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CFD modelling of start-up fuelling phase accounting for all hydrogen refuelling station components

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Hydrogen fuelling
Challenges

- Onboard storage pressure in the range 35-70 MPa.
- Fuelling time 3-4 minutes from 2 to 70 MPa.
- Temperature increase due to compression, Joule-Thomson effect, etc.
- Safety limits for fuelling to preserve tank integrity (UN GTR#13):
    - Hydrogen temperature ≤85°C;
    - Maximum pressure 125% of the nominal working pressure (NWP);
    - SoC ≤ 100%.
- Only LDV fuelling protocols (SAE J2601) are available for ≤10 kg (NWP=70 MPa).
- No protocol for HDV – only high-level safety requirements (SAE J2601/2).
- Understanding of underlying phenomena is needed to develop fuelling protocols.
- Validated modelling tools are needed for entire equipment of hydrogen refuelling station (HRS) not only onboard storage tanks.

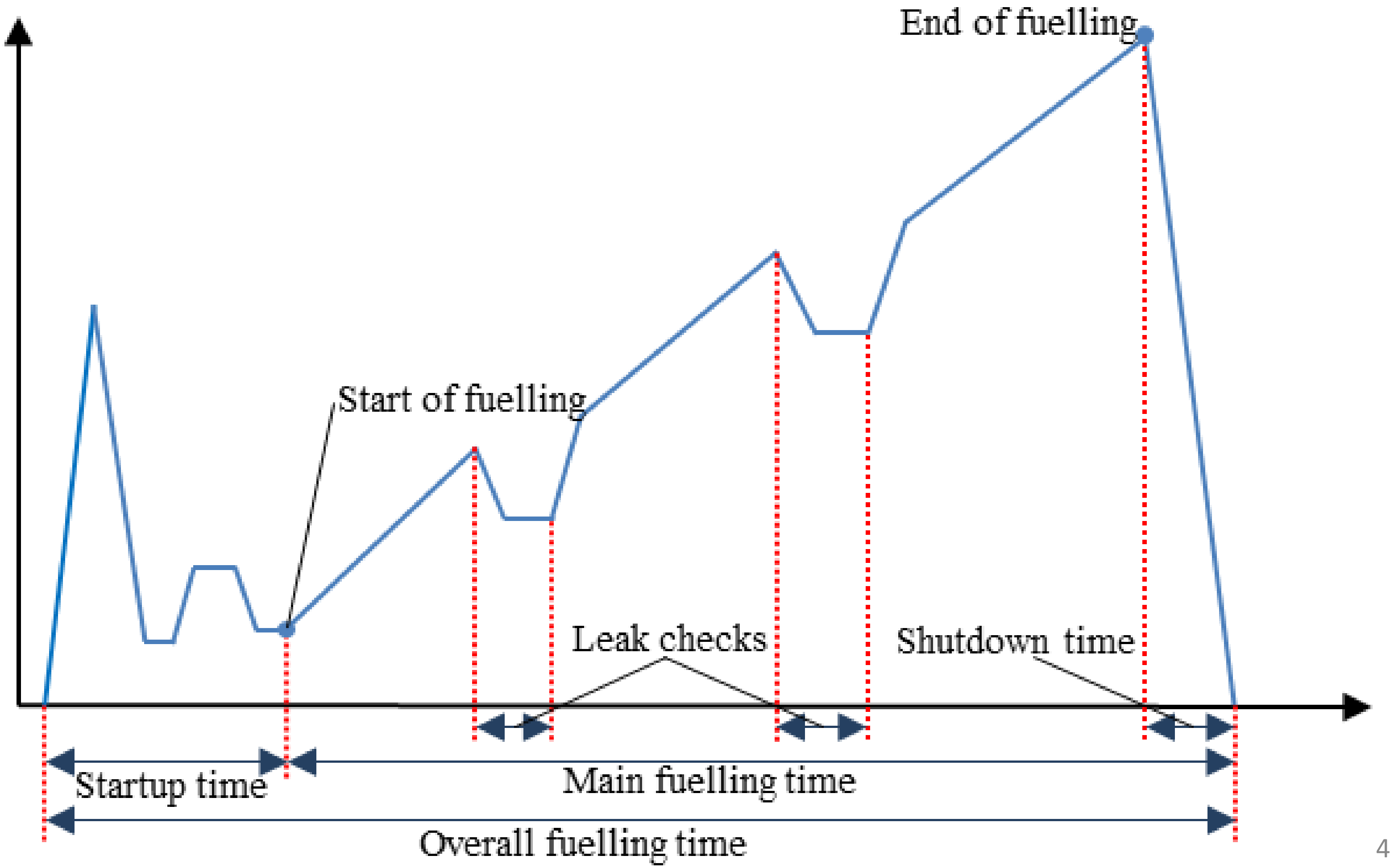
Hydrogen fuelling
Modelling

- Current thermodynamic / 0D models:
  - Fast, may include the entire HRS
  - Only average hydrogen pressure and temperature in the HRS and FCEV components
  - Not capable to predict temperature non-uniformity, e.g. in conformable tanks
  - Limited availability of model validation description
  - Examples of modelling tools: H2FillS (NREL), H2-Fill (Wenger Engineering), SOFIL (Air Liquide), Hyfill (Engie)
- Current CFD models:
  - Simulate distribution of parameters in hydrogen storage tanks
  - Comparatively long simulation time, even limited to onboard storage tank only
  - Examples: Melideo et al. (2015), Charolais et al. (2021), Carrere et al. (2021), etc.
  - No CFD models for entire equipment of HRS

