Series of workshops on safety of cryogenic hydrogen transfer technologies

Progress in modelling and development of fuelling/bunkering procedures

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CFD model of refuelling through the entire equipment of an HRS

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Gaseous hydrogen refuelling
Challenges

- Refuelling of cars, buses, trucks, trains, ships, and planes is a challenge.
- Onboard storage pressure 35-70 MPa.
- Refuelling time 3-4 min from 2 to 70 MPa (Clean Hydrogen Partnership, US DoE).
- Refuelling regulated limitations: T < 85°C, P < 125% of NWP, SoC < 100%.
- Only light-duty vehicle fuelling protocol (SAE J2601) is available: < 10 kg.
- Heavy-duty vehicle protocols (SAE J2601/2): only high-level safety requirements.
- Temperature increase due to compression, Joule-Thomson effect, etc.
- Fundamentally based tools to underpin fuelling protocol development are needed.

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Gaseous hydrogen refuelling

Modelling through entire equipment of HRS

- Understanding heat and mass transfer during refuelling through the entire equipment of HRS is essential for the development of inherently safer protocols.
- Validation against the NREL refuelling experiments by Kuroki et al. (2021).
- Test No.1 was used to compare the two models’ performance for 195 s refuelling.
- Test No.2 was used to simulate the start-up phase of 14 s duration.
- Aim: develop and validate the CFD models that can be used as engineering tools to design HRS equipment parameters and develop refuelling protocols.

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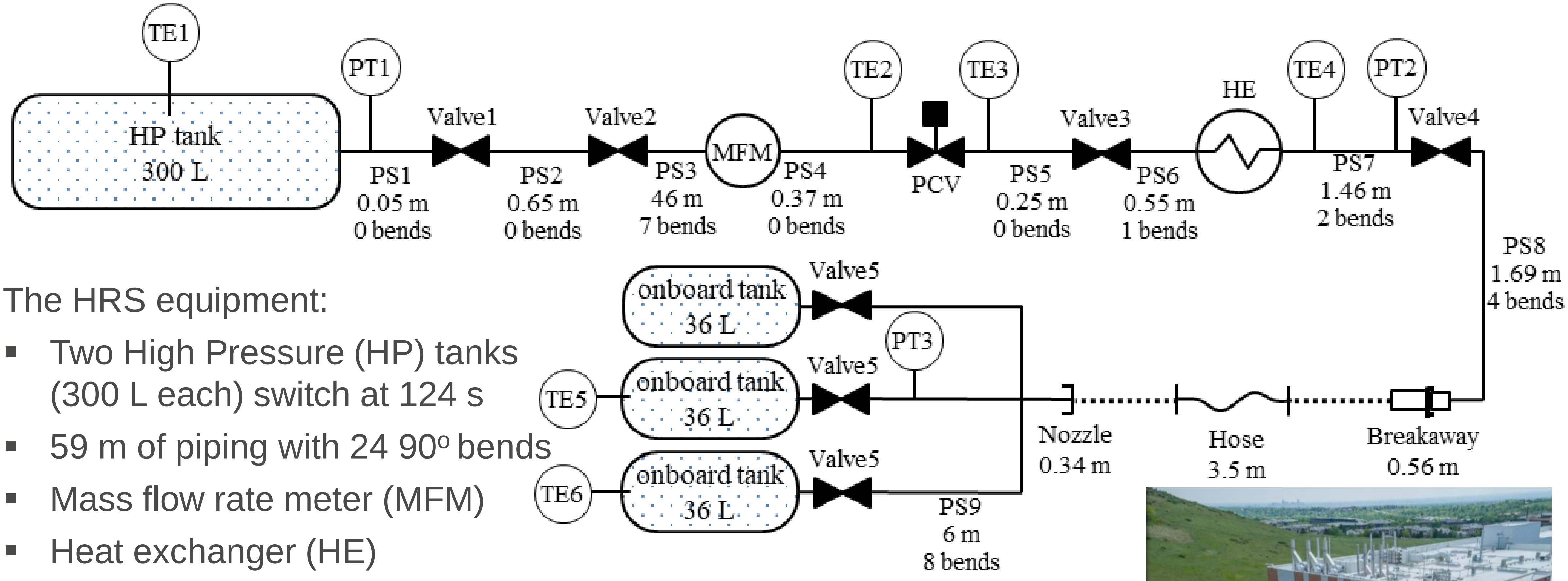
Validation experiments

Diagram of entire HRS equipment



The HRS equipment:

- Two High Pressure (HP) tanks (300 L each) switch at 124 s
- 59 m of piping with 24 90º bends
- Mass flow rate meter (MFM)
- Heat exchanger (HE)
- Pressure control valve (PCV) and 5 other valves
- Breakaway, hose, nozzle, and
- Three 36 L capacity onboard storage tanks.

