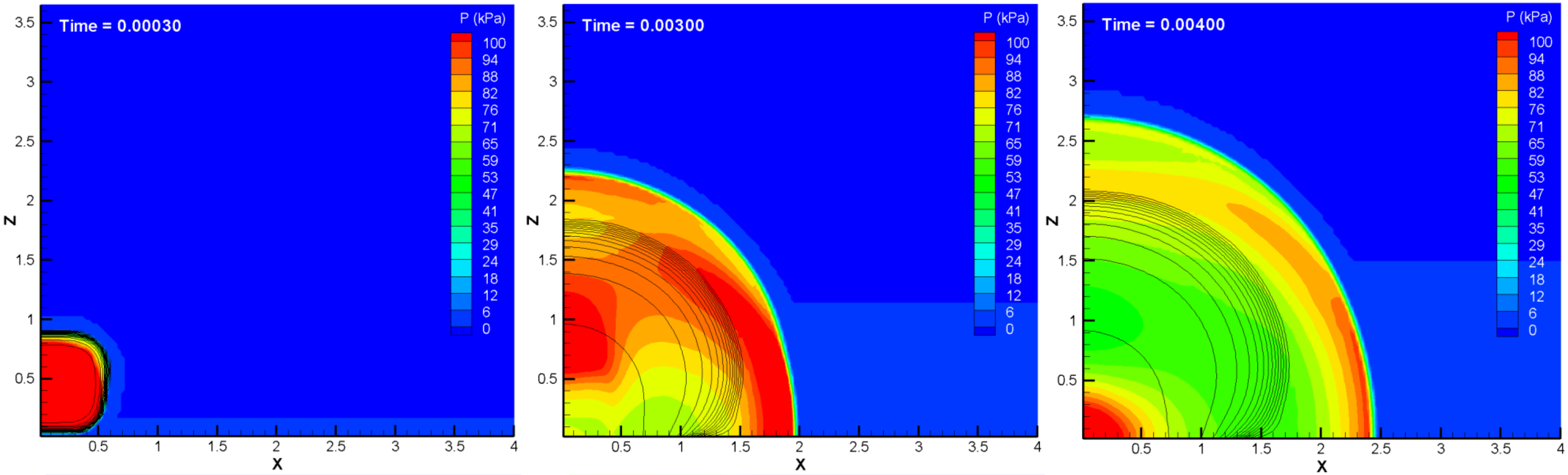
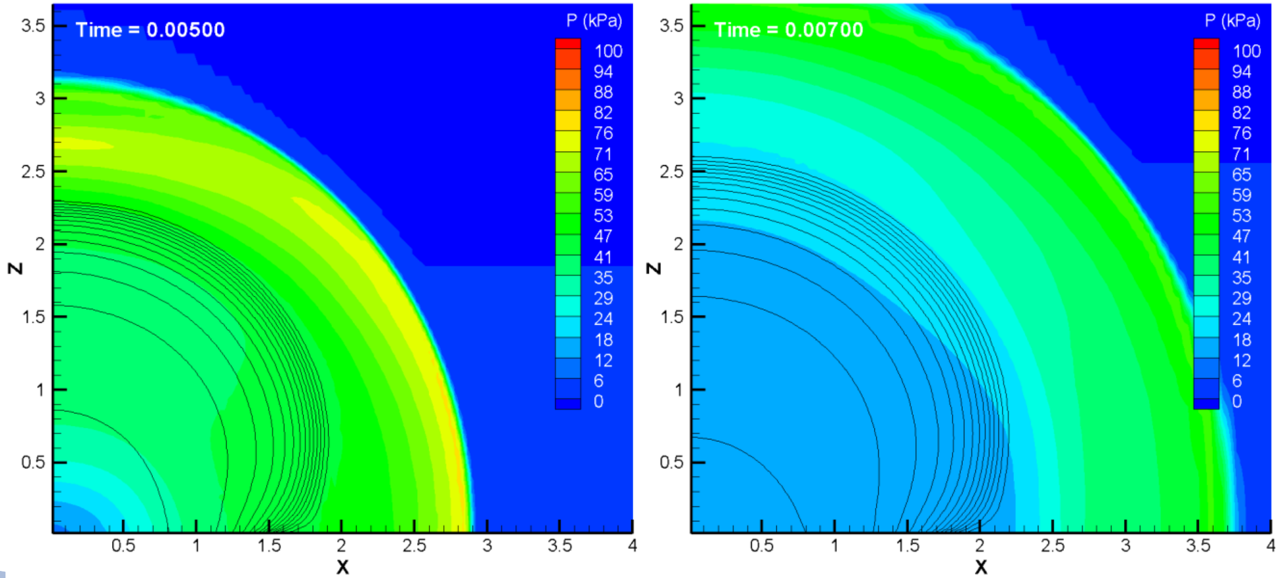
- Liquid is formed also in Hot BLEVE
  Color contours: **Liquid mass fraction**, Black lines: H_2 volume fraction

