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LES model of pressure recovery phenomena in a large-scale LH2 storage at HRS

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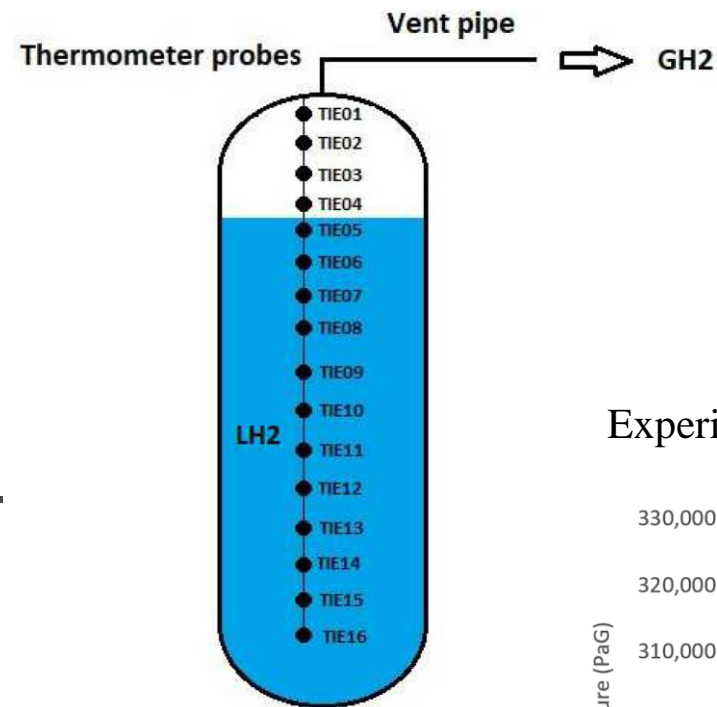- Results and discussions

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Introduction

- Clean energy plays a crucial role in a global scale for a range of industries.

- Comprehension of physical phenomena occurred during hydrogen transport, storage and distribution is required.

- Phenomena can be studied via numerical method (CFD).

- Contemporary tools are required to be established to characterise the liquid hydrogen evaporation in tank during the transport, storage and fuelling process.

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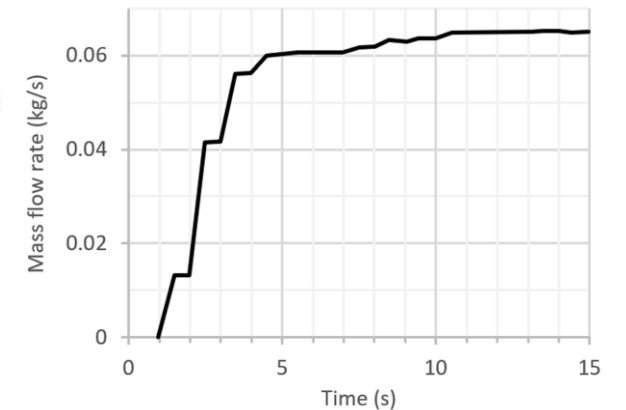
Validation experiment
Hydrogen flashing

- Hydrogen flashing experiment were conducted at JAXA Noshiro Rocket Testing Centre.

- Liquid hydrogen (LH2) tank sized 30 m3 (80% filled) had dimensions 7.622m of height and 2.3 m of internal diameter.

- Initial pressure was 321,800 PaG.

- 16 thermocouples were installed in LH2 tank (4 probes in gaseous area, 12 probes in LH2 zone).
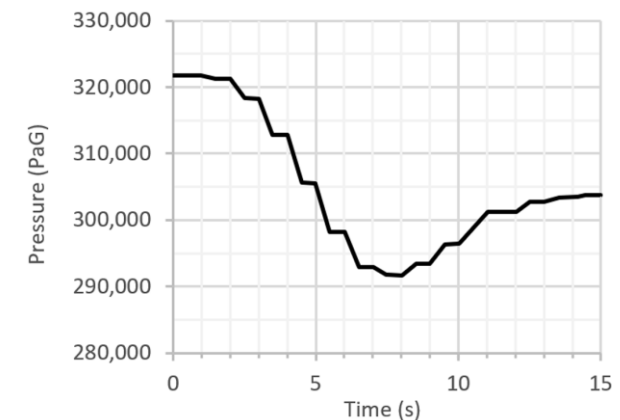
Schematic diagram of LH2 tank with 16 thermocouples

Experimental mass flow rate (15 s)