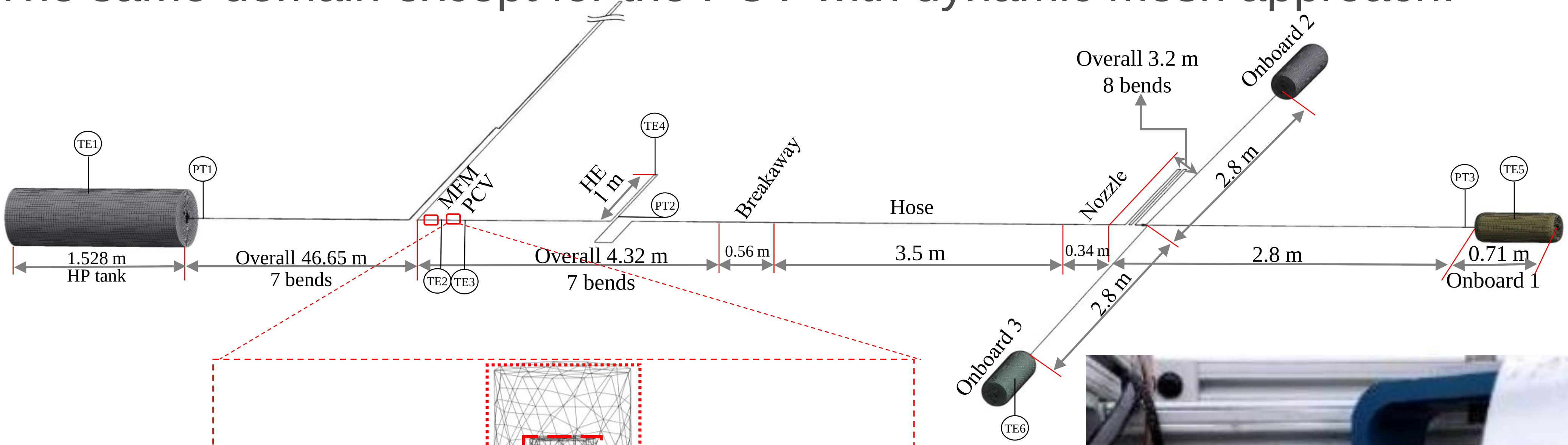
CFD model
Numerical details

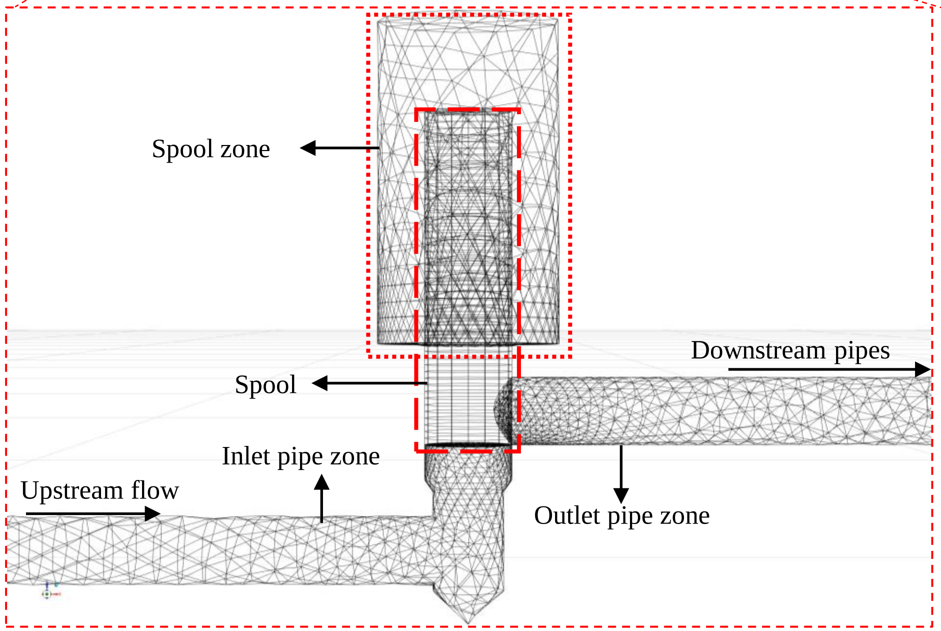
- ANSYS Fluent 2023R1 is used as a CFD engine.
- Governing equations: conservation of mass, momentum and energy.
- The standard k-ε model is applied to simulate flow turbulence.
- NIST real gas EoS.
- Boundary conditions: non-slip, impermeable walls, 3rd kind boundary condition for energy equation, h=7 W/m^2K, ambient temperature 23°C.
- 3D conduction in tank/pipe walls by ANSYS Fluent "Shell conduction" technique.
- The SIMPLE algorithm was applied for pressure-velocity coupling.
- Convective terms were discretised using the pressure-based implicit solver and first-order upwind numerical scheme.
- Two models are developed in this study, based on:
  - the fixed values of variables, and
  - the use of dynamic mesh

CFD model

Calculation domain

The same domain except for the PCV with dynamic mesh approach.