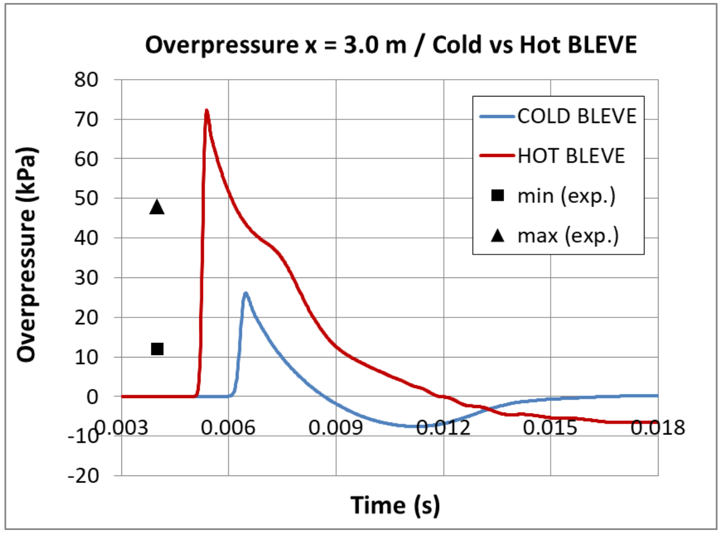




2^{nd} scenario: 11bar / full vapor / Hot

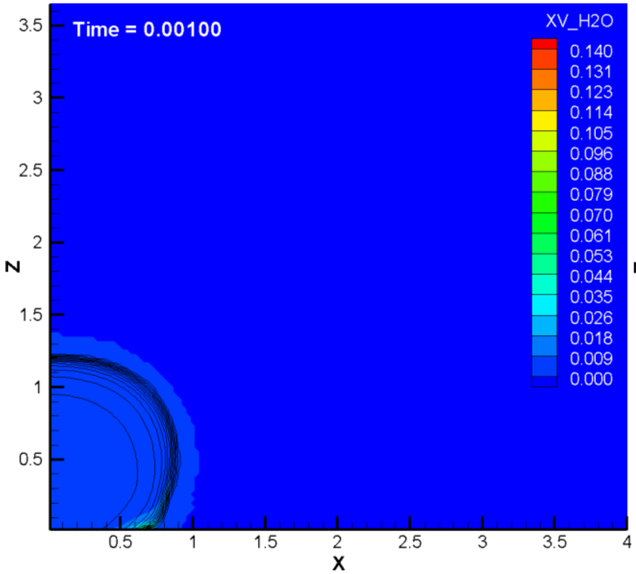
- Color contours: **Overpressure**, Black lines: H_2 volume fraction