Experimental pressure in vent pipe

Reference:
- Kangwanpongpan, T., Makarov, D., Cirrone, D., Molkov, V., LES model of flash-boiling and pressure recovery phenomena during release from large-scale pressurised liquid hydrogen storage tank, International Journal of Hydrogen Energy, 2023, Article in Press, https://doi.org/10.1016/j.ijhydene.2023.07.126.
- Tani, K., Himeno, T., Sakuma, Y., Watanabe, T., Kobayashi, H., Toge, T., Unno, S., Kamiya, S., Muragishi, O., Kanbe, K., Pressure recovery during pressure reduction experiment with large-scale liquid hydrogen tank, International Journal of Hydrogen Energy, Volume 46, Issue 57, 2021, pp. 29583-29596. https://doi.org/10.1016/j.ijhydene.2020.12.184.
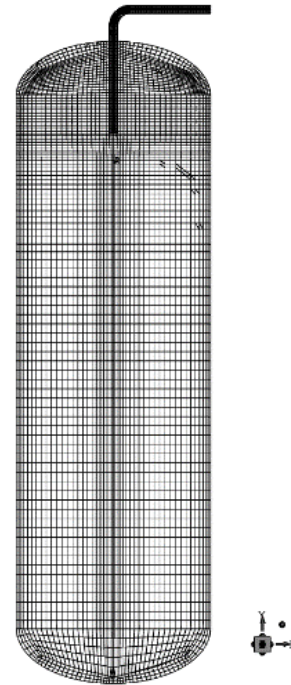
CFD model
Mesh & Initialization

- Mesh

  - CFD model performed via ANSYS FLUENT 2020R2.

  - 251,272 hexahedral control volumes used to create numerical mesh.
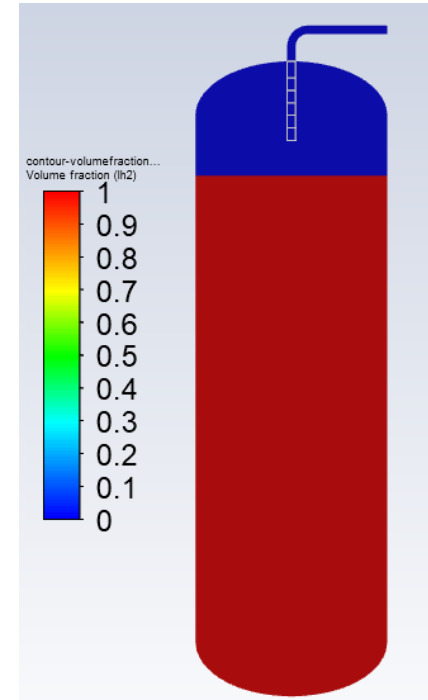
- Initialization

  - Initial LH2 level is 6.248 m from the bottom.

  - Initial LH2 temperature is 26.3 K.

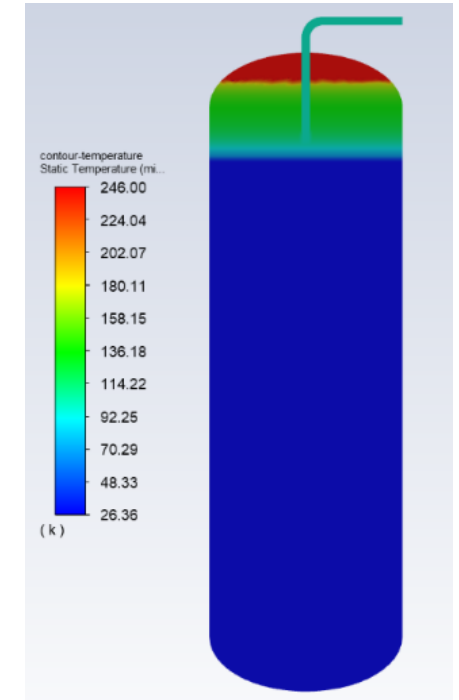 - Initial GH2 temperatures in ullage is set equal to experiment (thermocouples TIE01-TIE04).

Initialization

Numerical mesh

Volume fraction (LH2)

Temperature (in K)

contour-volumefraction...
Volume fraction (lh2)

1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

contour-temperature
Static Temperature (mi...