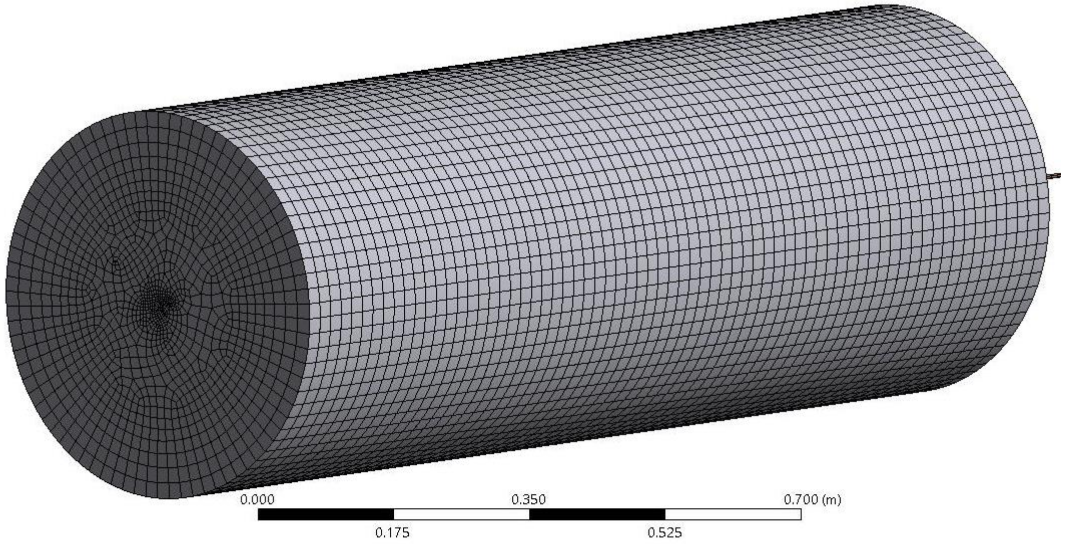


CFD model

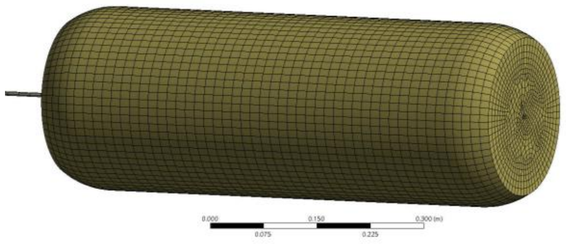
Calculation domain discretisation

- Hexahedral mesh: 207,252 CVs.
- Maximum CV size: 3 cm (close to the walls of the tank).
- 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

PCV and HE modelling (fixed values)

Pressure Control Valve (PCV):

- Hydrogen velocity in PCV is changed dynamically to match the experimental pressure. The algorithm developed using the “fixing the value” capability of ANSYS Fluent (original UDF programmed using C++ code).

Heat exchanger (HE):

- HE is modelled using its experimentally measured equivalent length and diameter. Temperature control follows experimentally measured temperature dynamics at HE outflow. Temperature control relies on the “fixing the value” function of ANSYS Fluent (original UDF programmed using C++ code).

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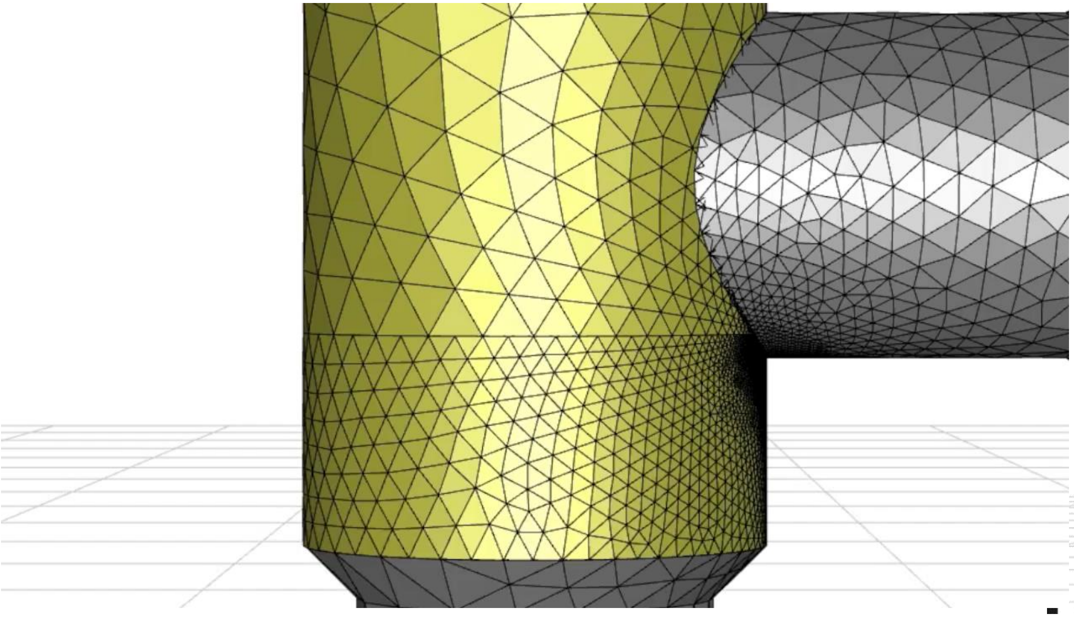
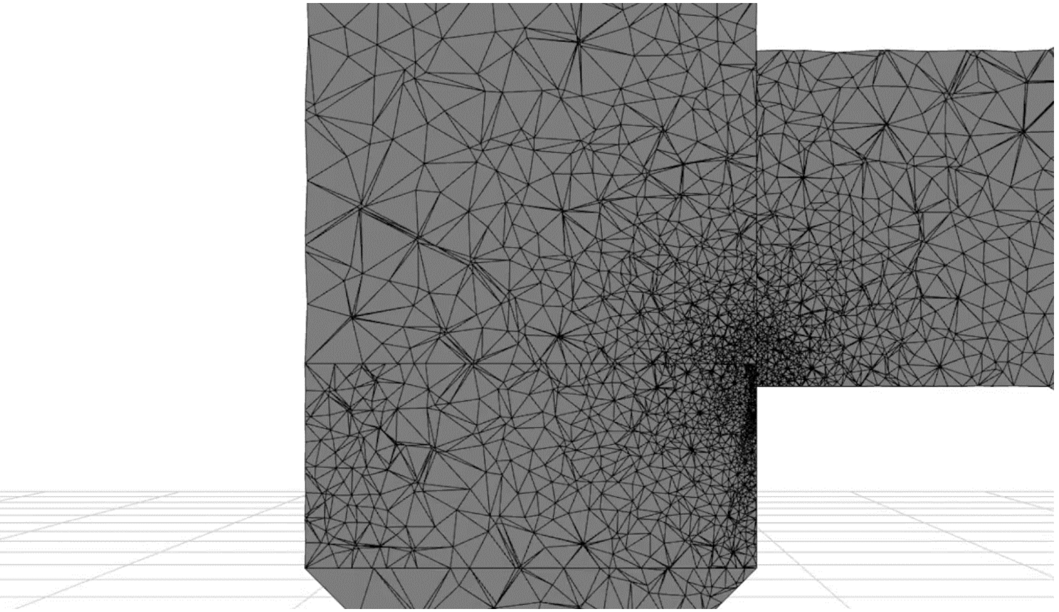
CFD model
Dynamic mesh for PCV spool movement (Method No.2)