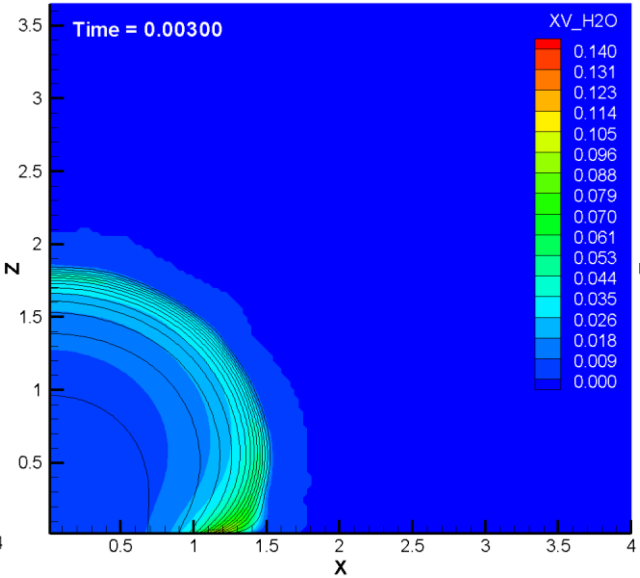



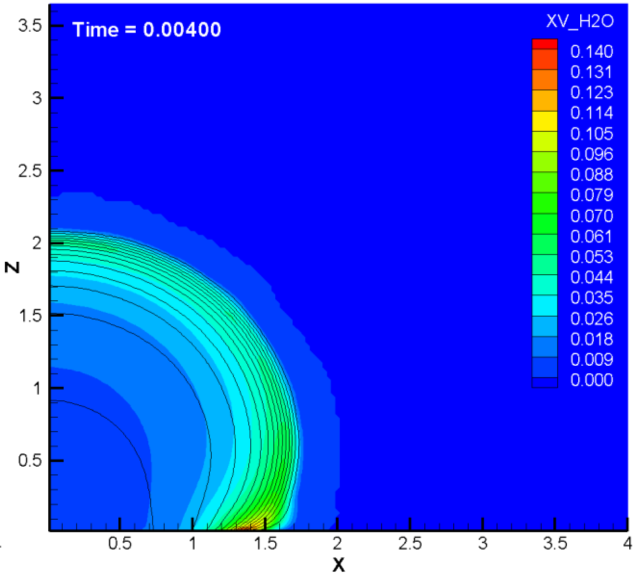


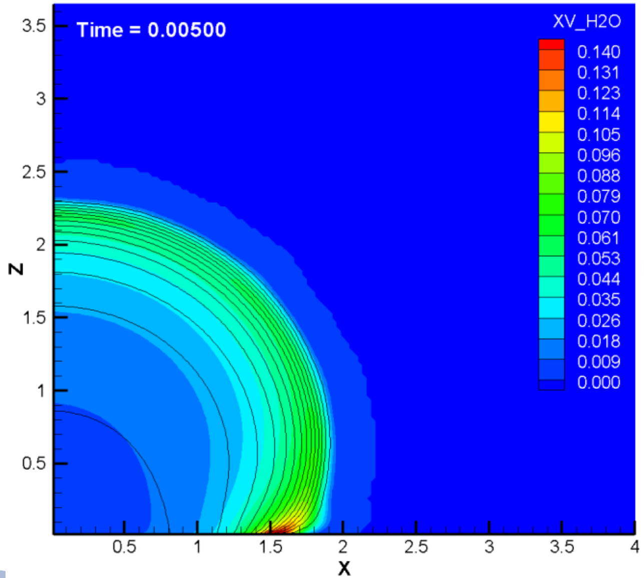
2nd scenario: 11bar / full vapor / Hot

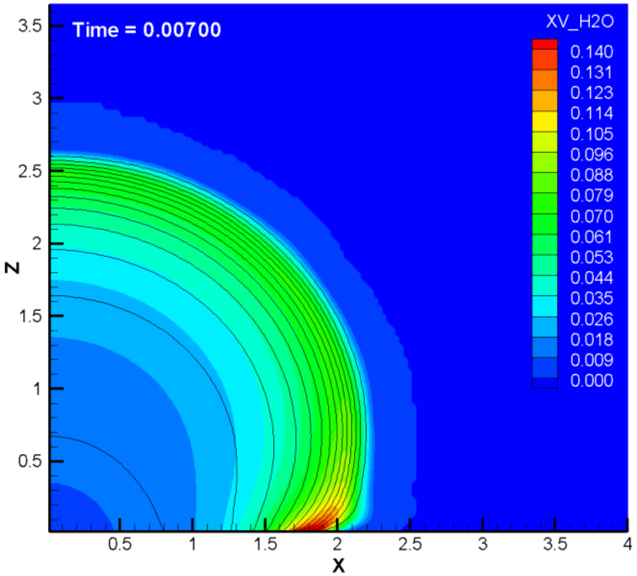
- Color contours: **H2O volume fraction**, Black lines: H_2 volume fraction

