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LH2 refuelling at HRS: modelling approach and CFD simulations results

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Outline

- The modelling approach of LH2 refuelling through the entire set of equipment of Hydrogen Refuelling Station (HRS) is presented.
- The thermodynamic model of LH2 transfer from HRS storage to pump exit is described. The advantages of transforming hydrogen from equilibrium to non-equilibrium “sub-cooled” state (sLH2) during compression at pump are utilised.
- The two-phase 3D transient CFD model for LH2 refuelling from the pump exit to onboard storage tanks (verified against the conceptual LH2 fuelling protocol).
- The CFD model encompasses all HRS components downstream of the LH2 pump exit, including automatic PCV (directly connected in the model to the pump exit), pipes with bends, breakaway, nozzle, manifold, and two onboard storage tanks.
- Due to the absence of published experimental data, the simulations are verified against the conceptual LH2 refuelling process dynamics (mass flow rate, P, T).

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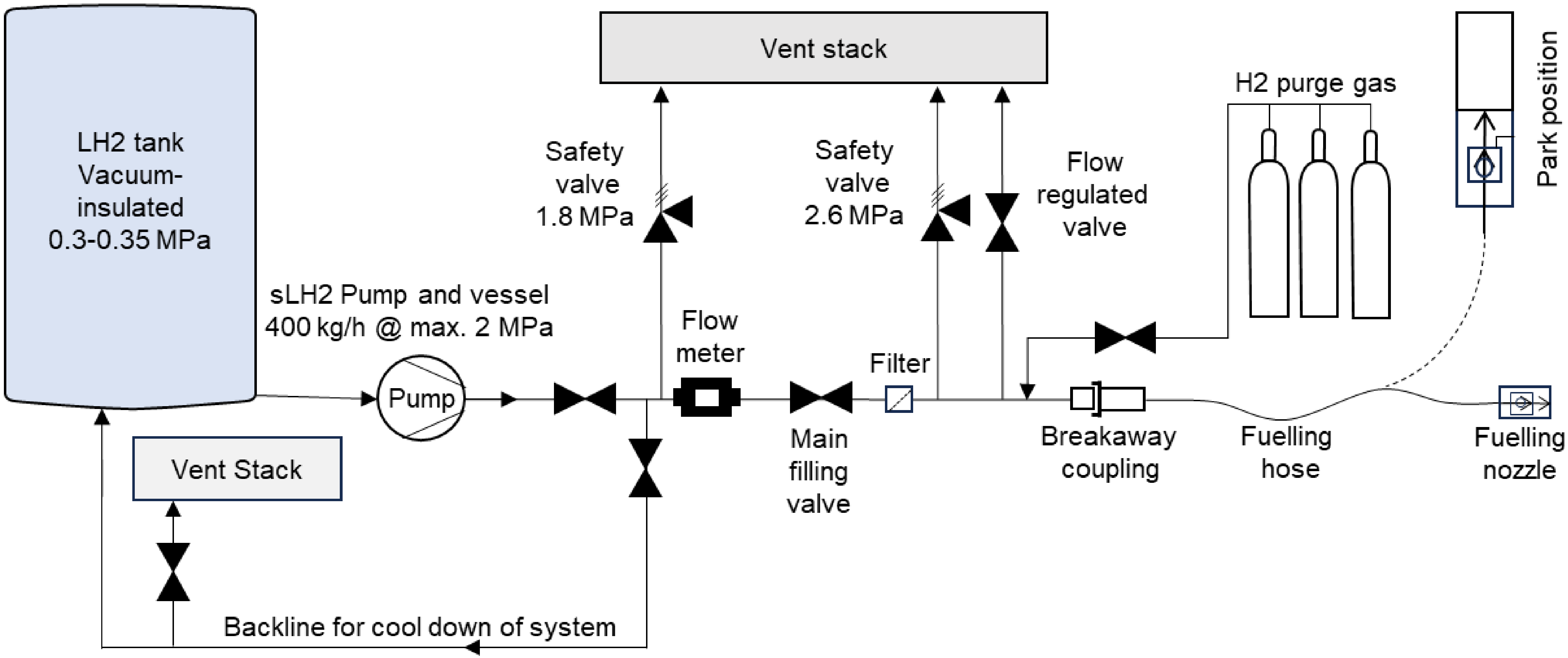
The state-of-the-art
Studies related to LH2 refuelling modelling

- To date, the CFD modelling of LH2 tank filling has been restricted to the process dynamics in the storage tank itself. Components of the LH2 HRS equipment and their effect on pressure and temperature dynamics were not considered.
- Examples of such studies are:
  - In 2022, Wei et al. conducted a numerical simulation and analysis of the LH2 storage tank filling process under sloshing conditions by **coupling the sloshing model with the phase-change model**.
  - In 2022, Kang et al. performed simulations of the initial charging process of the LH2 tank for vehicles using a **2D CFD model**. Only the first **1.2 s** were analysed.
  - In 2023, Ma et al. proposed a four-node mathematical model to examine **the no-vent-filling performance of LH2 under microgravity** conditions.
- There are few publications focussing on the boil-off phenomenon, e.g. Petitpas (2018), Al Ghafri et al. (2022).

The state-of-the-art

Schematic of an exemplary LH2 refuelling station equipment

Source: Maus S, Schäfer S. Technology Pitch: Subcooled Liquid Hydrogen. NOW CEP Heavy Duty Event, April 21st 2021.



The aim: modelling of entire LH2 refuelling station

The aim is achieved by addressing the following objectives

- **Getting insights** into the concept of efficient LH2 refuelling (sLH2).
- Development of a **universal modelling approach** that comprises elements of **thermodynamic modelling** and **transient 3D two-phase flow CFD** simulations.
- Modelling **for the first time** the LH2 refuelling from HRS storage tank **through the entire HRS equipment** down to the onboard storage tanks.
- **Reproduction** by the model of the **conceptual LH2 refuelling protocol** derived from unpublished experimental observations.

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The concept of efficient LH2 refuelling

LH2 pump to achieve sub-cooled liquid hydrogen (sLH2)

- LH2 pump is a core component of an LH2 refuelling station that can enable the sLH2 fuelling technology if properly implemented.
- The existing literature lacks knowledge on the modelling of LH2 pumps, impeding deeper insight and optimisation of their functionality (Qiu et al., 2023).
- LH2 possesses distinct physical properties compared to gaseous hydrogen, resulting in the design and operational disparities between LH2 pumps and gas compressors. *Firstly*, LH2, is stored near saturation with low latent heat. This necessitates pre-compression in LH2 pumps to **prevent cavitation**, thus leading to a more complicated pump design. *Secondly*, during pump operation, hydrogen undergoes compression from near-saturated liquid to high-pressure sLH2, eventually reaching a supercritical state. This complex interplay of temperature, pressure, and phase change fundamentally alters fluid flow and heat transfer within the pump cylinder, diverging from gas compressor behaviour.