- PCV mesh: 37K CVs (closed) to 49K CVs (100% open).
- CV volume size: 10^{-4} mm^3 ~ 3×10^{-3} mm^3.



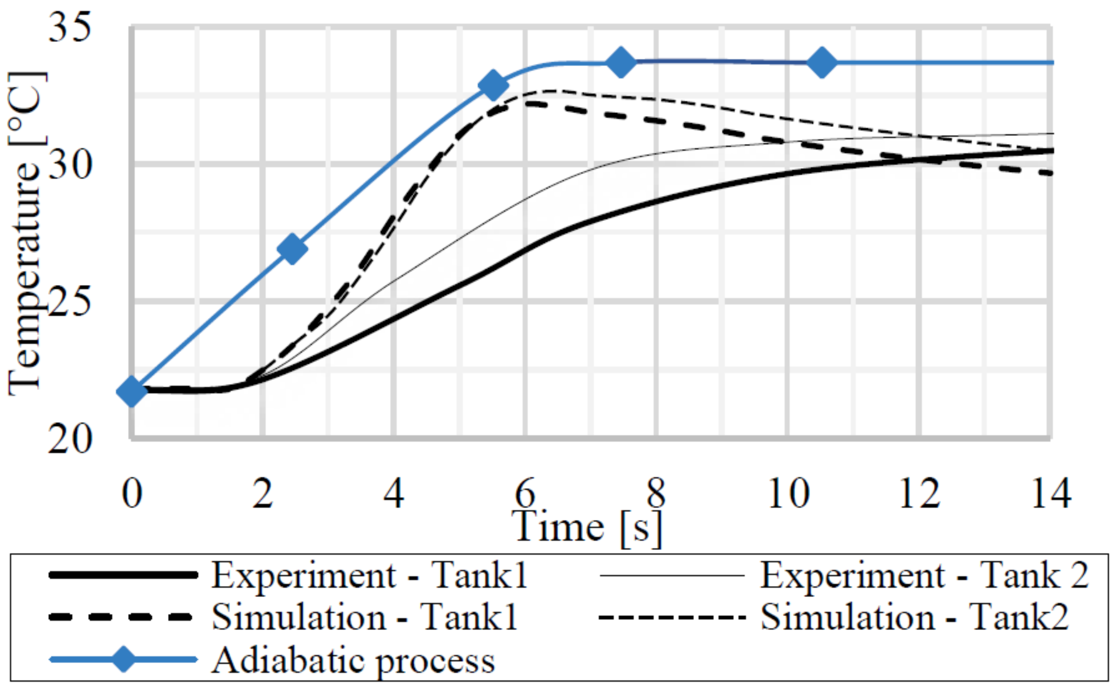
PCV boundary mesh



PCV cross-section mesh

Simulations versus experiment
Start-up phase 14 s of Test No.2 (1/2)

- The initial conditions and the results of the Test No.2 start-up phase were used.
- The “fixed values” method is used to control the flow rate and HE temperature.
- The simulation of 14 s takes about 2 hours on a 32-core CPU running at 2.3 GHz.
- While the simulated temperature transients were correct in a physical sense, i.e., the temperature in the tank was reduced after stopping fuelling (at 6 s) due to heat losses to the tank walls, it did not match the experimental temperature demonstrating “growth”.
- Test temperature was reproduced only when a triple-moving averaging (TMA) was applied to the simulated temperature, which is a common experimental practice (Hart et al., 2022).