246.00
224.04
202.07
180.11
158.15
136.18
114.22
92.25
70.29
48.33
26.36

(k)

Theoretical method
Governing equations

- The continuity equation: $\quad \frac{\partial(\alpha_G \rho_G)}{\partial t} + \nabla \cdot (\alpha_G \rho_G \vec{v}_G) = (\dot{m}_e - \dot{m}_c)$

- Conservation of volume fractions: $\quad \alpha_G + \alpha_L = 1$

- Energy source term: $\quad S_{energy} = -\dot{m}_{transfer} L_{heat} \qquad \dot{m}_{transfer} = (\dot{m}_e - \dot{m}_c)$

- Latent heat of vaporization: $\quad L_{heat} = (h_G^s - h_L^s)$

- Phase change model: (Lee's model)

  For evaporation ($T_L > T_{sat}$): $\qquad$ and for condensation ($T_G < T_{sat}$):

  $$\dot{m}_e = r_e \alpha_L \rho_L \frac{(T_L - T_{sat})}{T_{sat}}, \qquad \dot{m}_c = r_c \alpha_G \rho_G \frac{(T_{sat} - T_G)}{T_{sat}},$$

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Theoretical method
Gas and liquid properties

- GH2 properties:
  - GH2 density is determined via the Peng-Robinson EoS:

$$p = \frac{RT}{V-b} - \frac{a}{V(V+b)+b(V-b)}$$

  - GH2 specific heat capacity (Cp,G) is determined by the sum of ideal gas and correction term. The ideal gas specific heat is presented by [Leachman et al. 2009]:

$$C_{p,G}^0 = 10{,}950 - (40.3)\,T + (0.6641)\,T^2 - (0.00268)\,T^3 + (3.468 \times 10^{-6})\,T^4$$

- LH2 properties:
  - LH2 density is determined assuming it as depending on saturation temperature [NIST database]: $\rho_L = 73.168 + 0.8712\,T - 0.0484\,T^2$
  - Specific heat capacity of LH2 (Cp,L,sat) is fitted to selected properties of hydrogen [McCarty et al. 1981] assuming LH2 is at saturation state:

$$C_{p,L,sat} = 10{,}563 - 645.59\,T + 29.466\,T^2$$

References:
- Leachman, J.W., Jacobsen, R.T., Penoncello, S.G., Lemmon, E.W., Fundamental equations of state for parahydrogen, normal hydrogen, and orthohydrogen, J. Phys. Chem. Ref. Data, Vol. 38, No. 3, 2009.
- NIST Chemistry Webbook, NIST Standard Reference Database Number 69, available at https://webbook.nist.gov/chemistry/
- McCarty, R.D., Hord, J., Order, H.M., Selected properties of hydrogen (engineering design data), Technical Report, U.S. Department of Commerce/National Bureau of Standards Monograph 168, 1981.

Theoretical method
Saturation temperature

- For evaporation, the saturation temperatures vary with pressures. The saturation temperature is modelled as polynomial function of absolute pressures (1 – 6 bar) fitted to NIST database presented as:

$$T_{sat} = 17.1 + (3.797 \times 10^{-5})\, P - (5.198 \times 10^{-11})P^2 + (3.3 \times 10^{-17})\, P^3$$
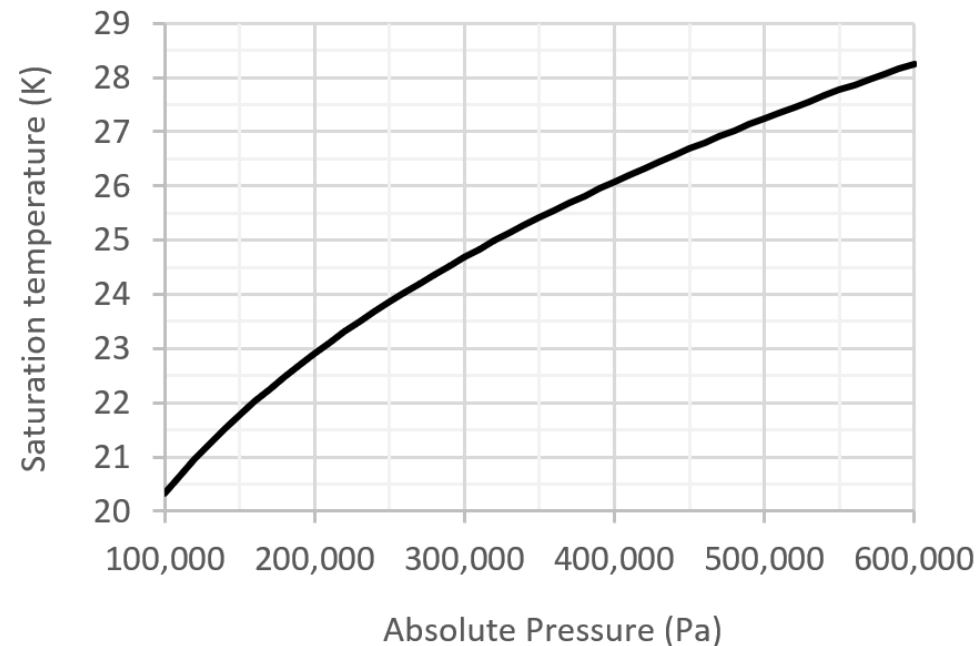