Hydrogen fuelling

Start-up phase

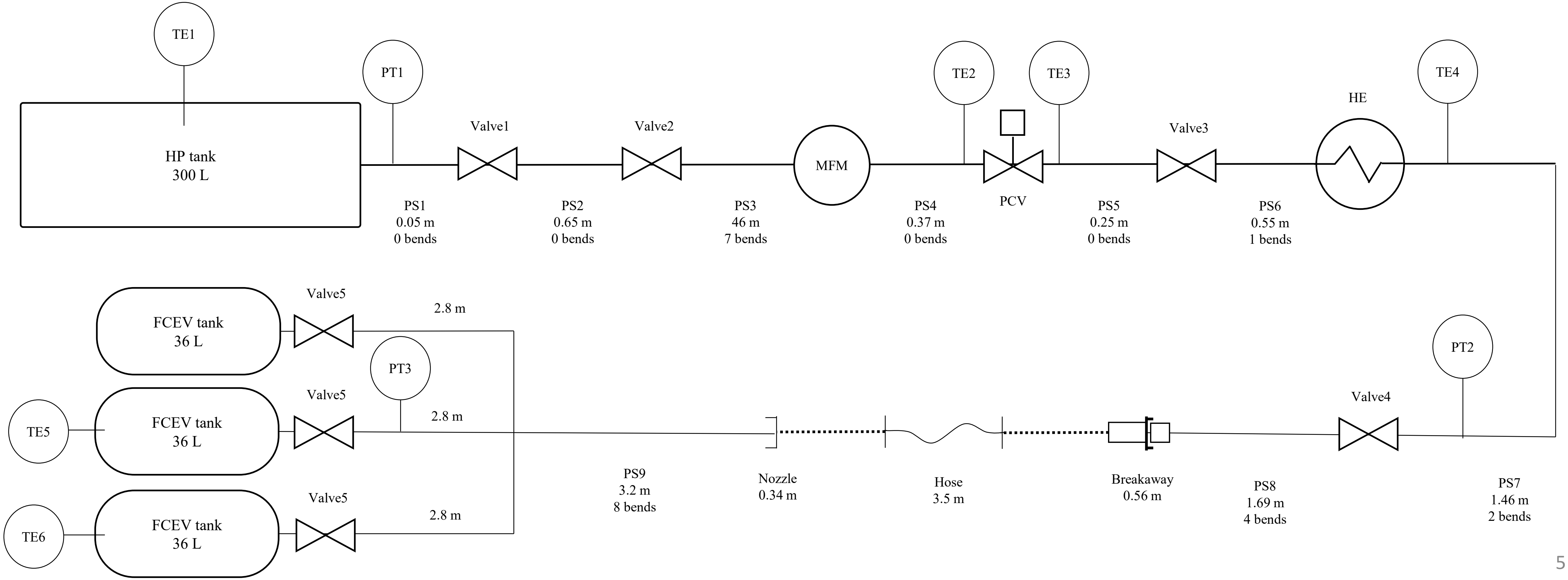
- The start-up phase begins after the user initiates fuelling (SAE J2601).
- Can include a connection pulse, leak check, etc.
- Measures any decrease of pressure in the fuelling line.
- Determines if it is safe to start fuelling or not.



Validation experiment

NREL (Kuroki et al., 2021)

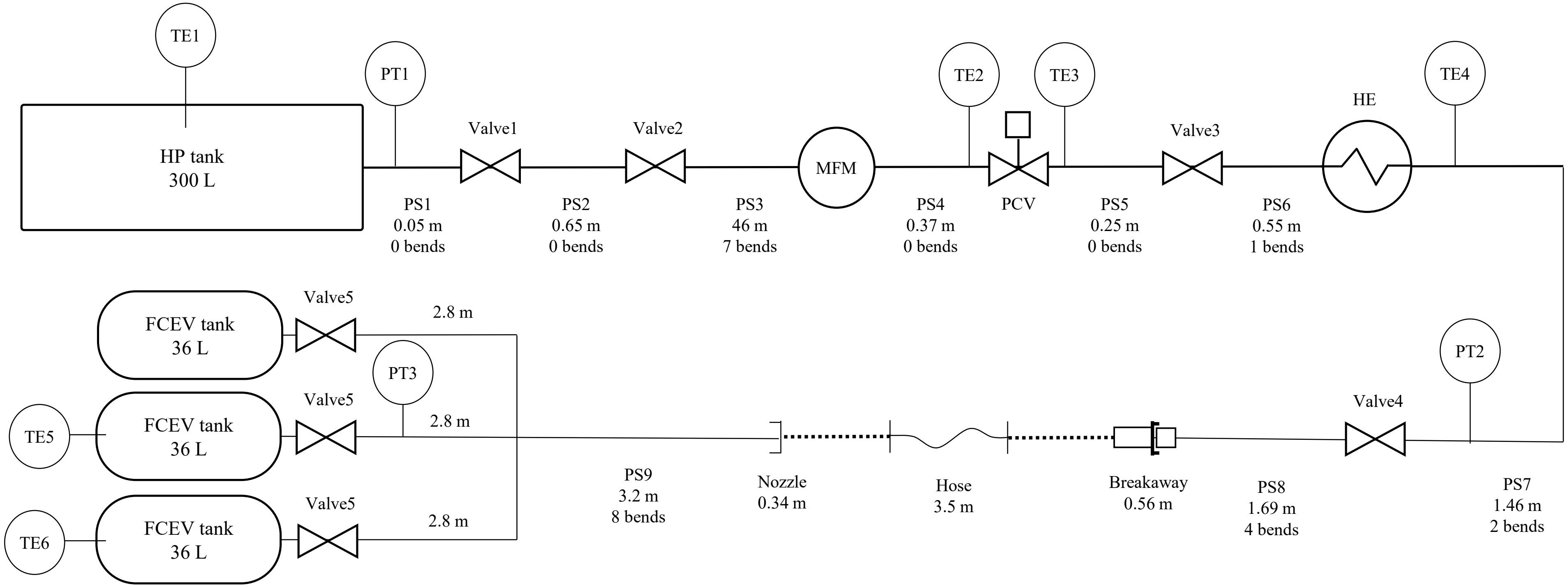
HRS and FCEV components: 6x300 L high-pressure (HP) tanks, Pressure Control Valve (PCV), Precooler heat exchanger (HE), Breakaway, Nozzle, Hose, Pipes, 3x36 L onboard tanks, etc.



Validation experiment

Initial conditions

- High pressure (HP) tank: 17.5°C, 880 bar
- FCEV onboard tank: 23°C, 60 bar
- Ambient temperature: 23°C
- Average Pressure Ramp Rate (APRR) 19.8 MPa/min



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CFD model
Equations

- 3D conservation equations: mass, momentum, energy
- Standard k−ε model, NIST real gas EoS
- Boundary conditions:
  - Non-slip, impermeable walls
  - 3rd kind boundary condition for energy equation, h=7 $W/m^2/K$
  - Ambient temperature 23°C
- Numerical details:
  - 3D conduction in tank and pipes (ANSYS Fluent “Shell conduction” functionality)
  - Pressure-velocity coupling: SIMPLE algorithm
  - First-order upwind numerical scheme for convective terms

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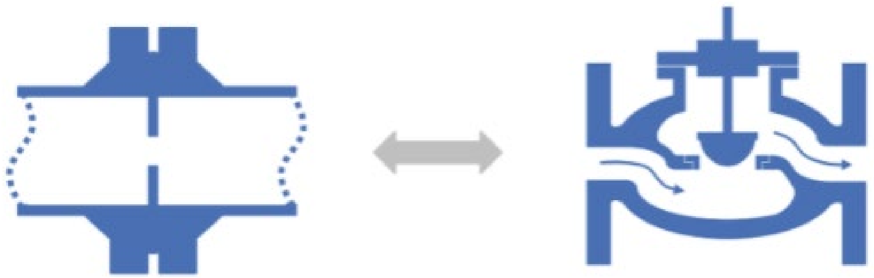
CFD model