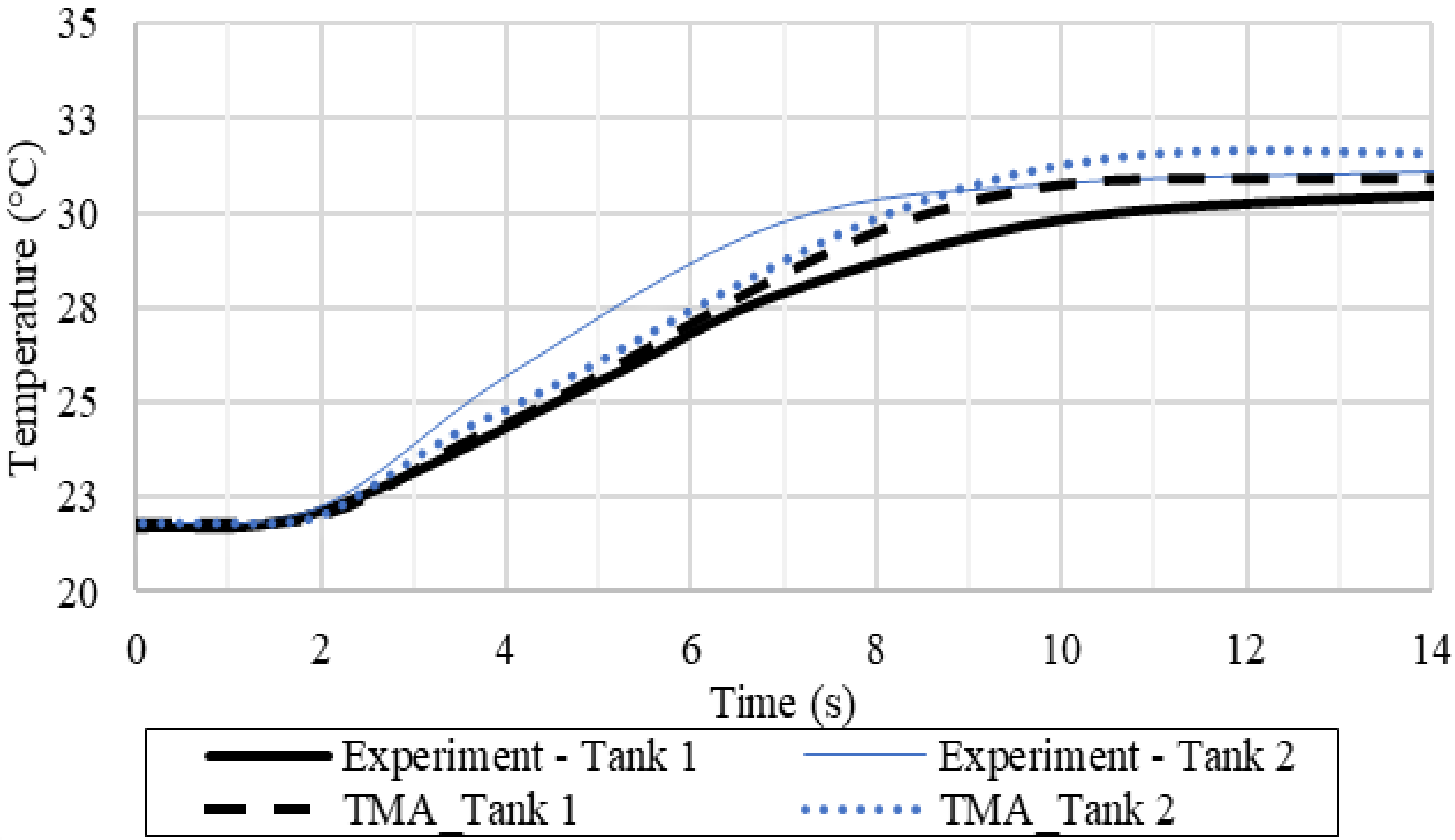


Simulations versus experiment

Start-up phase 14 s of Test No.2 (2/2)

Both simulated and experimental temperatures of hydrogen in Tank 2 are higher than in Tank 1. This can be explained by the difference in heat transfer in the piping to these tanks after splitting the flow. For both tanks stabilised simulated temperature after the start-up pressure pulse is higher than experimental data by about 1°C.