The concept of efficient LH2 refuelling

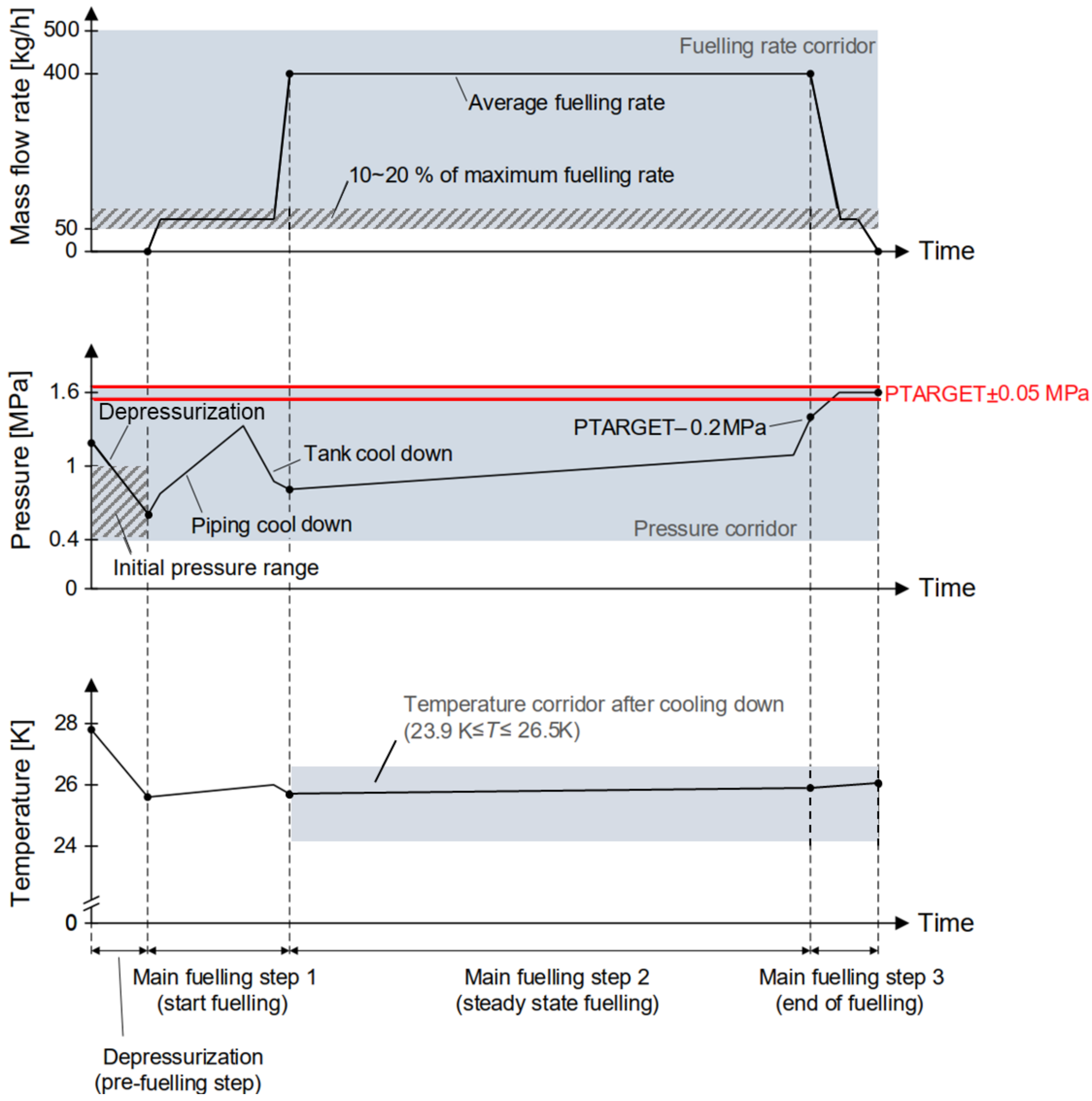
Complex heat and mass transfer

- Sub-cooled at the pump sLH2 flows through pipes and valves toward onboard tanks. Heat transfer and flow losses along the LH2 pathway are unavoidable.
- The fluid experiences multiple transformations throughout its journey along the entire pathway, including sub-cooled liquid phases, two-phase transitions, super-heated warming, non-uniform temperature distributions in a two-phase system, etc.
- The efficient sLH2 fuelling technology implies filling of vehicle tank with LH2 at a sub-cooled state, i.e. as liquid at a non-equilibrium state above the saturation curve on the P-T phase diagram. This non-equilibrium in the sense of vapour-liquid saturation state can be achieved by an increase of pressure in the pump. In this sub-cooled state **LH2 will flow as "non-vaporising" liquid** unless heat transfer from warmer equipment, especially at the start of refuelling, and will "return" LH2 from sub-cooled conditions to the saturation curve conditions.

The concept of efficient LH2 refuelling

Conceptual fuelling protocol: mass flow rate, P and T profiles

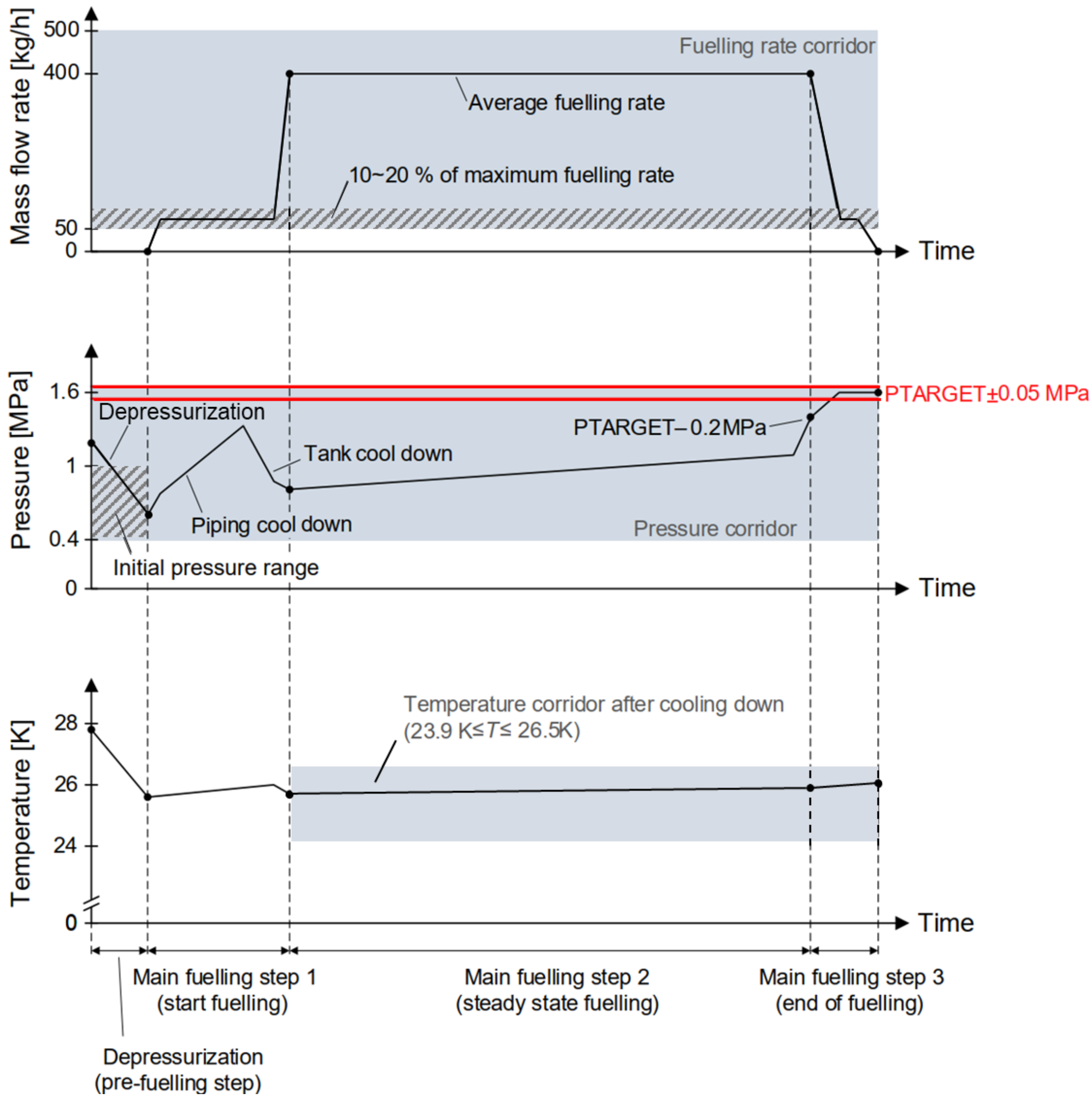
- Presented by Pizzutilo et al. (2022-2024).
- The pre-fuelling activities include purging and leakage testing (not shown in the diagram), and system depressurisation.
- During the depressurisation, the temperature drops due to vapour phase expansion and liquid phase cooling due to evaporation accompanying the pressure reduction.
- Three steps of the main refuelling:
  - Reduced mass flow rate (10-20% of maximum) to cool down piping and storage systems.
  - Refuelling with a targeted average fuelling rate of 400 kg/h, and finally
  - End of fuelling with reduction of mass flow rate to zero when pressure reaches 1.6+0.05 MPa.