Calculation domain 1/2

- 2x300 L HP tanks: L/D=1.062/0.6 m (cascade mode)
- 3x36 L FCEV tank: L/D=2.2x0.25 m
- Overall piping length: 63 m
- Valves length: 0.1 m,
- Valves ID calculated based on Cv



	Valve1	Valve2	MFM	PCV	Valve3	Cooling system	Valve4	Breakaway	Nozzle	Valve5
Flow coefficient (Cv value)	1.3	0.75	1.00	1.0	0.75	1.00	0.75	1.00	1.0	1.0

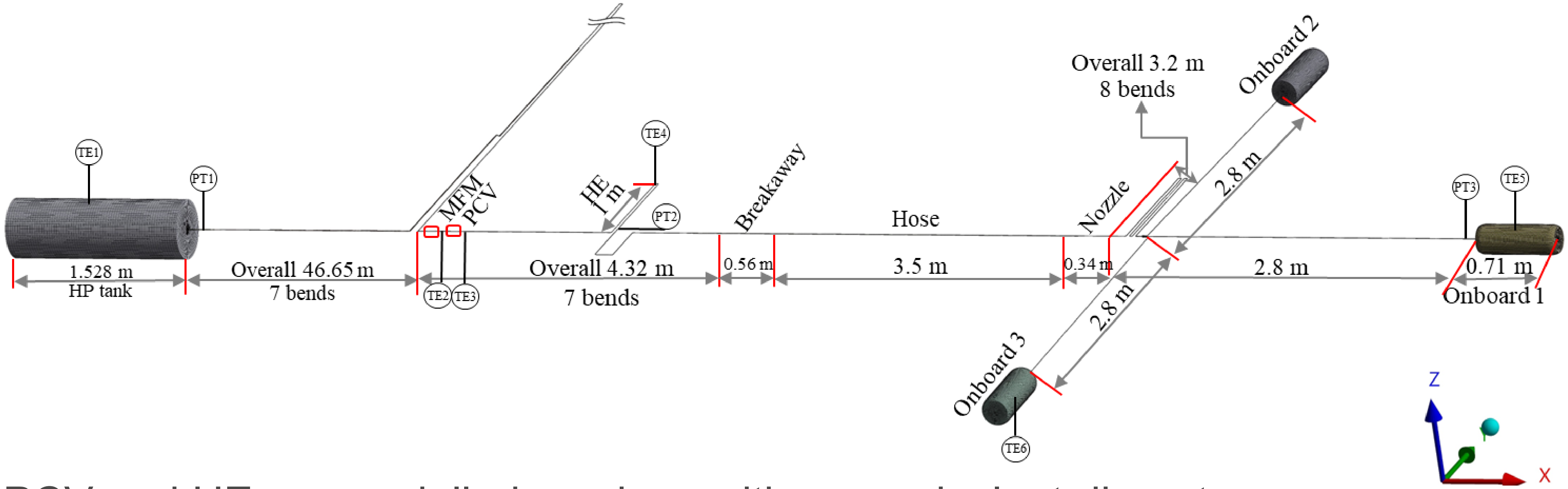
Ref.: Kuroki T. , Nagasawa K., Peters M., et al. (2021). Thermodynamic modeling of hydrogen fueling process from high-pressure storage tank to vehicle tank, IJHE, 46, pp. 22004–22017.

	L [m]	ID [m]	OD [m]	ρ [kg/m³]	c [J/(kg·K)]	λ [W/(m·K)]	Number of bends
Piping section 1							
Piping 1 (9/16")	5.3×10^{-2}	7.9×10^{-3}	14.3×10^{-3}	7900	659	16.7	0
Piping section 2							
Piping 2 (9/16")	17.0×10^{-2}	7.9×10^{-3}	14.3×10^{-3}	7900	659	16.7	0
Piping 3 (3/8")	47.6×10^{-2}	5.1×10^{-3}	9.5×10^{-3}	7900	659	16.7	0
Piping section 3							
Piping 4 (9/16")	384.3×10^{-2}	7.9×10^{-3}	14.3×10^{-3}	7900	659	16.7	0
Piping 5 (3/8")	4021.5×10^{-2}	5.1×10^{-3}	9.5×10^{-3}	7900	659	16.7	0
Piping 6 (5 tee fittings for 9/16")	34.0×10^{-2}	7.9×10^{-3}	31.6×10^{-3}	7900	659	16.7	5
Piping 7 (2 tee fittings for 3/8")	10.0×10^{-2}	5.1×10^{-3}	25.8×10^{-3}	7900	659	16.7	2
Piping section 4							
Piping 8 (3/8")	37.0×10^{-2}	5.1×10^{-3}	9.5×10^{-3}	7900	659	16.7	0
Piping section 5							
Piping 9 (3/8")	25.0×10^{-2}	5.1×10^{-3}	9.5×10^{-3}	7900	659	16.7	0
Piping section 6							
Piping 10 (3/8")	50.0×10^{-2}	5.1×10^{-3}	9.5×10^{-3}	7900	659	16.7	0
Piping 11 (1 tee fitting for 3/8")	5.0×10^{-2}	5.1×10^{-3}	25.8×10^{-3}	7900	659	16.7	1
Piping section 7							
Piping 12 (3/8")	106.0×10^{-2}	5.1×10^{-3}	9.5×10^{-3}	7900	659	16.7	0
Piping 13 (2 tee fittings for 3/8")	20.0×10^{-2}	5.1×10^{-3}	25.8×10^{-3}	7900	659	16.7	2
Piping section 8							
Piping 14 (3/8")	89.0×10^{-2}	5.1×10^{-3}	9.5×10^{-3}	7900	659	16.7	0
Piping 15 (4 tee fittings for 3/8")	20.0×10^{-2}	5.1×10^{-3}	25.8×10^{-3}	7900	659	16.7	4
Piping section 9							
Piping 16 (3/8")	280.0×10^{-2}	5.1×10^{-3}	9.5×10^{-3}	7900	659	16.7	0
Piping 17 (8 tee fittings for 3/8")	40.0×10^{-2}	5.1×10^{-3}	25.8×10^{-3}	7900	659	16.7	8
Other components							
Breakaway	56.0×10^{-2}	4.0×10^{-3}	24.9×10^{-3}	7900	659	5.0	0
Hose	350.0×10^{-2}	6.3×10^{-3}	12.6×10^{-3}	3694	558	1.5	0
Nozzle	34.2×10^{-2}	4.0×10^{-3}	27.6×10^{-3}	7900	659	5.0	0