Reference:
- NIST Chemistry Webbook, NIST Standard Reference Database Number 69, available at https://webbook.nist.gov/chemistry/

Results and discussions
Pressure recovery dynamics

- Pressure during 15 s is obtained from simulations, applying Lee's coefficient r=0.05 and 0.1.

- Using r=0.1 fitted to a variety of physical problem from literature review is not able to reproduce the pressure recovery phenomena (no strong pressure drop presented).

- For this specific LH2 flash-boiling problem, applying r=0.05 provided better agreement for pressure recovery to experiment.

Pressure recovery in LH2 tank
(r=0.05 and r=0.10)
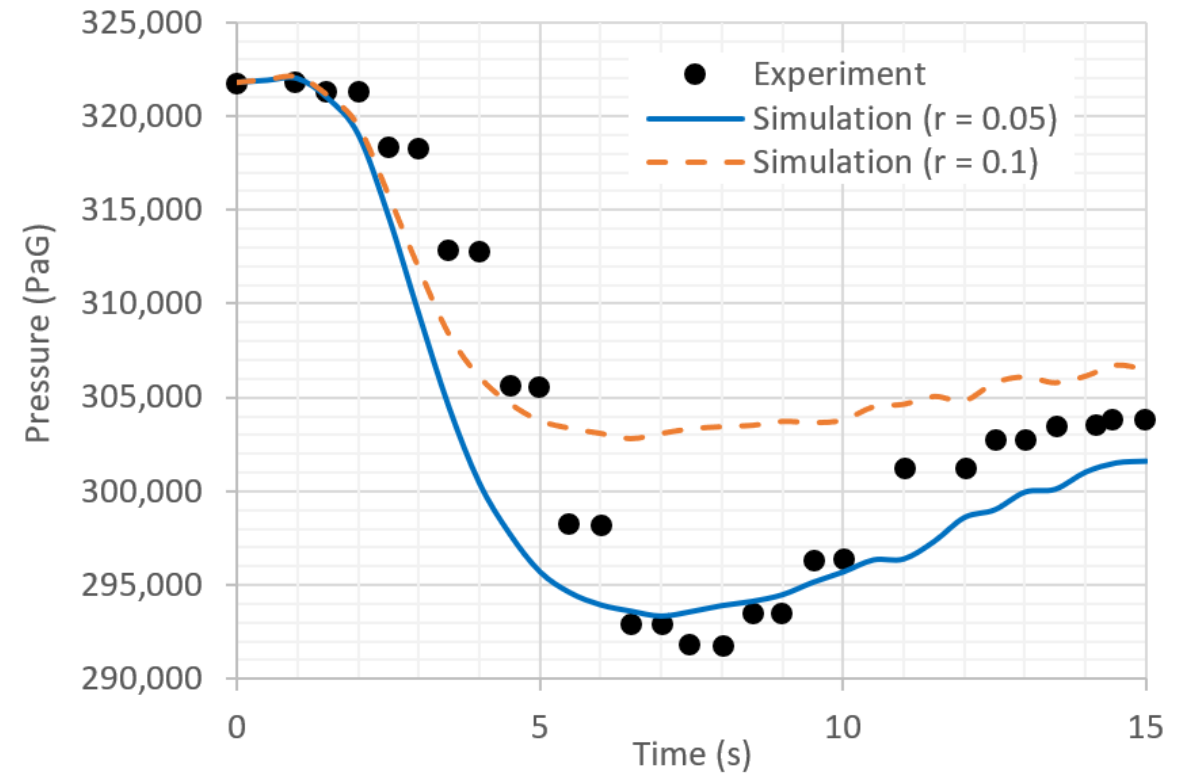
Results and discussions
GH2 phase temperature (ullage area, probe TIE01-TIE04)

- Simulated and experimental GH2 temperature are compared.
- Simulated GH2 temperature at probe TIE01-TIE03 are in good agreement with experiment (slightly fluctuated for TIE03 near the end of 15 s).
- At probe TIE04 (near initial LH2 surface), simulated GH2 temperature drops earlier and is smoother than experiment (sharp drop at 12.5 s), expected to be due to the absence of sharp phase transition between LH2&GH2 phase in reality (limited by control volume's numbers and sizes).