The concept of efficient LH2 refuelling

Conceptual fuelling protocol: mass flow rate, P and T profiles

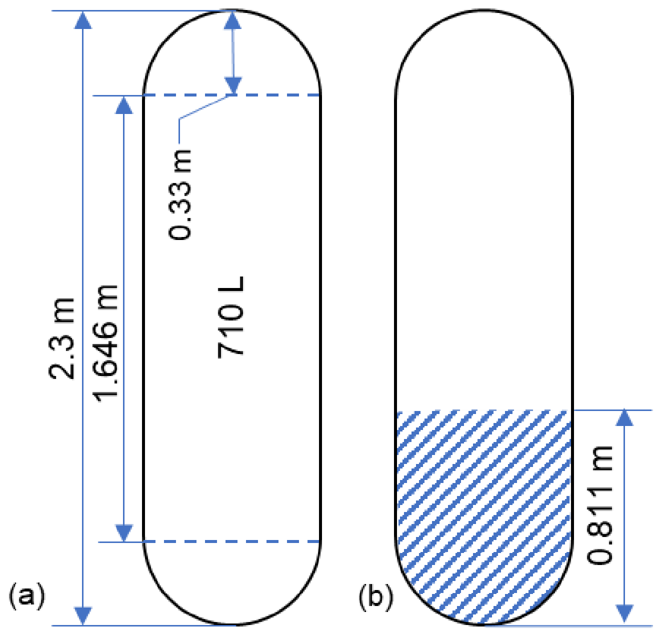
- The conceptual temperature corridor after cooling down is 23.9 K ≤ T ≤ 26.5 K. The fuelling protocol which is under development by ISO/TC197/WG35 "Liquid Hydrogen Land Vehicle Fueling Protocol" expects the supply sLH2 to ensure the cooling down of warm components and the condensation of gaseous hydrogen in the HRS. This would allow to avoid prematurely reaching the target pressure limit.
- One of the advantages of the sLH2 refuelling is that only one nozzle is required, as no gaseous hydrogen returns from onboard tank.
- The technology reduces the complexity of the refuelling hardware and of the protocol, compared to CGH2 and CcH2. This makes the technology of choice for efficient H2 storage .



Modelling problem formulation

Assumptions 1/3

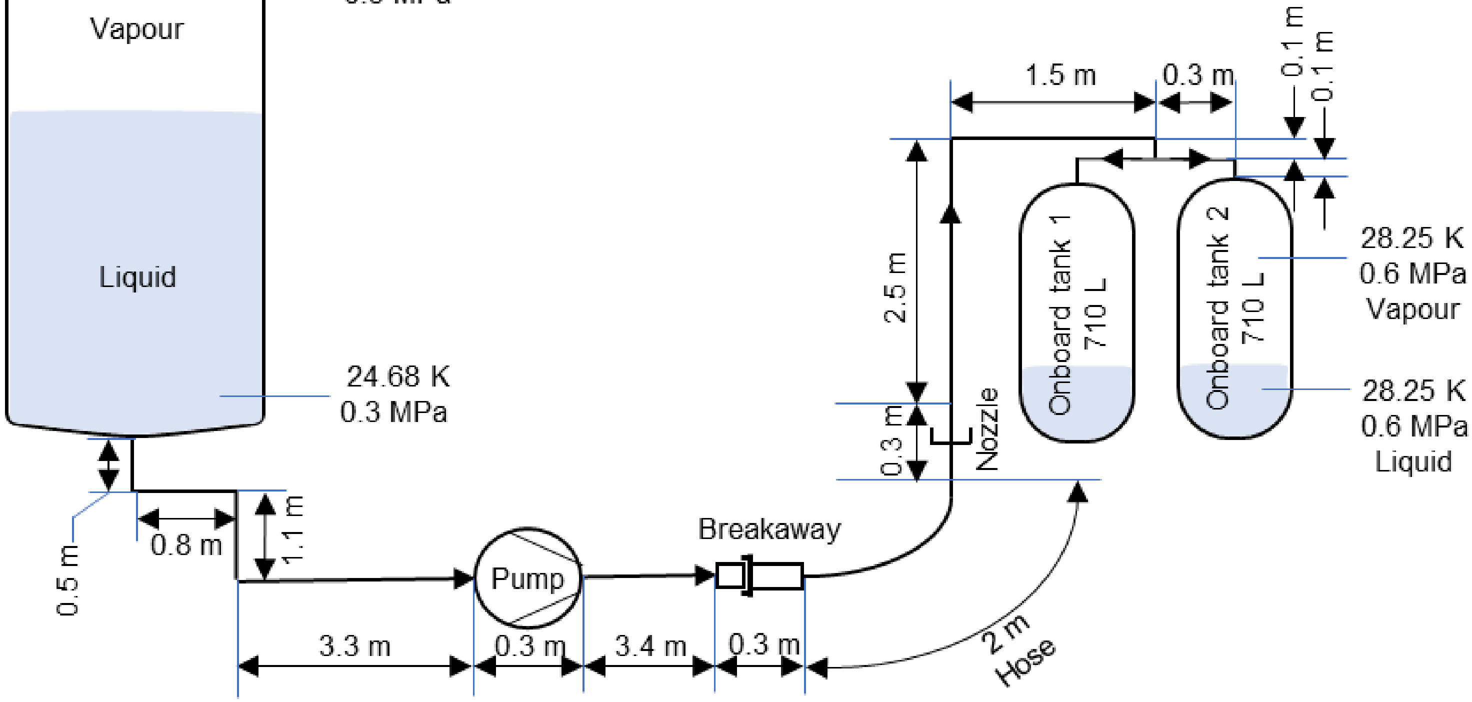
- The HRS storage tank is of 61.36 m^3 volume (4 tonnes of LH2 at 0.3 MPa abs. and saturated temperature of 24.68 K). Temperature within the HRS tank remains constant throughout the LH2 transfer process due to its large volume.
- There are two vertically installed onboard storage tanks, each of 0.71 m^3 (44 kg of LH2 at 100% SoC, 63 kg/m^3 at final pressure of 1.6 MPa and T=29 K). The internal length is 2.3 m and diameter is 0.66 m. The tanks are filled from the top. Internal walls of stainless steel of 3 mm thickness. Tanks are initially at 0.6 MPa abs. with temperature of 28.25 K (saturated temperature for 0.6 MPa abs.). The initial LH2 filling level in onboard tanks is 35% by volume.
- The value of heat flux of 1 W/m^2 is applied to all tank walls based on the review of published data.