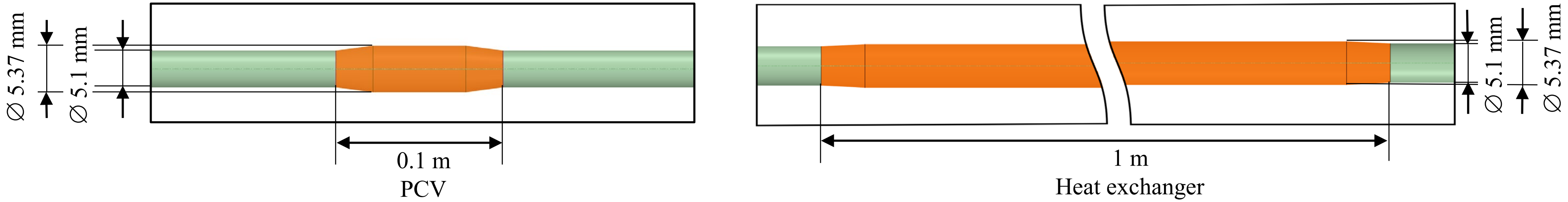
CFD model

Calculation domain 2/2

Entire equipment of HRS and FCEV storage tanks:



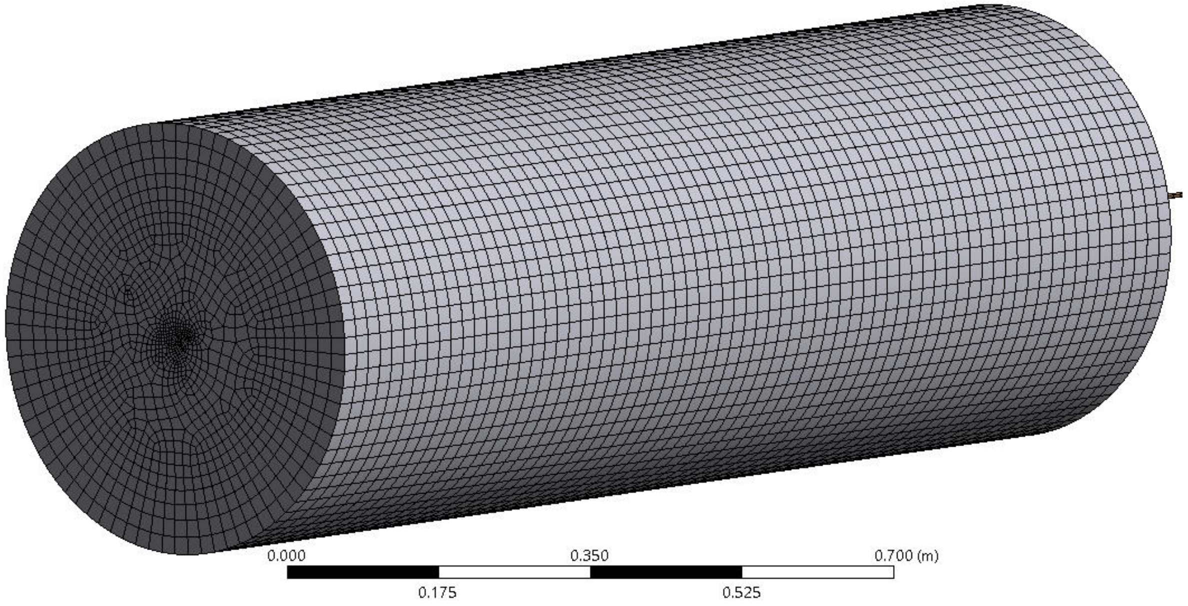
PCV and HE are modelled as pipes with an equivalent diameter:



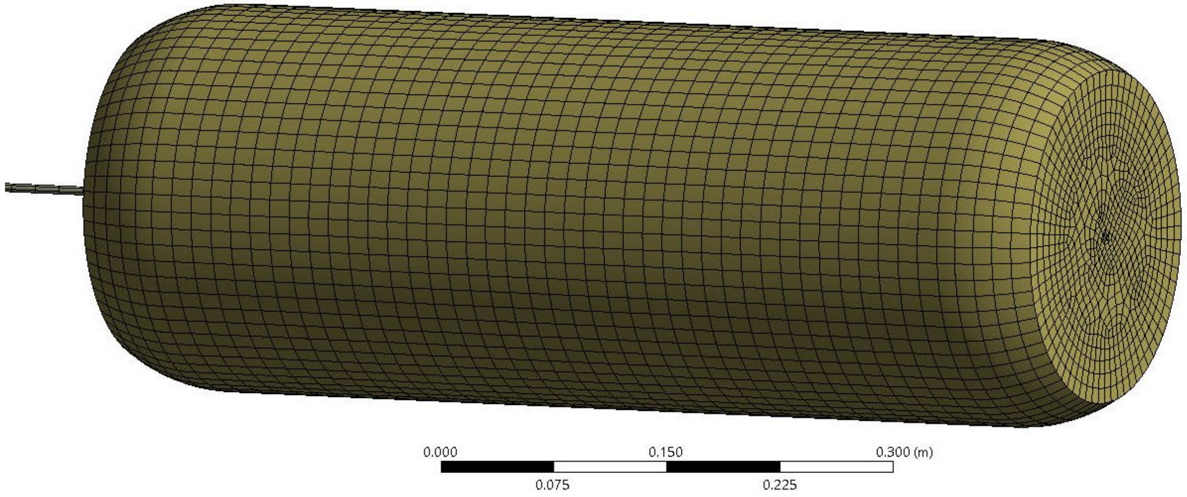
CFD model
Mesh

- Hexahedral mesh: 207,252 CVs.
- Minimum CV size: 3 mm (close to the centreline of the tanks).
- CV growth rate: 1.1 (towards the peripheral of the tanks).
- Mesh quality: 0.7 (min orthogonal quality).

HP tank at HRS



FCEV onboard tank.



CFD model

Modelling of PCV and HE

The pressure control valve (PCV) and heat exchanger (HE) are modelled using in-house algorithms.