Experimental and simulated GH2 temperature
(probes TIE01-TIE04)
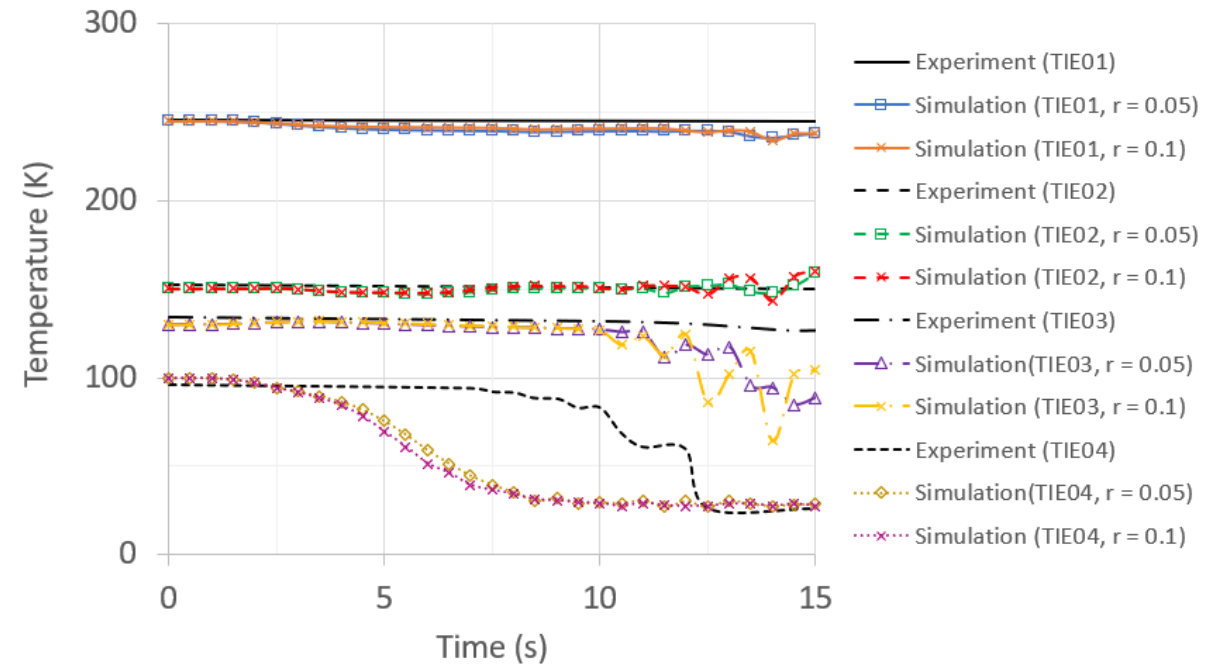
Results and discussions
LH2 phase temperature (LH2 zone, probe TIE05-TIE08)

- Similar trend of simulated temperatures are presented at probe TIE06 – TIE08.

- At end of 15 s, simulated temperatures are different from experiment by around 0.1K at probe TIE05 – TIE08 (inside LH2 zone), excepts 0.2 K at probe TIE06.