Modelling problem formulation
Assumptions 2/3

The heat transfer rate at the breakaway is 15 W (Maus and Schäfer, 2021). Piping and instrumentation diagram (PID), equipment parameters and initial conditions:

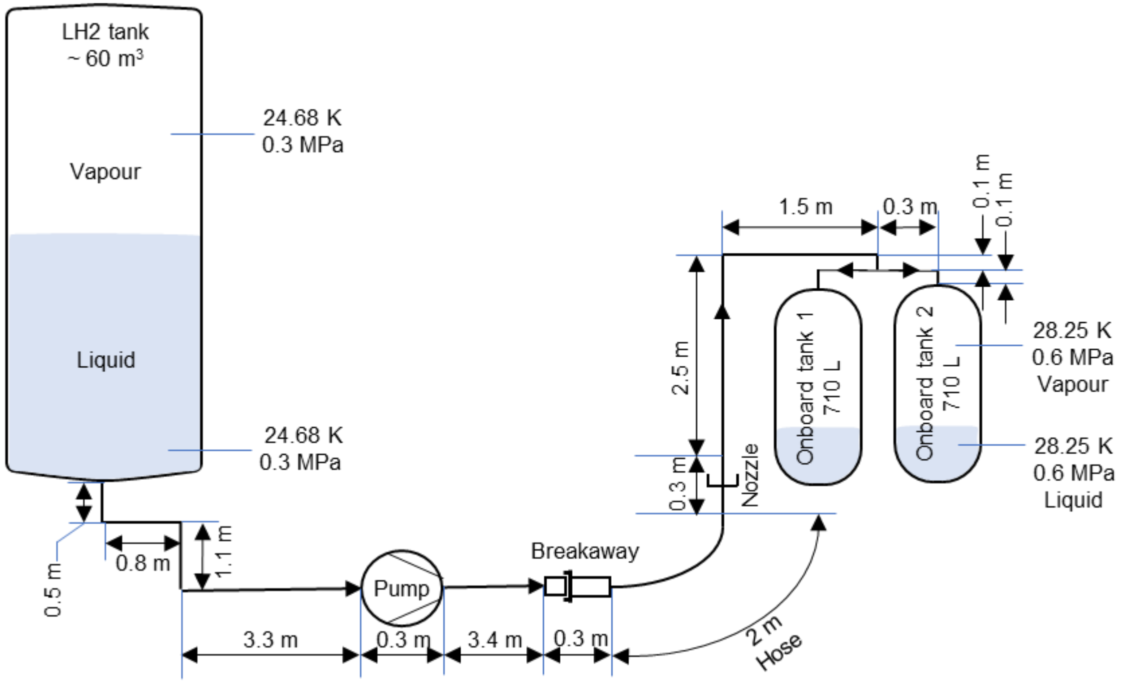
	HRS Reservoir	Pipe 1	Pump	Pipe 2	Breakaway	Hose	Nozzle	Pipes 3, 4	Tanks 1, 2
Length [m]	10	0.5/0.8/1.1/3.3	0.3	3.4	0.3	2	0.3	2.5/1.5/0.1/0.3/0.1	2.3
Diameter [m]	2.78	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.66
P_i [MPa (g)]	0.3	0.3	2.0	0.6	0.6	0.6	0.6	0.6	0.6
T_i [K]	24.68	24.68	27.01	88.0	88.0	88.0	88.0	88.0	28.25
Heat flux [W/m^2]	1.0	0.6	N/A	0.6	636.6	0.6	0.6	0.6	1.0
LH2 fraction*	N/A	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.35



Modelling problem formulation

Assumptions 3/3

- The LH2 reservoir at HRS and all components down to the pump are assumed to be filled in by LH2 at 0.3 MPa(a) and saturation temperature of 24.68 K.
- The components between the pump and the onboard tanks, i.e. nozzle, breakaway, hose, and connection pipes, are filled with gaseous hydrogen.
- The initial pressure downstream the pump is the same as in onboard storage tanks, i.e. 0.6 MPa(a). However, a higher initial temperature of piping of 88 K is assumed (higher than 28.25 K, i.e. the saturated temperature for 0.6 MPa(a), and even higher than the critical point temperature of 33.2 K above which LH2 cannot exist). This is to reflect that the pipes were pre-heated by external heat flux before the start of refuelling.



Thermodynamic model (1/4)
From the HRS reservoir to the pump exit

- Because of the complexity of the inclusion of the pump into the CFD model, the process in the pump as well as in the HRS reservoir will not be simulated by CFD.
- For the purposes of the thermodynamic modelling, the pump inlet parameters are assumed to be equal to the HRS tank's initial condition during the entire process (due to a large reservoir volume).
- The LH2 from the HRS reservoir comes to the pump to be compressed to the sLH2 state. This is possible as compression time is comparatively short, and the process is often assumed as **adiabatic**, i.e. without heat exchange with the environment (especially for the pump submerged into LH2).
- Though the process in a real pump is **polytropic**, in the present study the compressed LH2 temperature is estimated based on the pump **isentropic efficiency definition** (the **isentropic process is the ideal reversible adiabatic** process with no heat transfer between the pump or environment).

Thermodynamic model (2/4)
Pump efficiency

- The isentropic efficiency of a pump is defined as the ratio of the work required to increase the fluid pressure up to a specified value in an isentropic process to the actual required work input: $\eta_c = w_s / w_a$.
- Assuming negligible change in kinetic and potential energies, the work input for an adiabatic process would be equal to the change in enthalpy (Cengel, 2004):

$$\eta_c \cong \frac{h_{2s} - h_1}{h_{2a} - h_1}$$

  where h_{2a} and h_{2s} are the enthalpies at the pump exit state in an actual and isentropic compression, and h_1 is the LH2 enthalpy of incoming to the pump flow.
- Based on the conceptual refuelling protocol (Pizzutilo et al., 2022-2024), the hydrogen temperature at the dispenser (few meters from the onboard tank) should be in the corridor of 23.9-26.5 K.

Thermodynamic model (3/4)

Pump exit conditions

- The efficiency of LH2 pumps is 55-80% (Franco and Giovannini, 2024).
- Using the NIST real gas model and assuming the pump's efficiency of 65%, the LH2 temperature at the pump exit may be estimated as follows.
- For upstream of the pump pressure 0.3 MPa(a) and saturation temperature of 24.68 K, and the maximum pump pressure of 2.0 MPa(a), the temperature at the *pump exit* is calculated as 26.98 K.
- The **expansion** of pump compressed LH2 in the downstream pipes, which are initially at 0.6 MPa(a), is assumed to be **adiabatic** due to the rapid nature of the process and the pipe insulation. The calculations show that the LH2 temperature after the expansion is **25.98 K**, i.e. within the recommended hydrogen temperature corridor of 23.9-26.5 K.