PCV:

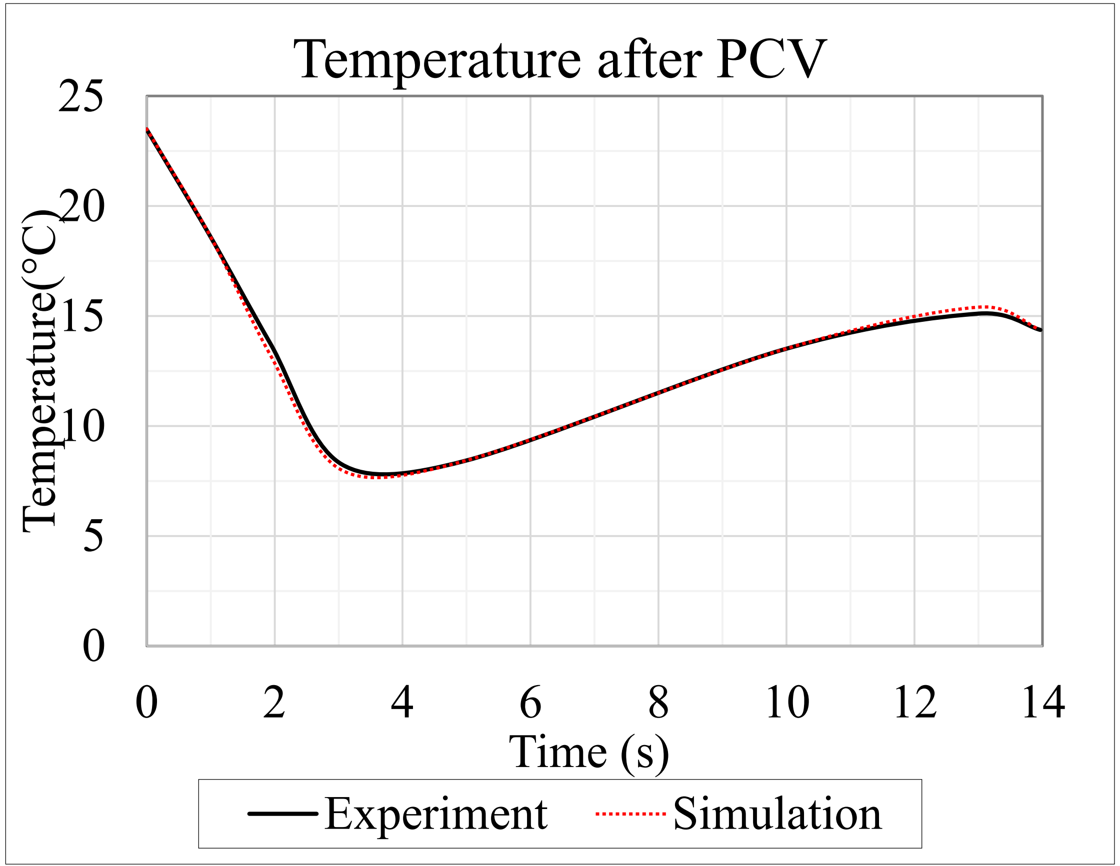
- Velocity in PCV is changed dynamically to match the experimental mass flow rate
- The algorithm uses the "*fixing the value*" Fluent capability (programmed using UDF C++ code)

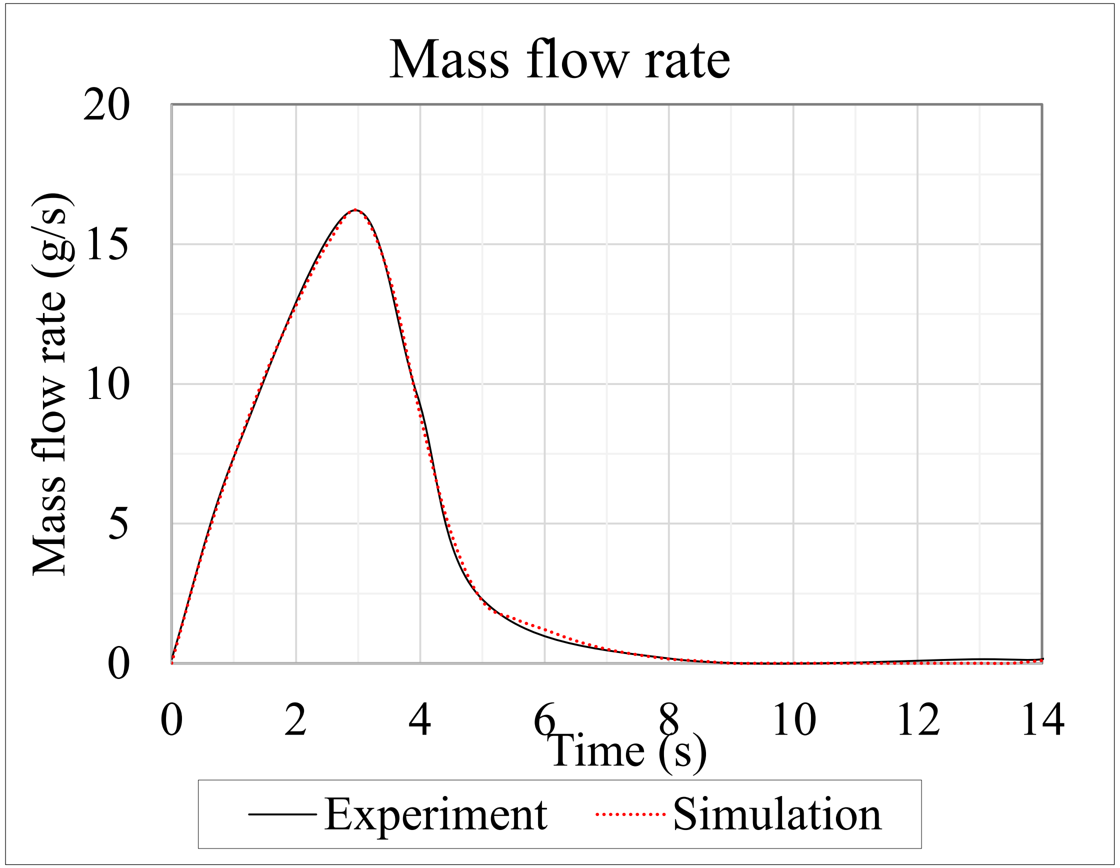
HE:

- HE is modelled using its experimentally measured equivalent length and diameter
- Temperature control follows experimentally measured temperature dynamics at HE outlet
- Temperature control relies on the "*fixing the value*" function of Fluent (programmed using UDF C++ code)

Simulations

Temperature at HE and mass flow rate at PCV (inputs)