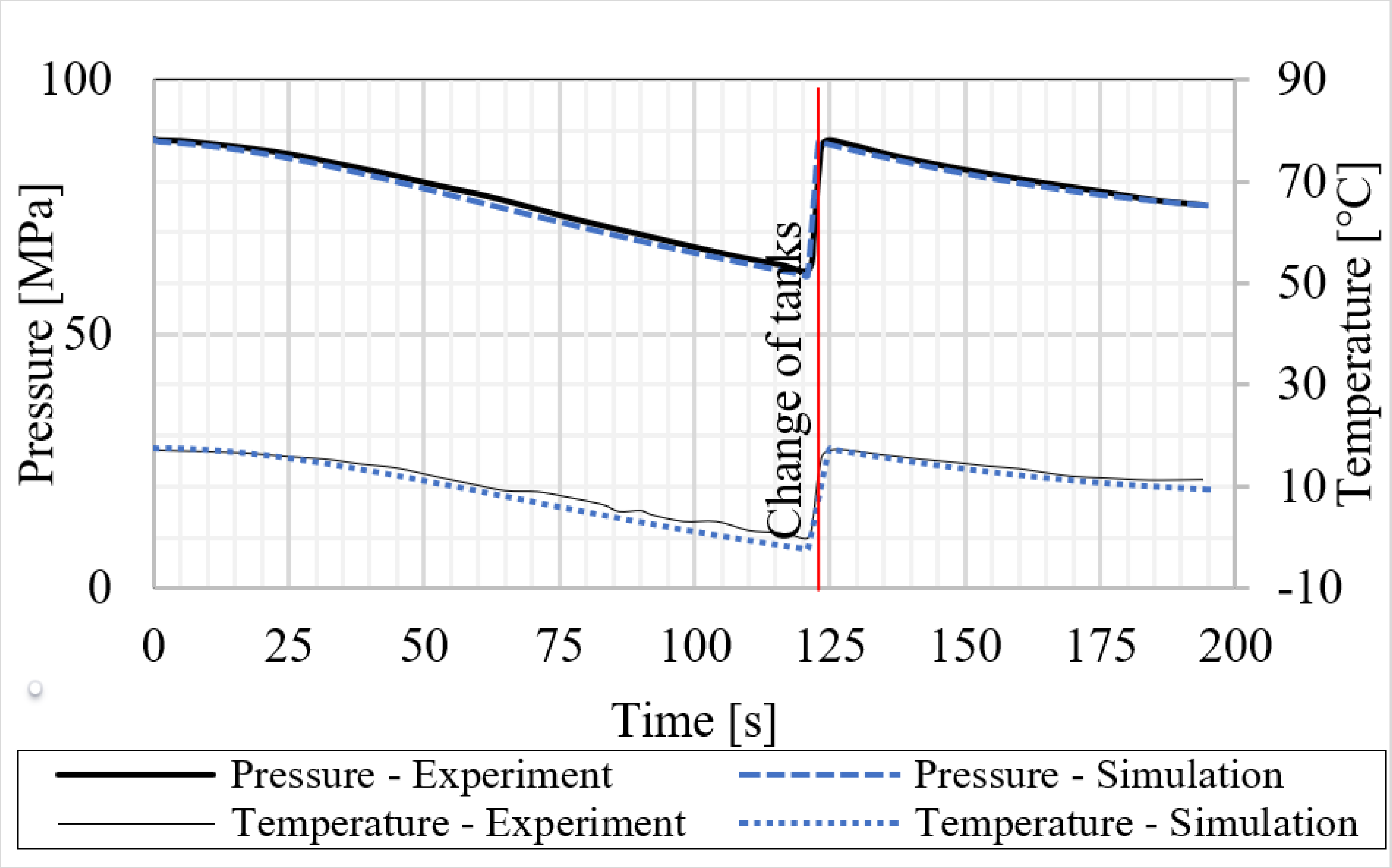
This is an excellent result considering that the measurement accuracy is ±1.5°C (Kuroki et al., 2021).



Simulations versus experiment

Full refuelling process of 195 s of Test No.1 (1/3)