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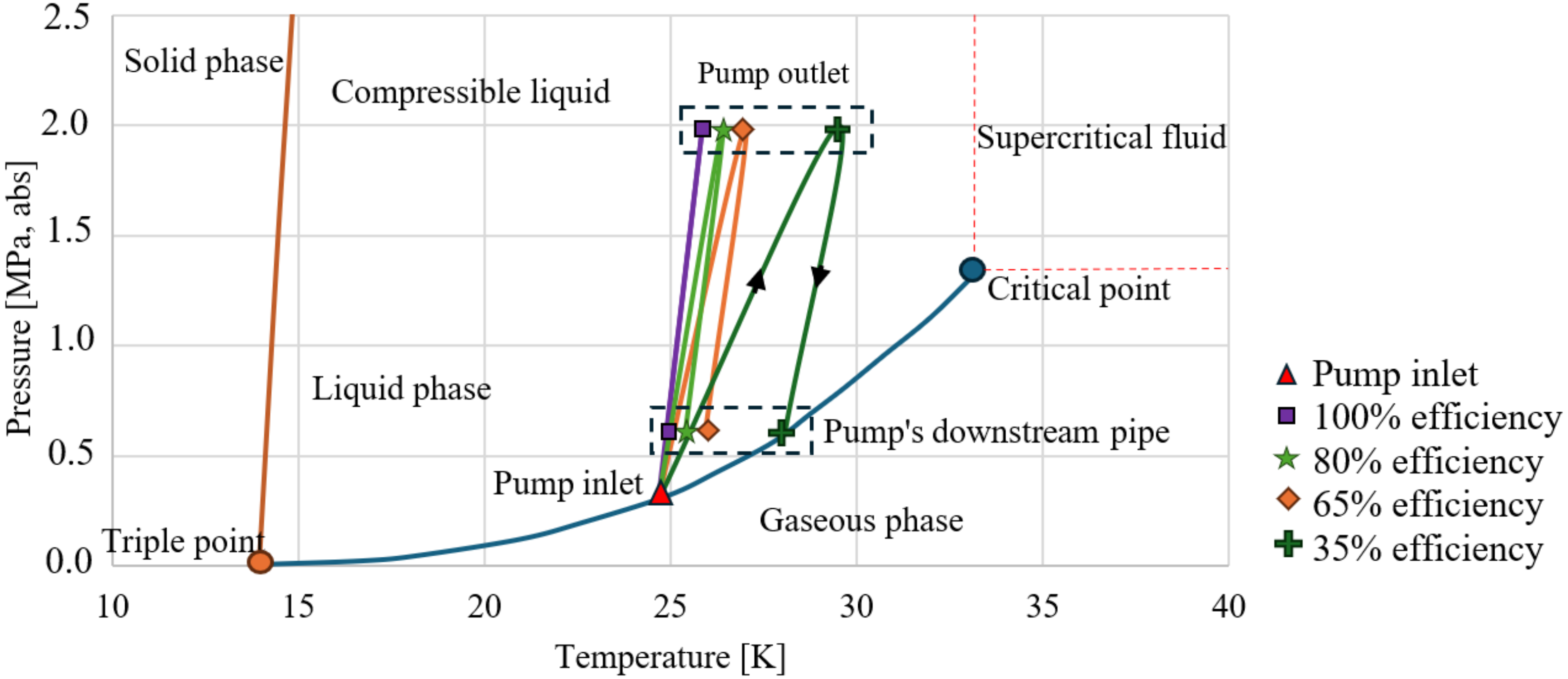
Thermodynamic model (4/4)

The phase diagram for hydrogen: pumps of different efficiency

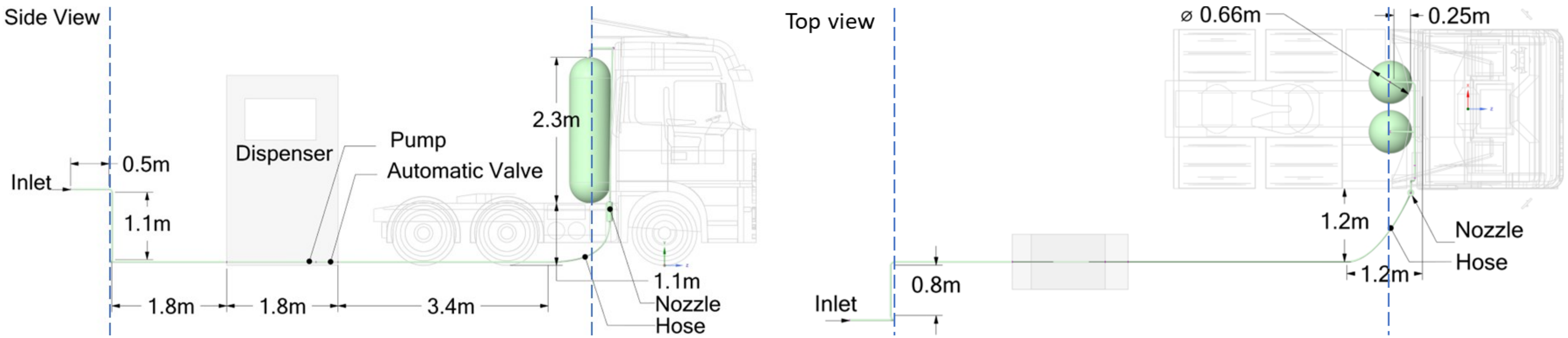
- LH2 is compressed from saturated condition in the HRS tank to maximum pump pressure 2.0 MPa(a), then expands to the pipe space at pressure 0.6 MPa(a).
- LH2 temperature increases after expansion in the downstream pipe space as the pump efficiency decreases. For 100%, 80%, 65% efficiency pumps, the LH2 in the pipe downstream of the pump is at a sub-cooled state (sLH2), i.e. above the saturated state curve.
- For 35% efficiency pump, LH2 temperature after expansion in the pipe reaches the saturated temperature of 28.25 K for 0.6 MPa(a), which is above the recommended LH2 temperature corridor.



CFD model

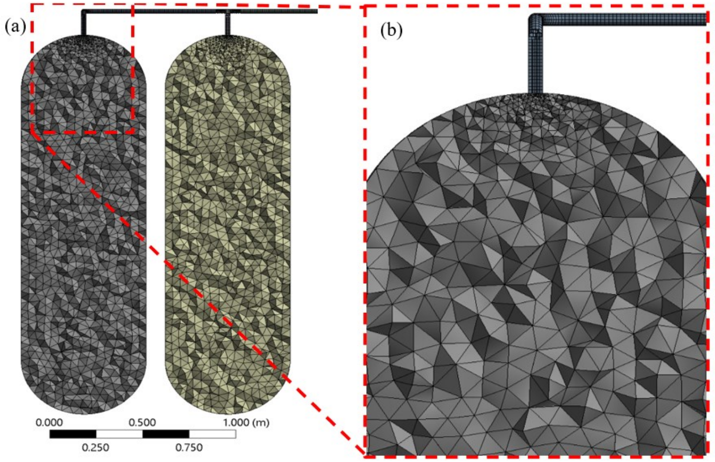
Geometry and calculation domain

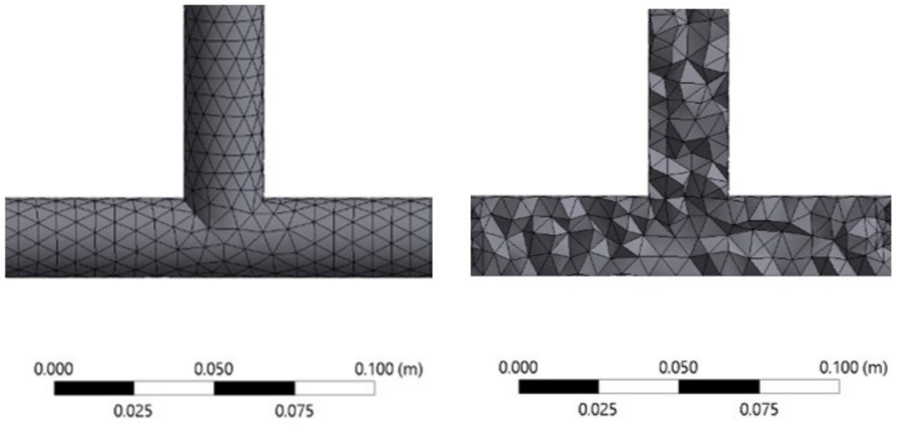
The calculation domain for CFD simulations was from the pump exit through equipment to the onboard storage tanks (hydrogen filled components are highlighted by green).