- Simulated saturation temperatures follows the experimental temperature and Tsat from NIST database, indicating an intensively flash-evaporation occurred at probes (not captured in simulation since no practical probes installed).
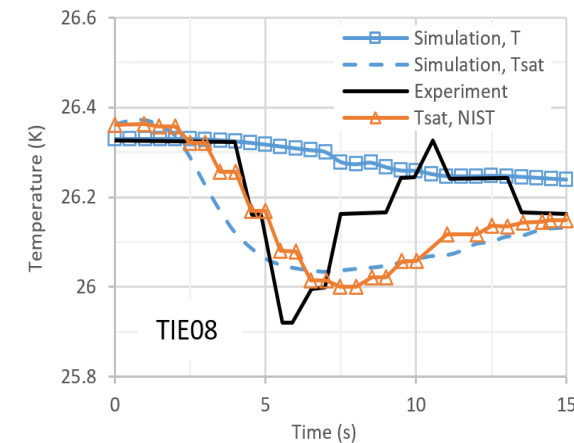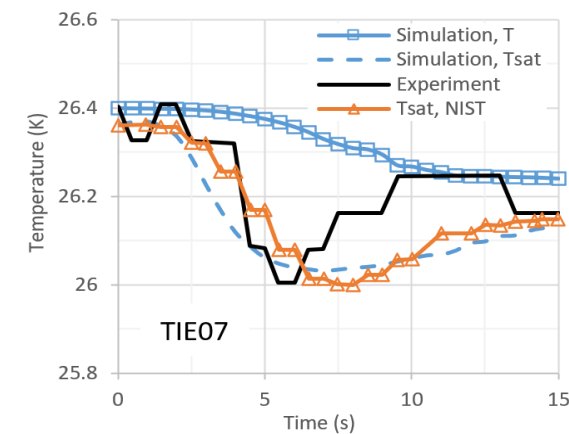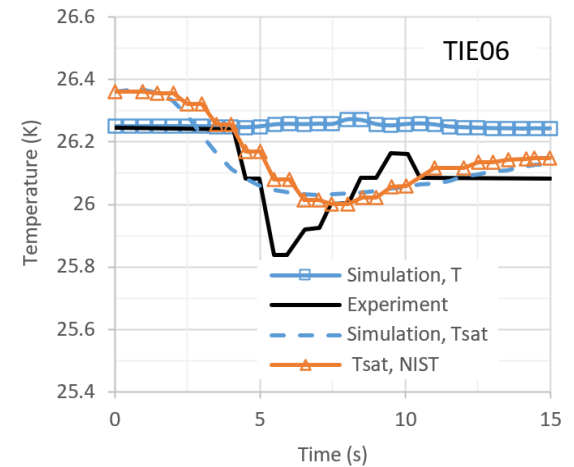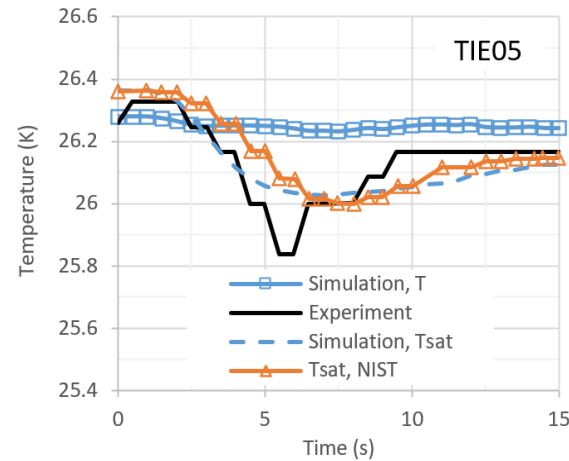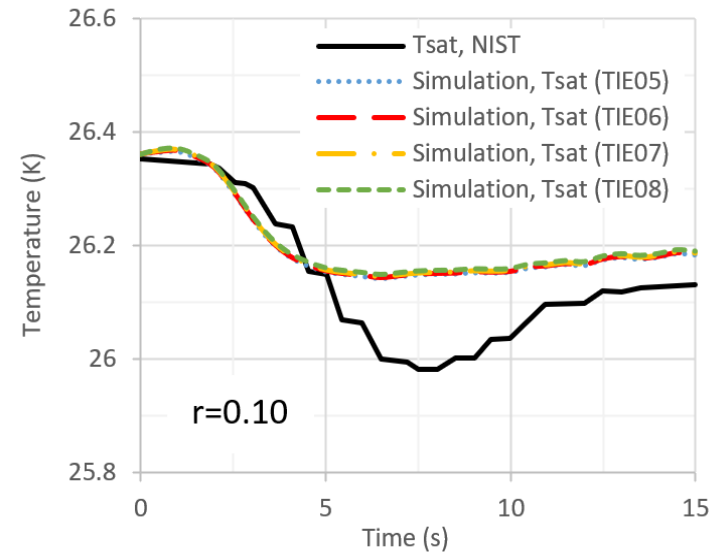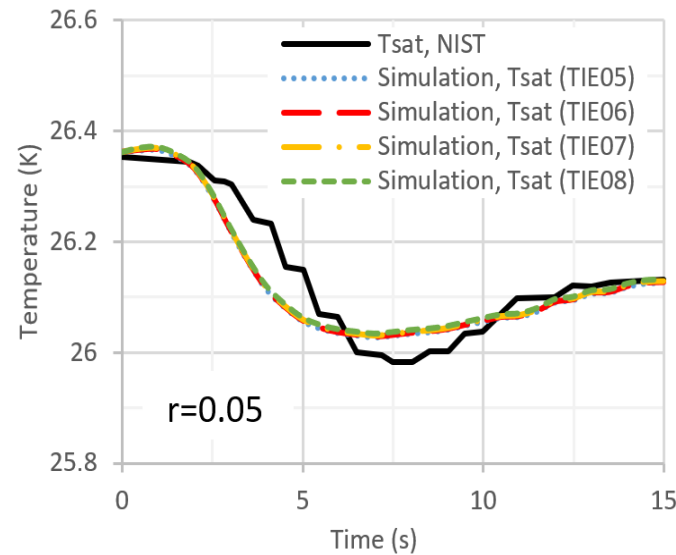
Results and discussions
Saturation temperature (LH2 zone, probe TIE05-TIE08)