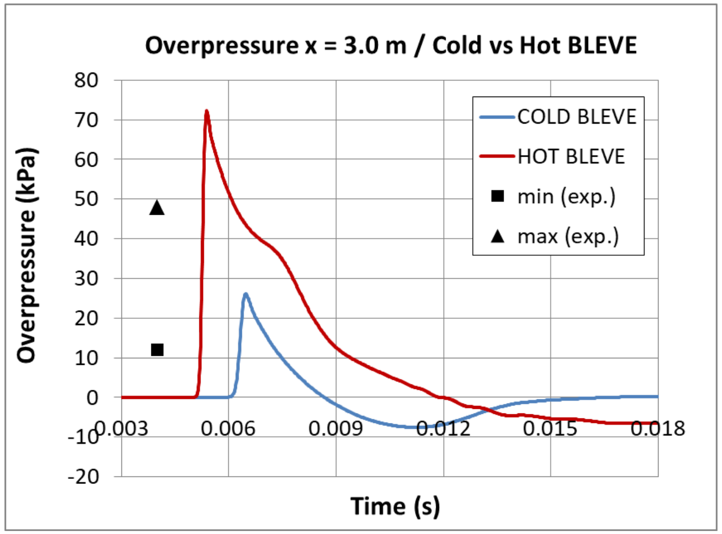












3^{nd} scenario: 11bar / liquid fractions

Cold BLEVE

- The effect of liquid fraction inside the tank was studied
- 4 cases were examined: Full vapor, Full liquid, 29 % and 50 % liquid fractions
- Cold BLEVE was examined first

3rd scenario: 11bar / liquid fractions

Cold BLEVE

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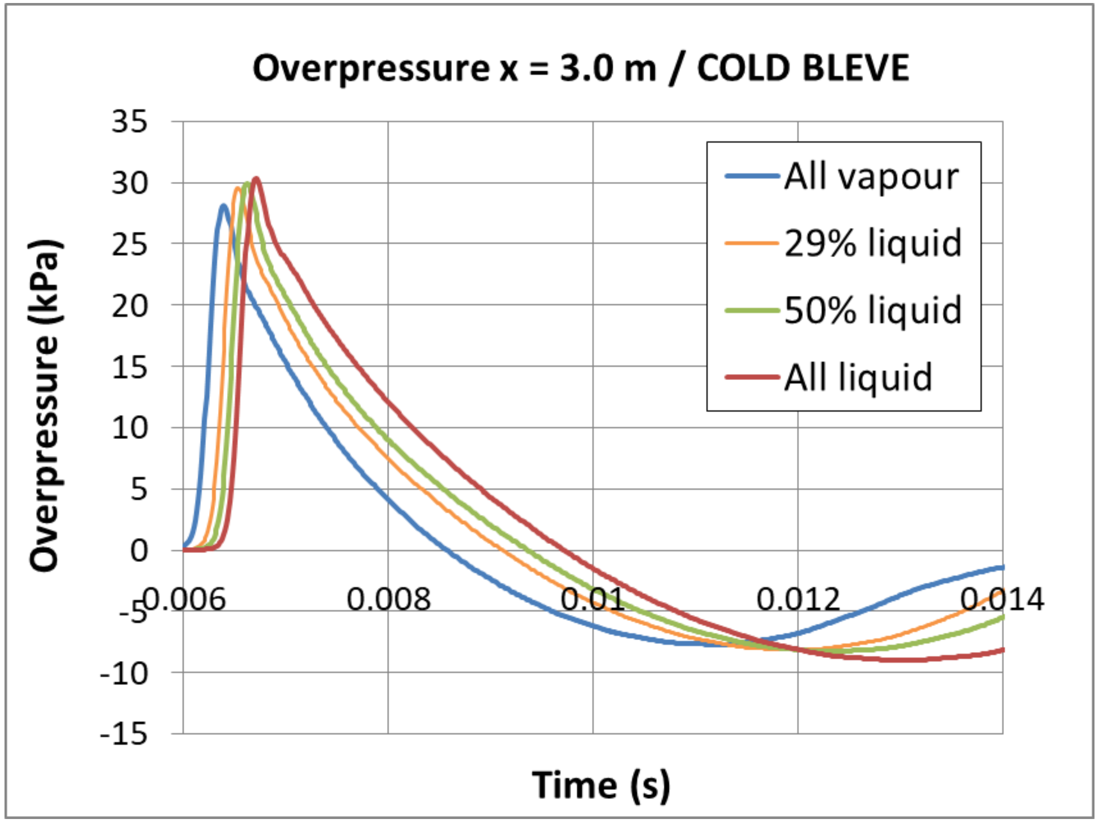