CFD model
Mesh

- Tetrahedral CVs are used to discretise the onboard tanks and the three-way manifold. Hexahedral CVs are used in pipes. The transition from tetrahedral to hexahedral mesh is by pyramidal CVs. The mesh is produced by ANSYS Mesher.
- The entire computational domain is meshed using 239,111 CVs with a minimum orthogonal quality of 0.5 (average 0.85). The minimum and maximum CV sizes in the onboard tanks are 0.5 cm and 5 cm respectively (growth rate is 1.2).
- Onboard tanks mesh (left), surface and central cross-section meshes of three-way manifold (right):





CFD model
Numerical details

- ANSYS Fluent 2023R1 is used as a CFD engine.
- The volume of fluid (VOF) model is applied to simulate the two-phase liquid-gas flow.
- Governing equations: continuity for volume fraction, shared momentum, shared energy.
- The SST k-omega turbulence model (recommended for VOF multi-fluid applications).
- The pressure-based implicit solver. The SIMPLEC algorithm for pressure-velocity coupling. Convective terms and volume fractions were discretised using a second-order upwind numerical scheme. The PRESTO discretization scheme is utilised for pressure discretisation.
- The time step was initially set as 0.001 s, and then gradually increased to 0.01 s to maintain the acceptable convergence of the simulations. The mass imbalance over the entire fuelling period is less than 1%, which is considered an indicator of good convergence and hydrogen conservation in the calculation domain.
- The simulation of 525 s of LH2 refuelling time takes about 14 days on a 72-core CPU node of Kelvin-2 (high-performance computing facilities in Northern Ireland).

CFD model

Numerical details: phase change model

- Lee's model (1980) is used to simulate evaporation and condensation.
- The explicit formulation for volume fraction in the multi-phase model is used while having a **"sharp interface" option** between the liquid and vapour phases.
- For condensation, when the saturation temperature is higher than the gas temperature ($T_{sat} > T_g$) the mass transfer rate from gas to liquid [kg/m^3/s] is:

$$\dot{m}_c = r_c \alpha_g \rho_g \frac{T_{sat} - T_g}{T_{sat}},$$

and for evaporation ($T_l > T_{sat}$) the mass transfer rate from liquid to gas is:

$$\dot{m}_e = r_e \alpha_l \rho_l \frac{T_l - T_{sat}}{T_{sat}},$$

where r_c and r_e are Lee's model coefficients (1/s). Lee's coefficient of **0.05** is selected, following Ulster's previous work on the pressure recovery phenomenon in the large-scale LH2 storage tank (Kangwanpongpan et al., 2023).

CFD model
Initial and boundary conditions

- Initial conditions are presented in Table.

	HRS Reservoir	Pipe 1	Pump	Pipe 2	Breakaway	Hose	Nozzle	Pipes 3, 4	Tanks 1, 2
Length [m]	10	0.5/0.8/1.1/3.3	0.3	3.4	0.3	2	0.3	2.5/1.5/0.1/0.3/0.1	2.3
Diameter [m]	2.78	0.025	0.025	0.025	0.025	0.025	0.025	0.025	0.66
P_i [MPa (g)]	0.3	0.3	2.0	0.6	0.6	0.6	0.6	0.6	0.6
T_i [K]	24.68	24.68	27.01	88.0	88.0	88.0	88.0	88.0	28.25
Heat flux [W/m^2]	1.0	0.6	N/A	0.6	636.6	0.6	0.6	0.6	1.0
LH2 fraction*	N/A	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.35

- The temperature in the onboard tanks is saturation temperature at 0.6 MPa(a), i.e. 28.25 K. The LH2 volume fraction in the pipes downstream of the pump is 0 (the pipes are warmed to 88 K i.e. above the critical temperature of 33.2 K for liquid phase existence). The heat fluxes at the pipe walls were used as thermal boundary conditions and presented in the Table. The values are typical for the LH2 tanks with multi-layer insulation and vacuumed space between inner and outer walls, e.g. 1-2 W/m^2 reported elsewhere, e.g. (Ahluwalia et al., 2023).

CFD model

Modelling of “pressure control valve” (PCV)

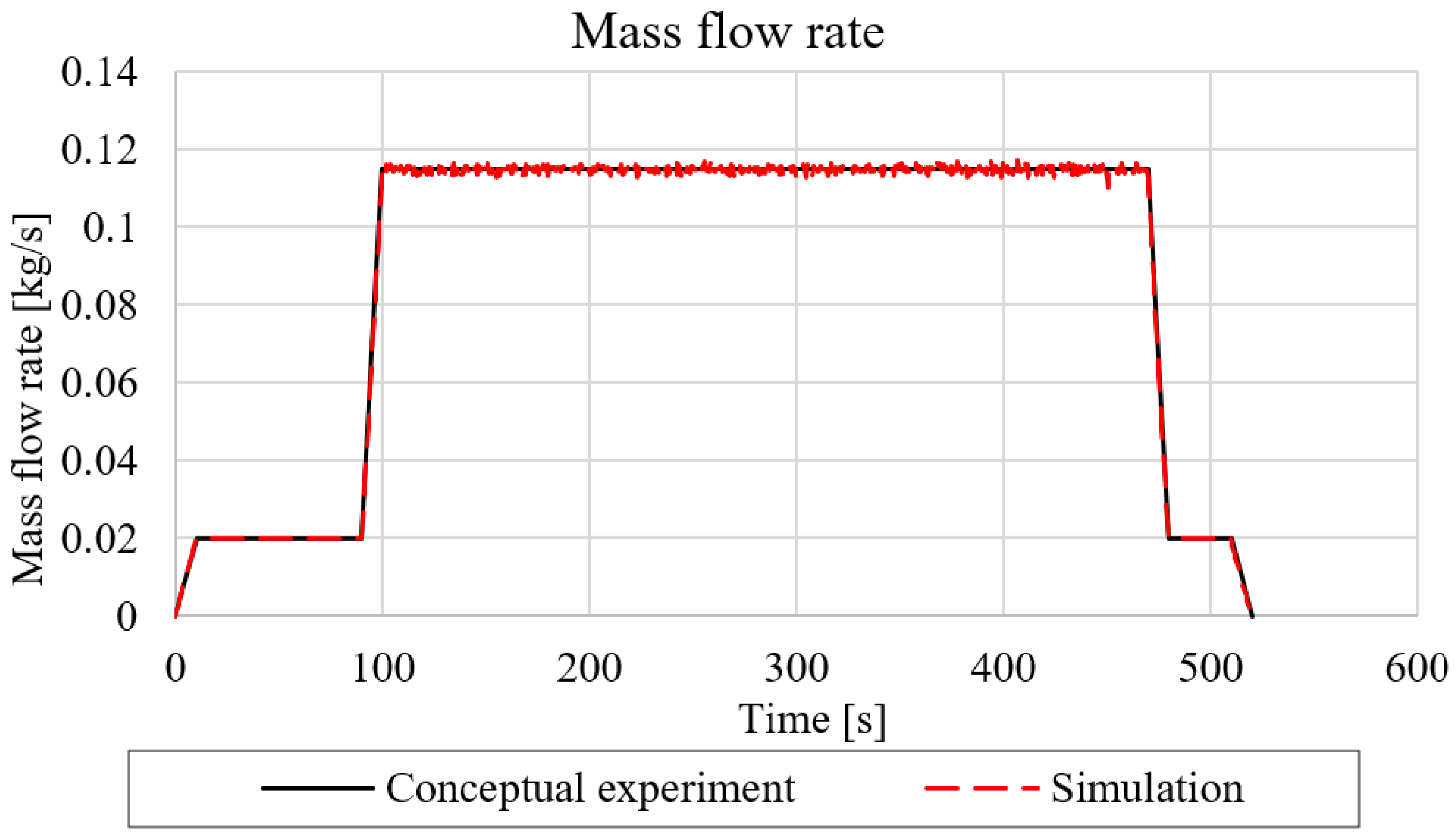
- The automatic PCV is represented as a porous media and the mass flow rate (MFR) as per the conceptual fuelling protocol is achieved by varying the porosity.
- This model introduces a sink into the momentum equations. The sink term includes two parts: a viscous (Darcy) loss term and an inertial loss term:

$$S_i = -\left(\frac{\mu}{\alpha} u_i + C_2 \frac{1}{2} \rho |u| u_i\right),$$

  where μ is the laminar viscosity, α is the viscous resistance, u is the velocity, ρ is the density, and C_2 is the inertial resistance. The coefficients α and C_2 in this sink term provide the control of MFR during simulations based on its prescribed value. α and C_2 are introduced using the UDF. The UDF is programmed to compute simulated MFR through the automatic valve and compare its value with the prescribed MFR to manipulate the porous media coefficients.
- The heat transfer in the PCV is disabled, allowing the porous model to function at enthalpy conservation, like a real throttling valve (Ebne-Abbasi et al., 2022).