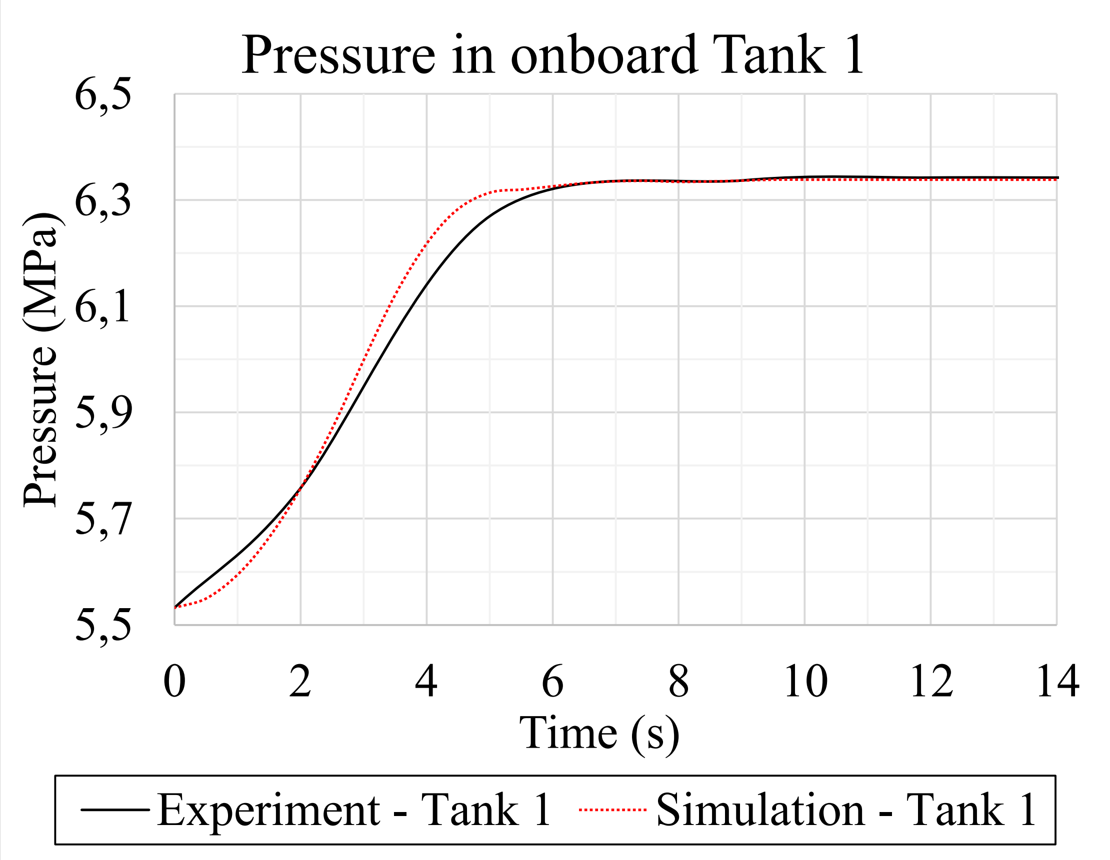


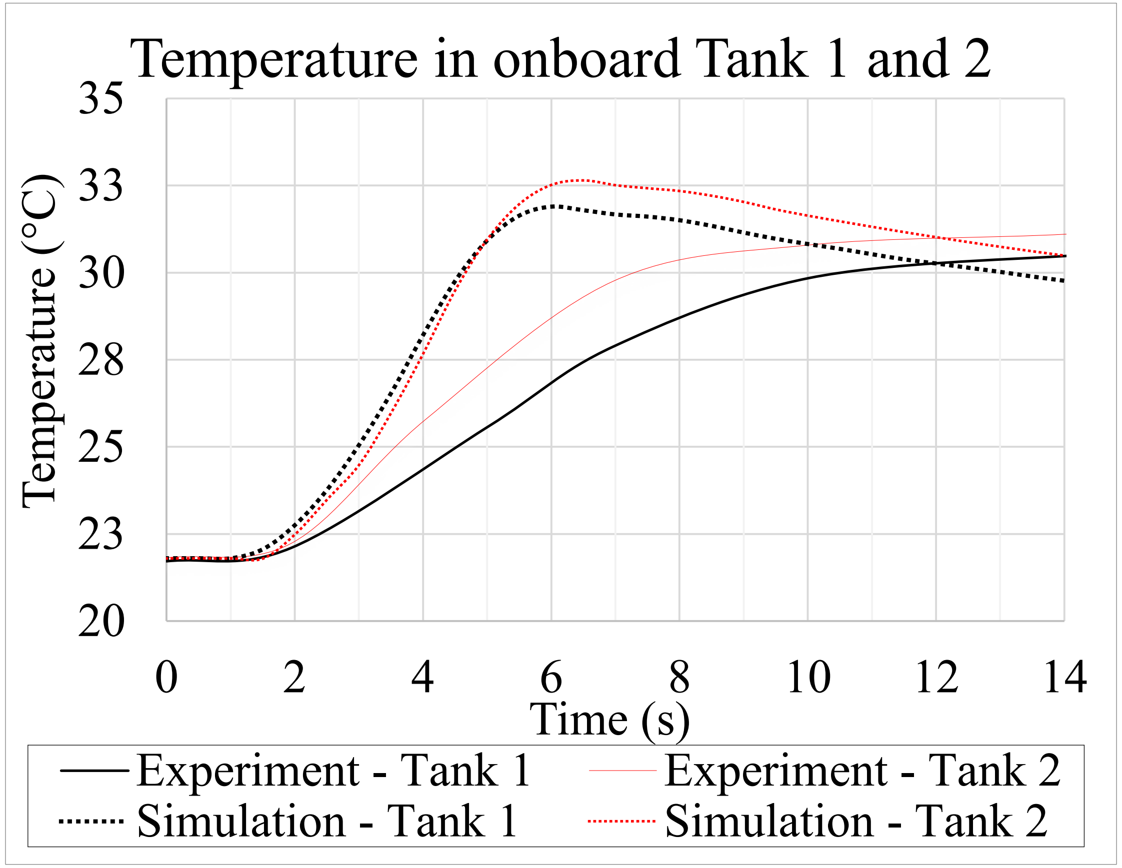


Simulations

Pressure and temperature in onboard tanks

Real simulated temperature



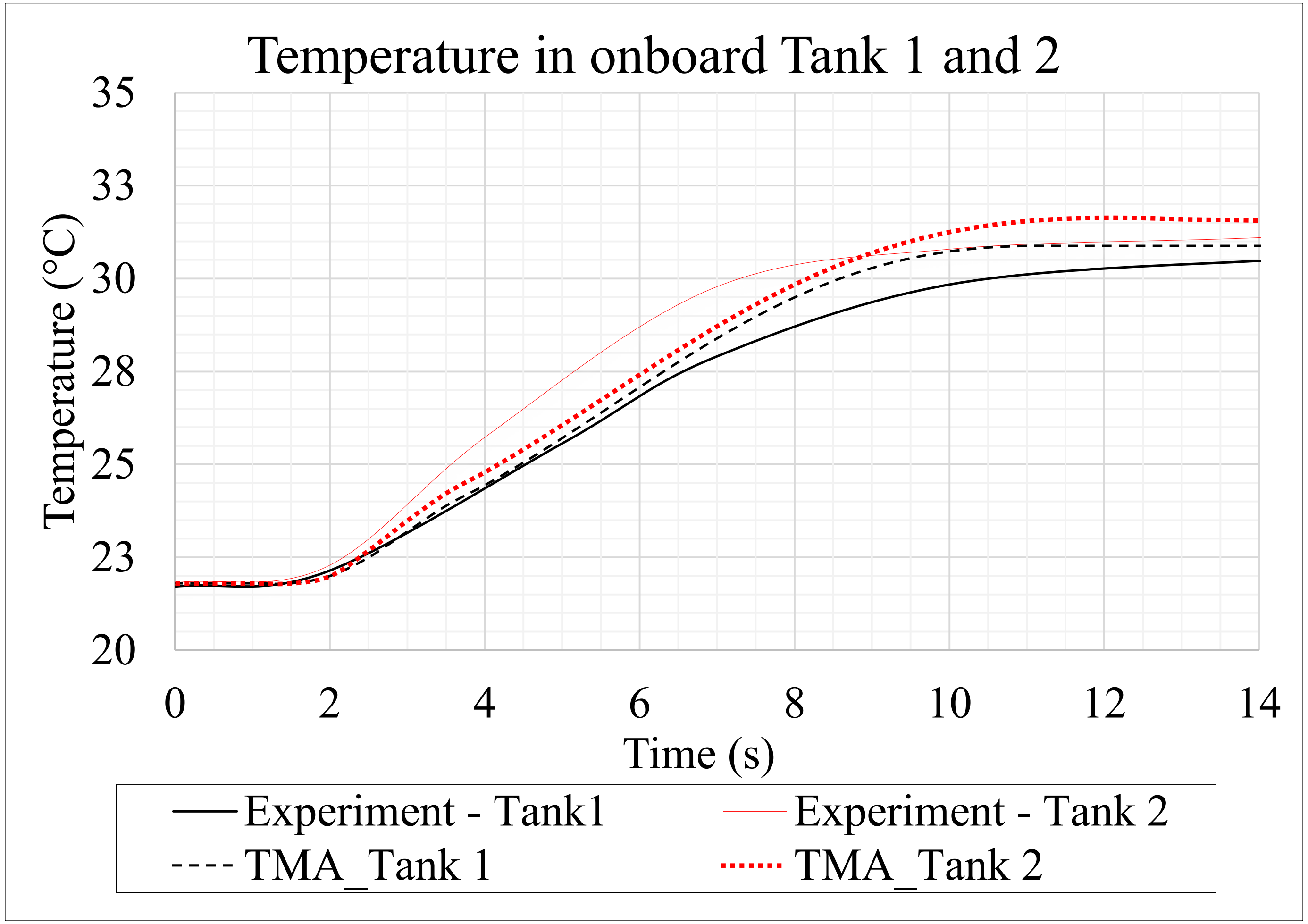


Simulations

What is “wrong” with simulated temperature? Nothing…

- Just follow procedures of experimentalists to reproduce their data.
- Triple Moving Average (TMA) is used to process simulation results in line with experimentalists results at PRHYDE project [PRHYDE Results as Input for Standardisation. Deliverable D6.7. 2022]

TMA simulated temperature



Conclusions

…of the first study in a series (start-up phase)

- For the first time a CFD model is developed to simulate hydrogen refuelling through entire equipment of HRS and FCEV.