- Small **increase** of maximum overpressure as the liquid fraction increases
- Maximum overpressure equal to 30 kPa at the all liquid case

3^{nd} scenario: 11bar / liquid fractions

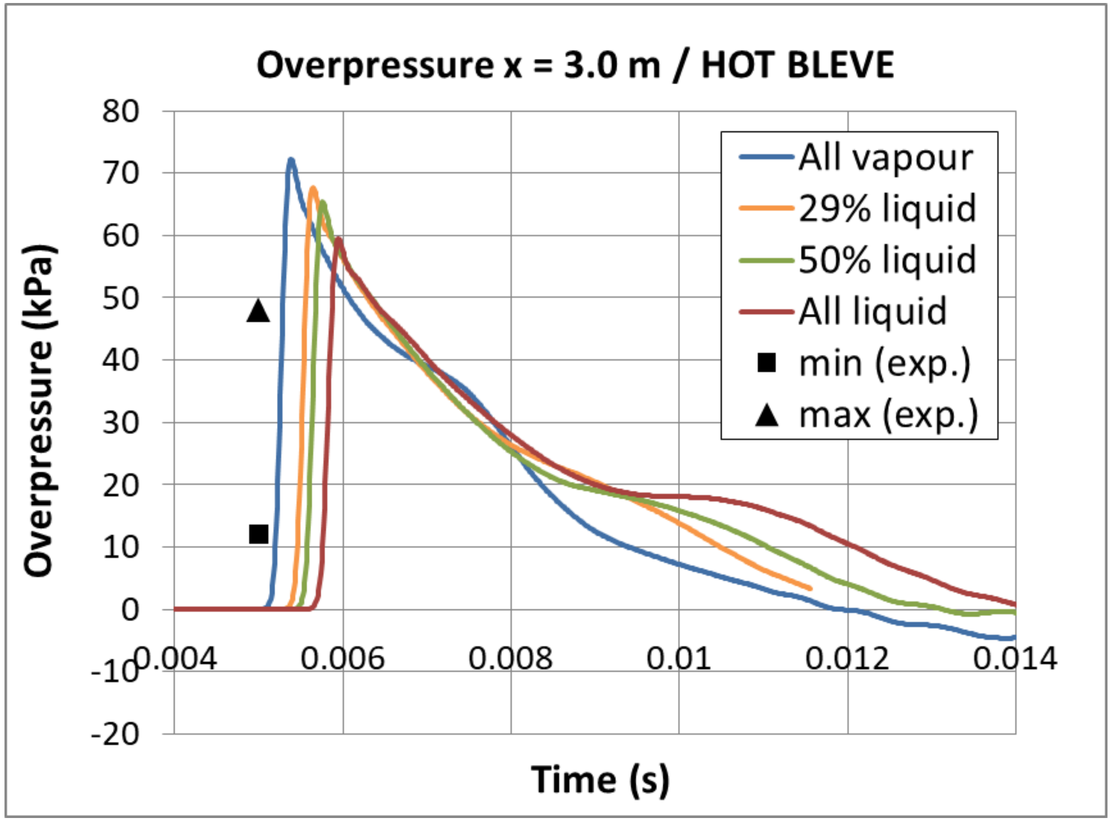
Hot BLEVE

- The effect of liquid fraction inside the tank was studied in **Hot BLEVE**
- The same 4 cases were examined: Full vapor, Full liquid, 29 % and 50 % liquid fractions