- Simulated saturation temperatures are the same for probe TIE05 – TIE08, showing nearly no influence from hydrostatic pressures.
- Simulated temperatures (r=0.05) follows trend of calculated Tsat using NIST data.
- When r=0.1 is used, slightly overestimation of saturation temperatures is reported.

Saturation temperatures at probes TIE05-TIE08
(simulations comparing to Tsat determined using NIST database)

Results and discussions
LH2 level dynamics from simulation

- LH2 level starts to grow at 4 s.
- LH2 level reaches the peak at 10 s.
- LH2 reaches the highest level at 10 s, later than the time having minimum simulated pressure (at 7s), indicating the slight delay of flash-boiling process.
- LH2 does not reach the protruding vent pipe (assuming intake at 6.672 m from tank bottom). Initial LH2 level was at 6.248 m

LH2 level during 15 s
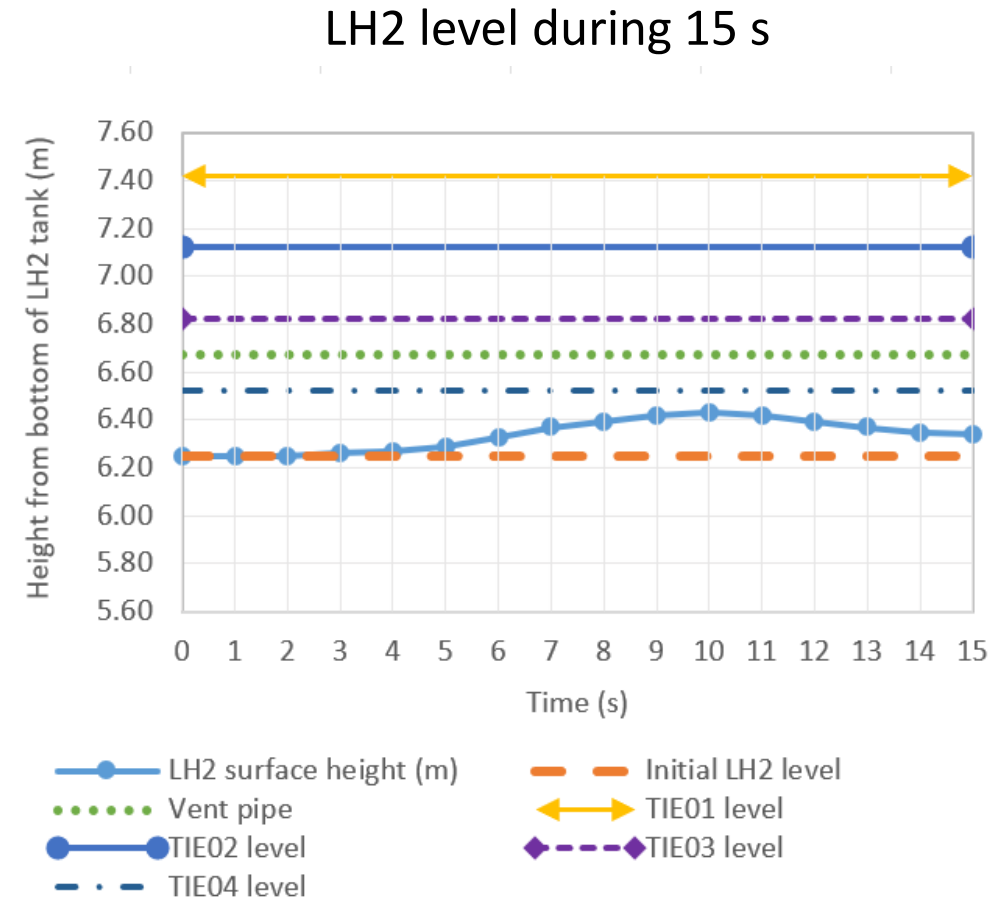
Results and discussions
LH2 volume fractions (to 15 s)

- Bubbles start to appear at 7 s, pressure reaches the minimum level at this time (291kPaG).
- Intensive boiling is presented at 10 s.
- At 15 s, there is a reduction of bubbles generated (represented by green & yellow color in volume fraction contour).