- The model is applied to simulate the start-up phase of fuelling using in-house UDF for mass flow rate at PCV and temperature at HE.
- Experimentally measured pressure and temperature in onboard storage are well reproduced (triple moving average is applied to simulated temperature following the experimental acquisition system).
- This model can be used, after further validation against experimental data of the full duration of Tests No.1 and No.2 of NREL (or other tests when available), as an affordable contemporary tool for development of inherently safer and efficient hydrogen fuelling protocols.

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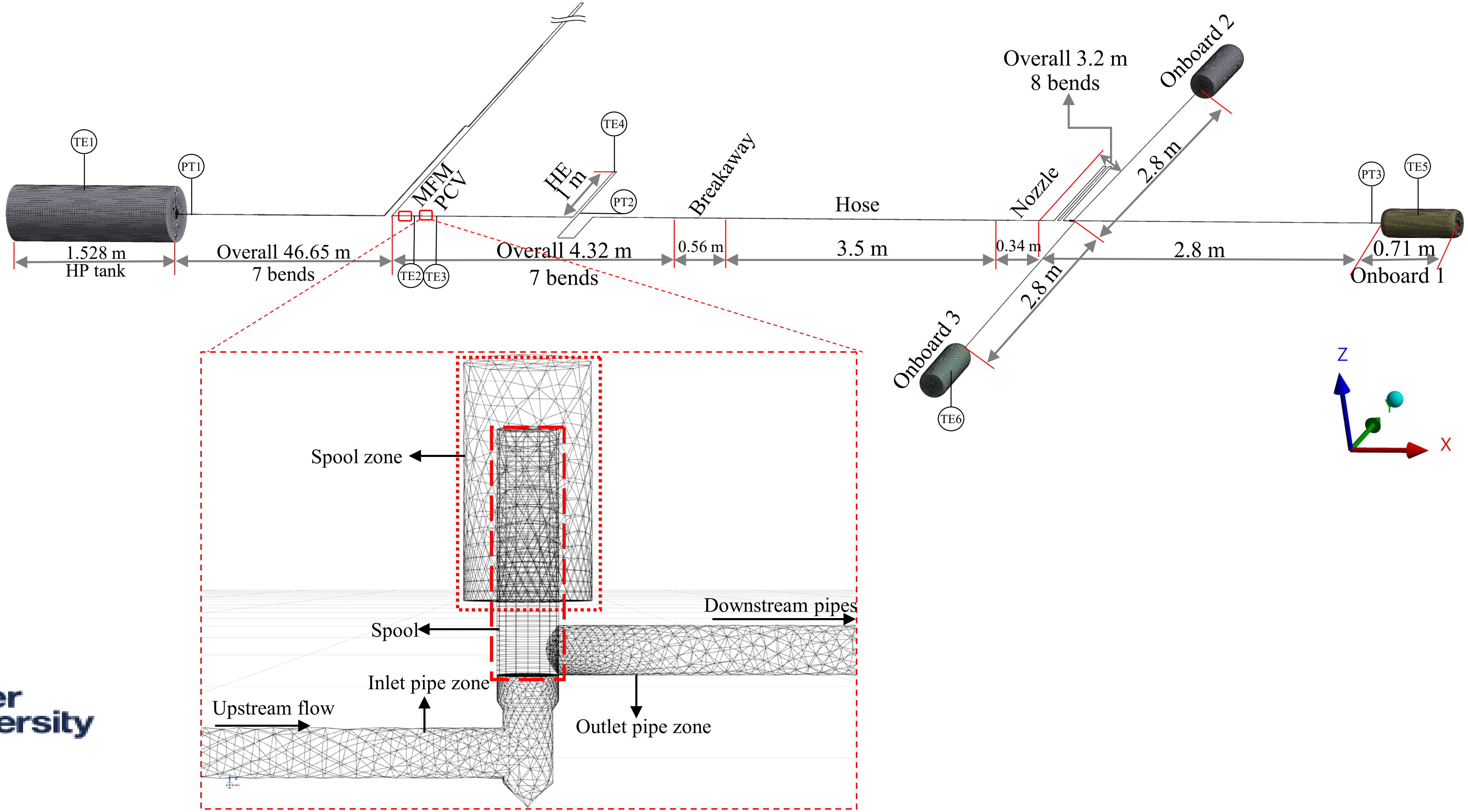
Information on ongoing research