3rd scenario: 11bar / liquid fractions

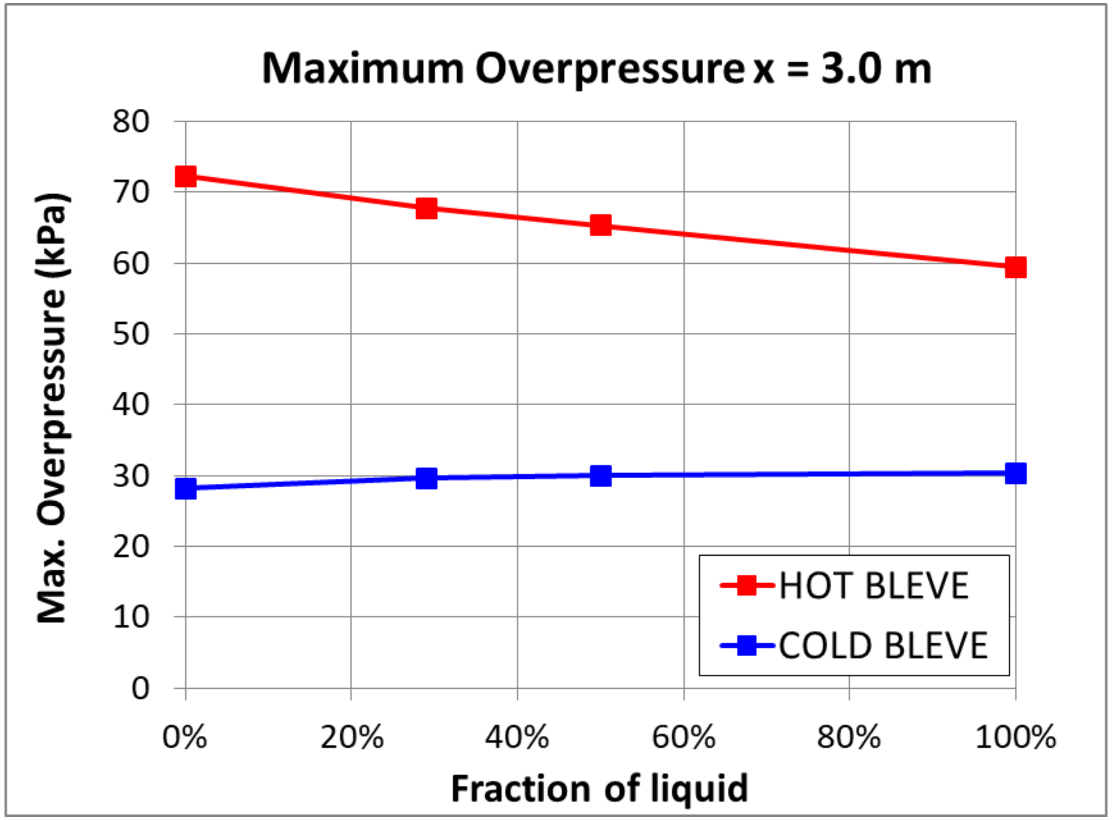
Hot BLEVE

- The effect of liquid fraction inside the tank was studied in **Hot BLEVE**
- The same 4 cases were examined: Full vapor, Full liquid, 29 % and 50 % liquid fractions
- Opposite effect of liquid fraction compared to Cold BLEVE
- Small **decrease** of maximum overpressure as the liquid fraction increases
  - The large amount of liquid delays the ignition and the temperature increase
- Maximum overpressure 72 kPa (all vapour) and minimum 60 kPa (all liquid)



3rd scenario: 11bar / liquid fractions

Cold vs Hot BLEVE



Conclusions

- Accurate BLEVE experiments are needed for model validation
- The exact position of tank and pressure measurement is very important
- k-ε is more suitable for BLEVE simulations due to the nature of the phenomenon
- N_2-O_2 condensation is important and need to be accounted for
- Maximum overpressure increase as the liquid fraction increases in Cold BLEVE but decreases in Hot BLEVE case

Thank you for your attention

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HPC ARIS

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