Results of CFD simulations
Mass flow rate (MFR)

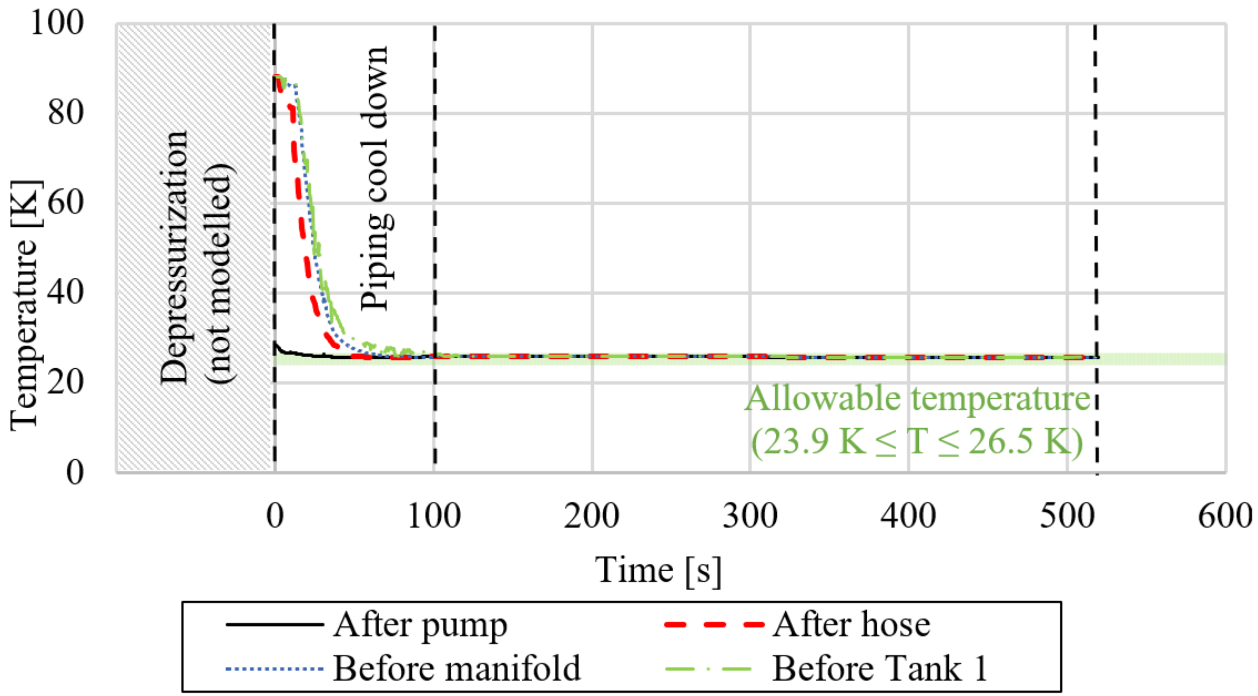
- The MFR in the conceptual refuelling protocol is digitised and used as an input to the UDF to regulate the porosity in the PCV.
- The simulated MFR deviates from conceptual MFR by less than 0.1%.
- This UDF can reproduce arbitrary MFR profile as required.



Results of CFD simulations

Temperature at locations of refuelling pathway in time

- The maximum pump pressure is 2.0 MPa(a). Temperature of sLH2 after expansion in the pipe, is calculated by the thermodynamic model as 25.98 K.
- This temperature is used as the inlet temperature for PCV in the CFD model. The simulated temperature after the PCV is shown by solid black line. The pipes, initially at 88 K, begin to cool down to the temperature of sLH2 of 25.9 K within the first 100 s. The temperature at different points of the refuelling pathway decreases from an initial 88 K to the acceptable range of 23.9-26.5 K during the main refuelling stage.



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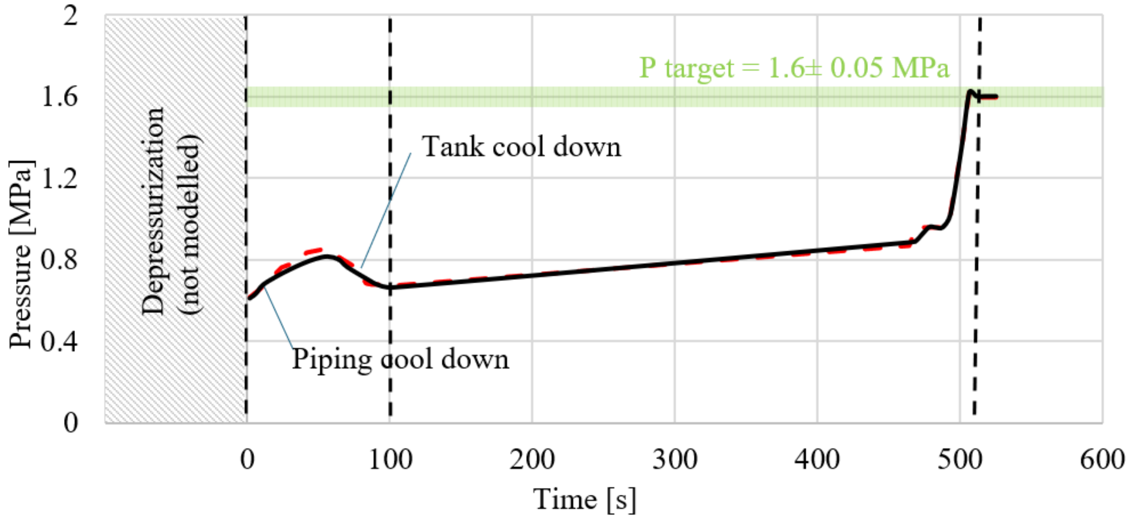
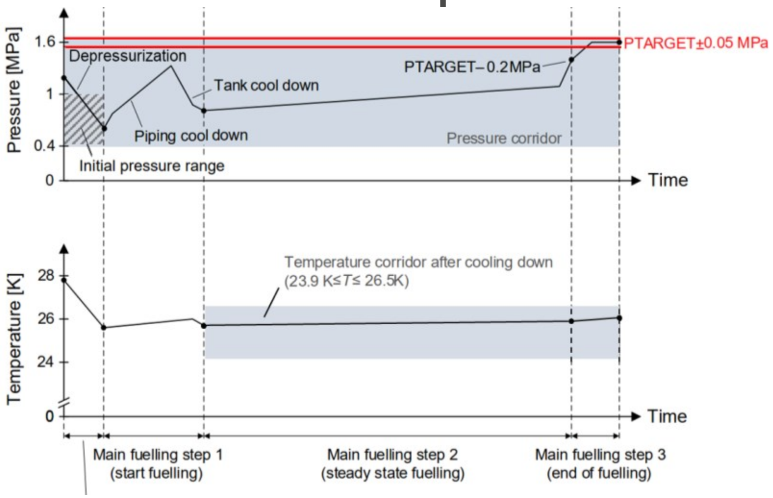
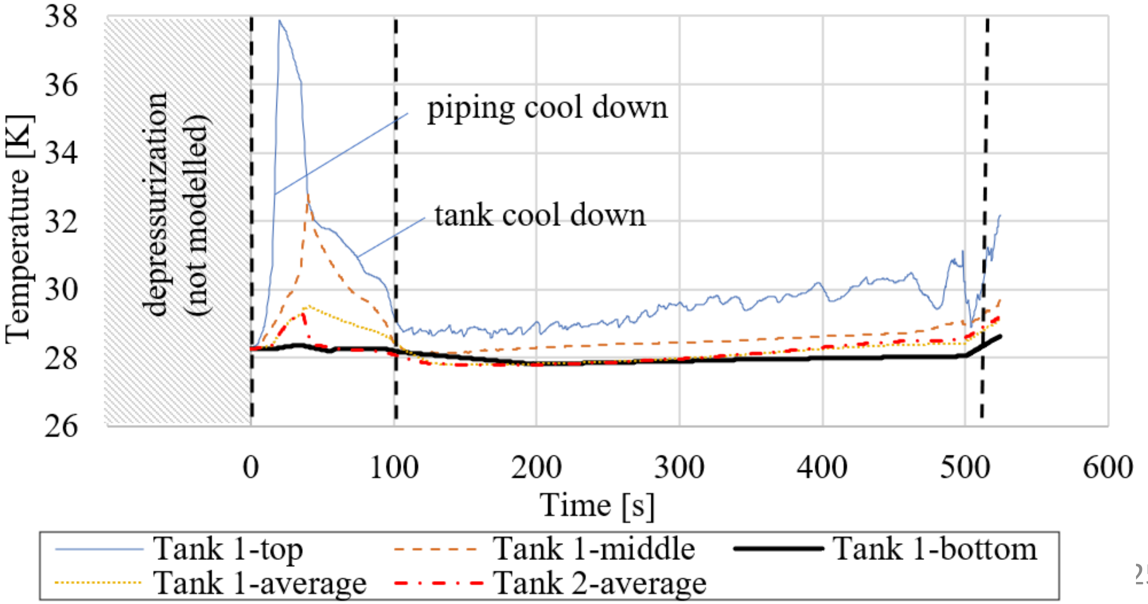
Results of CFD simulations