Simulated LH2 volume fraction at different times

contour-volume fraction ...
Volume fraction (lh2)

1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

$t = 0$ s $t = 7$ s $t = 10$ s $t = 15$ s
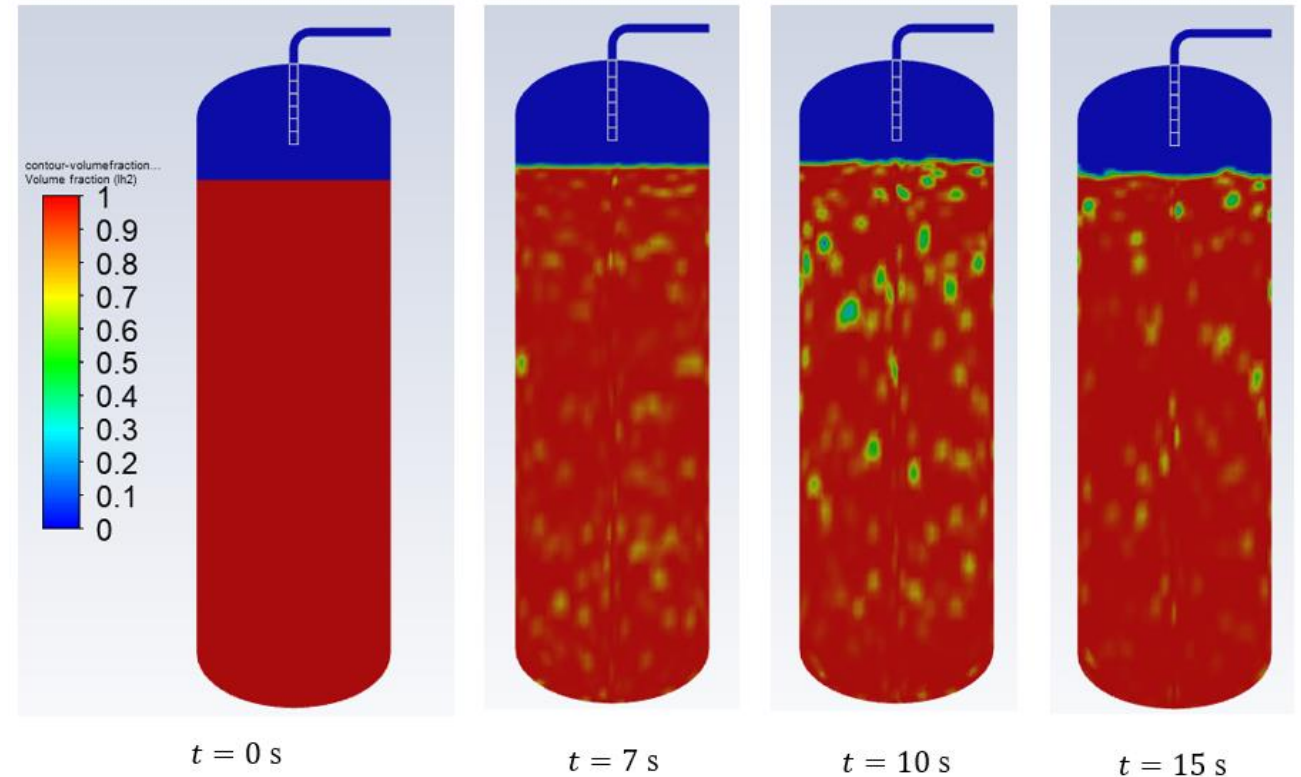
Conclusions

- A CFD model to predict pressure, temperature and liquid level inside a liquid hydrogen storage tank during venting is presented.
- CFD results were compared against experimental data from literature.
- Pressure recovery was reproduced applying Lee's model coefficient r=0.05 (during 15 s of boiling process).
- Simulated GH2 temperatures in ullage followed the experiment, excepts at probe near to LH2&GH2 interface due to complexity of phenomena in this area.
- Simulated LH2 temperatures at the start and end are close to experiment.
- When applying Lee's model coefficient r=0.05, simulated saturation temperature (Tsat) was close to Tsat fitted to NIST database.

Thank you very much

Acknowledgements:

This research has received funding from the Clean Hydrogen Partnership under grant agreement No. 101101381 (ELVHYS). The project is supported by the Clean Hydrogen Partnership and its members. UK participants in Horizon Europe Project ELVHYS are supported by UKRI grant No.10063519 (University of Ulster) and No.10070592 (Health and Safety Executive).

Disclaimer:

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