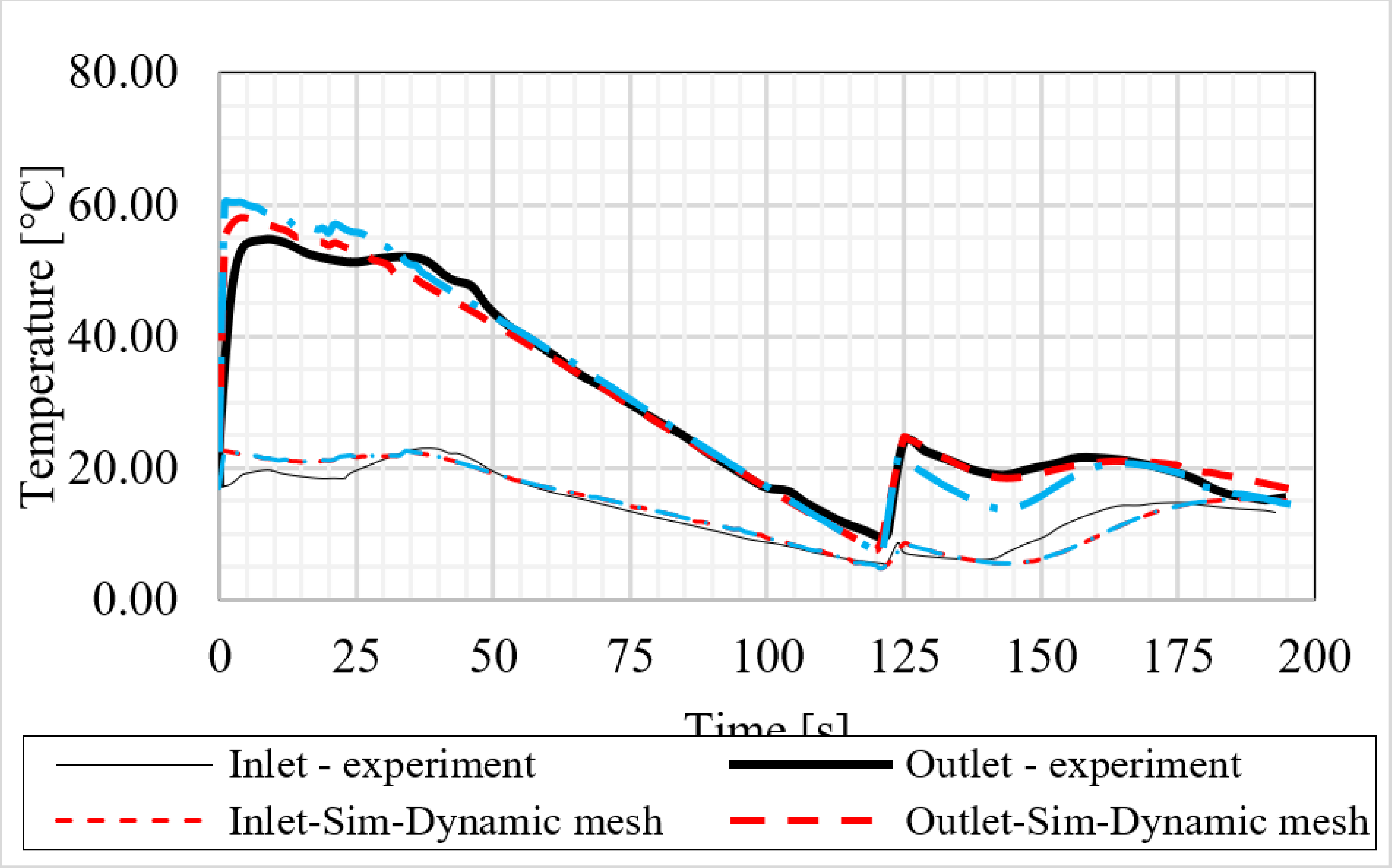
Experimental and simulated pressure and temperature in HP tank (change at 124 s).



Simulations versus experiment

Full refuelling process of 195 s of Test No.1 (2/3)

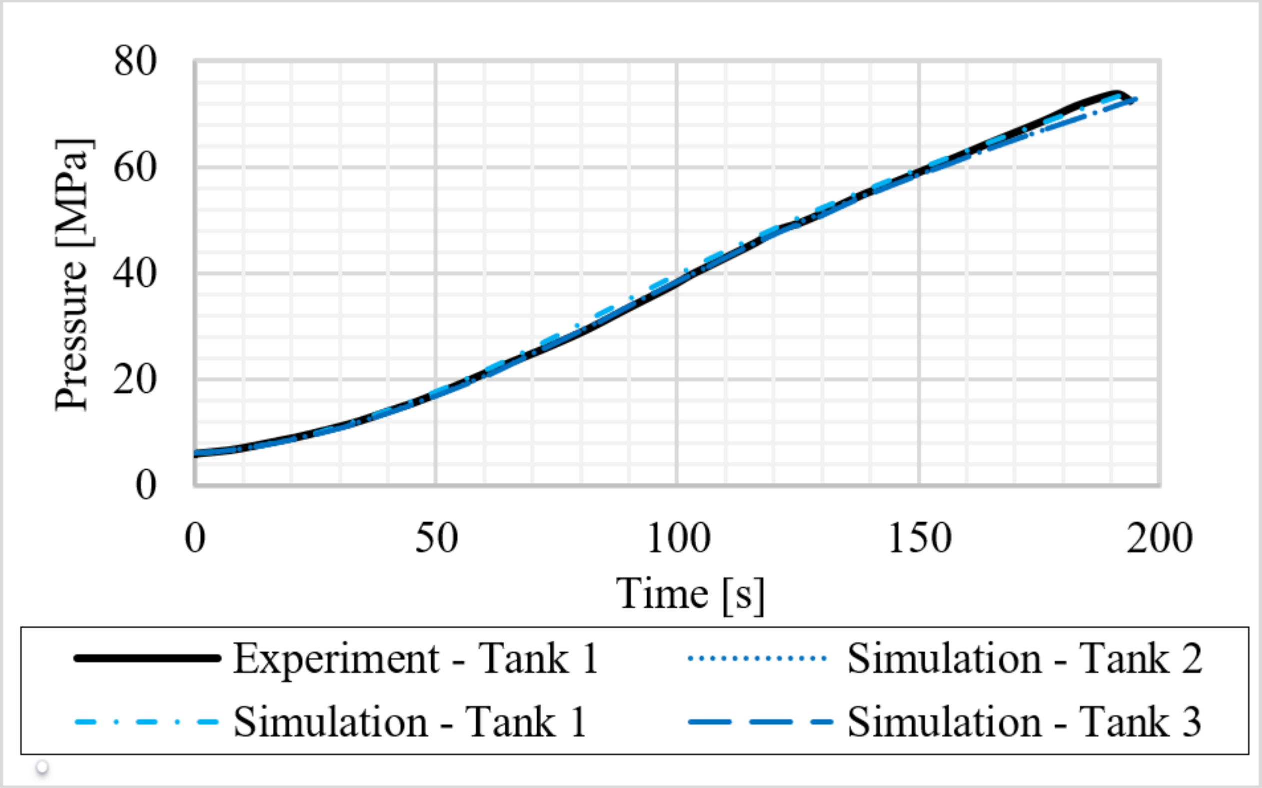
Experimental and simulated temperature upstream and downstream of the PCV.