Onboard tank pressure and temperature dynamics

- The initial pressure in both onboard storage tanks is 0.6 MPa(a). The difference in pressure between two tanks is minimal.
- Temperature in the ullage space is, as expected, somewhat higher.
- LH2 temperature is decreasing at some moments due to evaporation.







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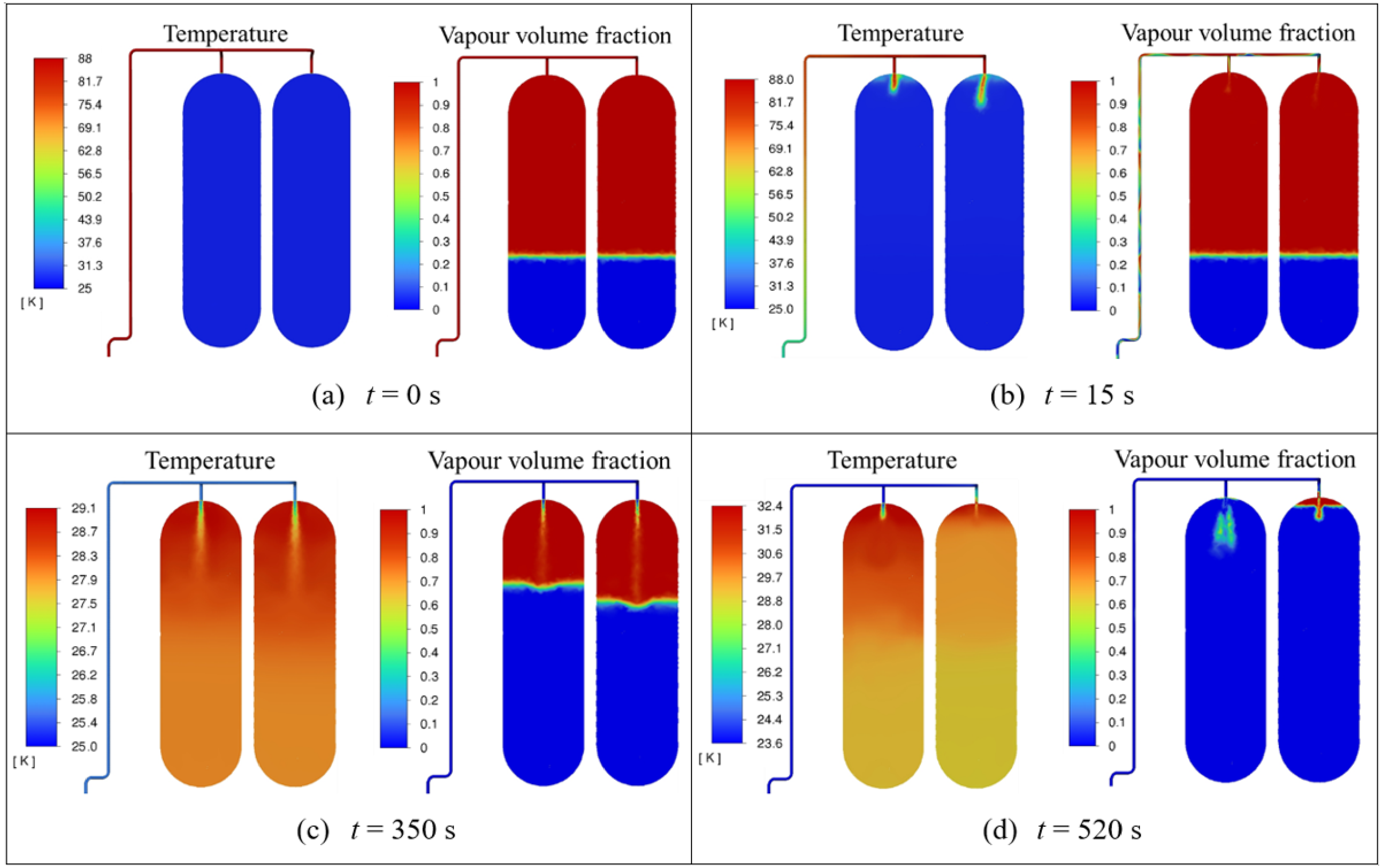
Results of CFD simulations

Temperature and vapour volume fraction in time (cross-section)



Conclusions

- The ***originality*** of this work is in the **development for the first time** of the novel modelling approach for LH2 refuelling through the entire equipment of HRS. This includes a thermodynamic model for equipment from the HRS reservoir to the pump exit, and a contemporary 3D two-phase CFD model from the pump exit to the onboard storage tanks. The concept of efficient refuelling to SoC=100% using sLH2 is verified through the insights provided by the thermodynamic model and the results of CFD simulations.
- The ***significance*** of this study lies in the creation of the model that can serve as a **contemporary engineering tool** for the design of efficient and inherently safer (1) LH2 refuelling station equipment and (2) refuelling protocols. This study provides valuable insights into the underlying physical phenomena of heat and mass transfer during LH2 refuelling at HRS, enhancing our understanding and even visualisation of the process by means of CFD.
- The ***rigour*** of this work is in the verification of the CFD simulations against a conceptual LH2 refuelling protocol published elsewhere.

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