Full duration of Test No.1 with dynamic mesh in PCV



Information on ongoing research

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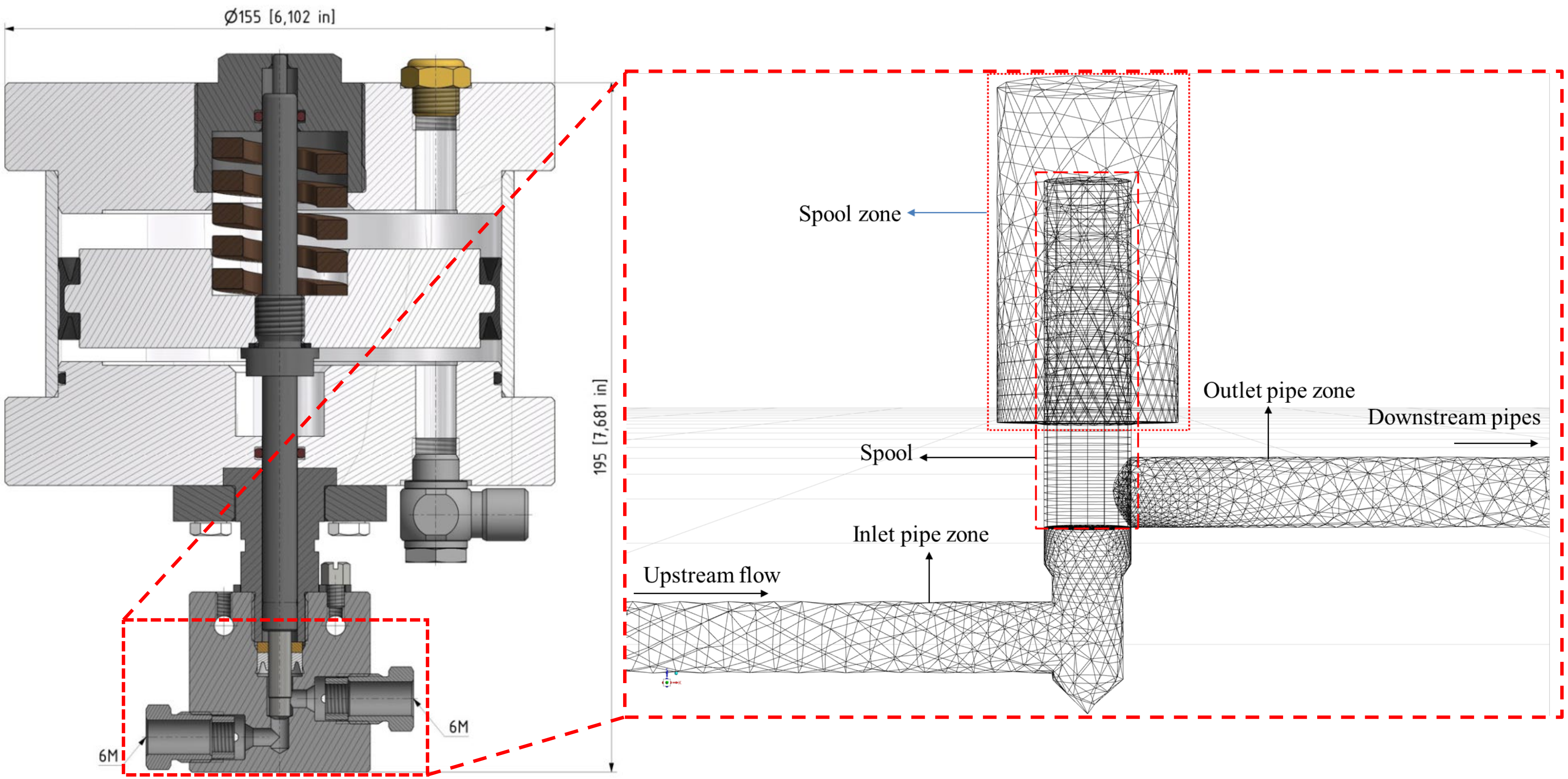

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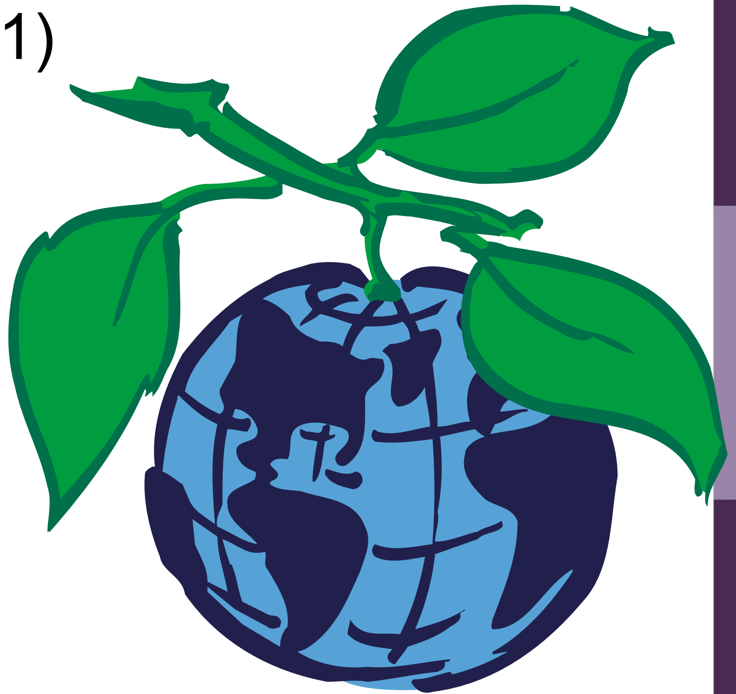

Thank you!