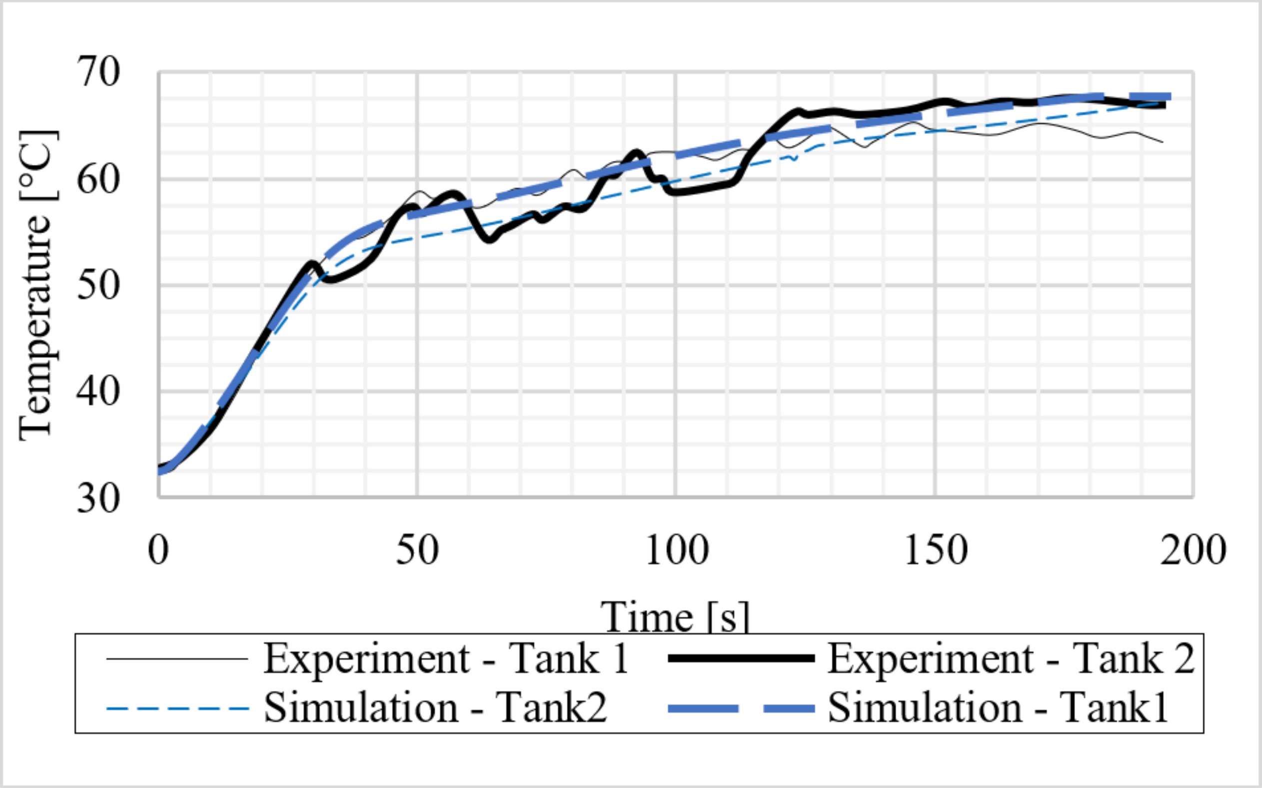


Simulations versus experiment

Full refuelling process of 195 s of Test No.1 (3/3)

Experimental and simulated pressure and temperature in onboard tanks.





Simulations of the full refuelling process take 2 days on a 32-core CPU.

Conclusions

- The ***significance*** of work is in the development of the first CFD model for the simulation of heat and mass transfer during fuelling through the entire equipment of HRS.
- The ***rigour*** is in the validation of simulations against Kuroki et al. (2021) tests, including the start-up phase (14s duration) and refuelling process of 195 s duration.
- The ***originality*** is in using different methods and numerical know-how, including the fixed values and dynamic mesh technique.
- The CFD model offers an affordable contemporary tool for developing inherently safer and efficient hydrogen refuelling protocols.

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