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European Hydrogen Safety Panel (EHSP)
Clean Hydrogen JU Webinar "Computational Fluid Dynamics (CFD) for hydrogen safety analysis ", 07 December 2022

CFD model of refuelling through the entire equipment of Hydrogen Refuelling Station

Seeding research of Ulster University (doctoral study of Mr H Ebne-Abbasi under supervision of Dr D Makarov and Prof V Molkov)

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Member of European Hydrogen Safety Panel (EHSP)

Acknowledgements to researchers contributed to this study and relevant papers:

- Ebne-Abbasi H, Makarov D, Molkov V. CFD modelling of the entire fuelling process at a hydrogen refuelling station. ***Proceedings of the 10th International Seminar on Fire and Explosion Hazards (ISFEH10)***, Oslo, Norway, 22-27 May 2022. Paper ID92.
- Ebne-Abbasi H, Makarov D, Molkov V. CFD model of refuelling through the entire HRS equipment: the start-up phase simulations. ***International Conference on Hydrogen Safety***, Quebec, Canada, 19-21 September 2023 (to be submitted).
- Kuroki T. , Nagasawa K., Peters M., et al. (2021). Thermodynamic modeling of hydrogen fueling process from high-pressure storage tank to vehicle tank, ***International Journal of Hydrogen Energy***, 46, pp. 22004–22017.

Presentation outline

- The problem of CFD simulations of refuelling through the entire HRS equipment
- Validation experiments by NREL
- The CFD model: numerical details
- Simulations versus experiment: start-up phase
- Simulations versus experiment: entire refuelling process

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The problem of CFD modelling of HRS

The state-of-the-art

- Refuelling is still a technological challenge for all hydrogen-powered vehicles:
  - Cars
  - Buses
  - Trucks
  - Trains
  - Ships
  - Planes
- Refuelling protocols for more than 10 kg onboard storage are not available.
- Reduced models of fuelling cannot simulate temperature non-uniformity in tanks, etc.
- Current CFD models are focused on simulation of only onboard tank fuelling.
- Simulations of refuelling through entire equipment of HRS was not even considered.
- Challenge of long simulation time (only tank fuelling takes usually few weeks).
- CFD model of entire HRS could be a powerful tool for development of protocols.

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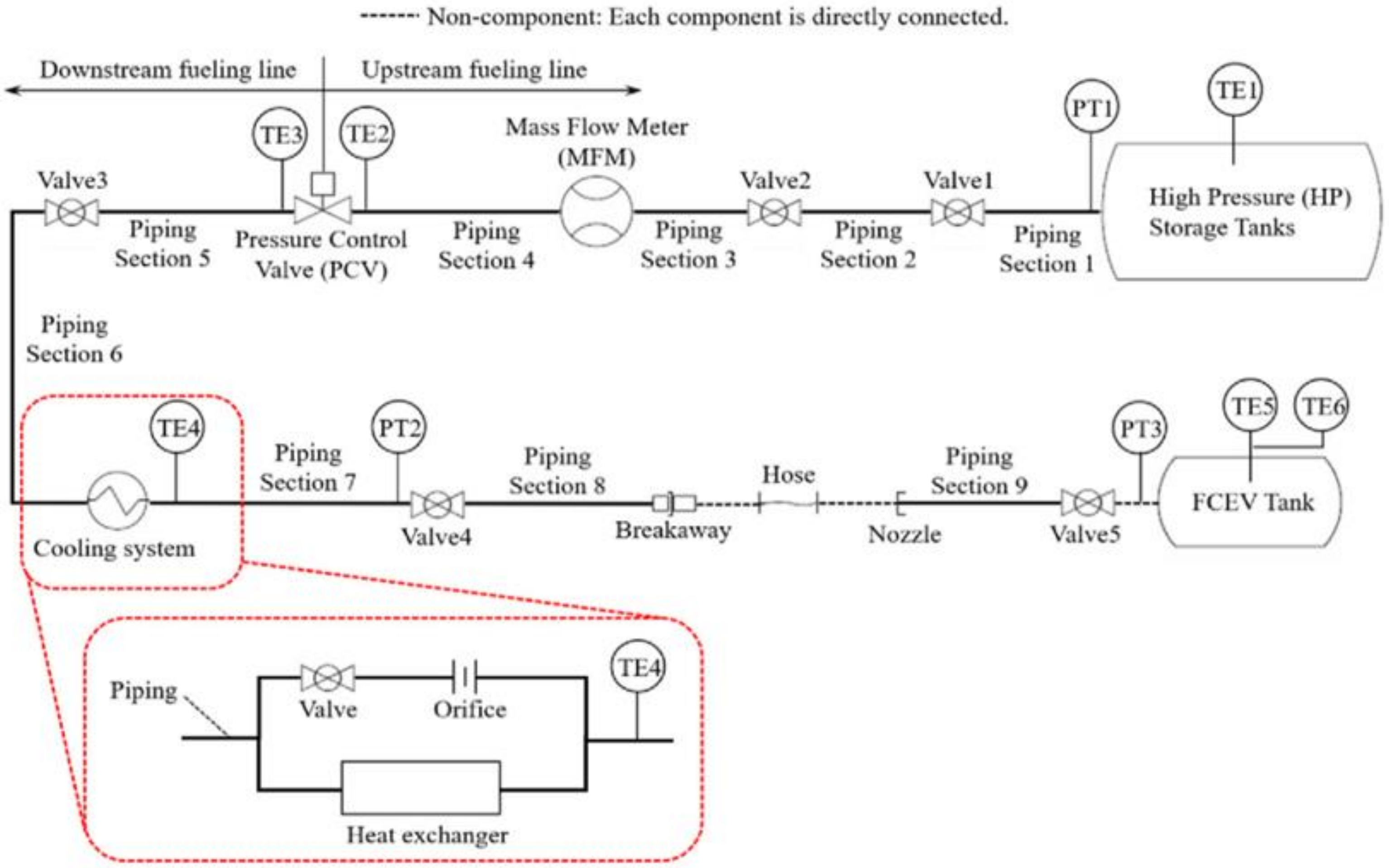
Validation experiments by NREL

Probably the only tests available in the public domain

Experimental study of the entire HRS equipment and three onboard storage tanks (Kuroki et al., 2021):

- Hydrogen Infrastructure Research Facility (HITRF) at the National Renewable Energy Laboratory's (USA)
- HRS and vehicle components:
  - 6×300 L high pressure (HP) tanks
  - 9 piping sections with bends
  - Pressure control valve (PCV)
  - Five other valves
  - Mass flow meter (MFM)
  - Precooler heat exchanger (HE)
  - Breakaway
  - Hose
  - Nozzle
  - 3×36 L onboard storage tanks
- Initial conditions:
  - HP tank: 17.5°C, 880 bar
  - Onboard tanks: 21°C, 55 bar
- Ambient temperature: 21°C
- Average Pressure Ramp Rate (APRR): 21.1 MPa/min



The CFD model: numerical details

RANS

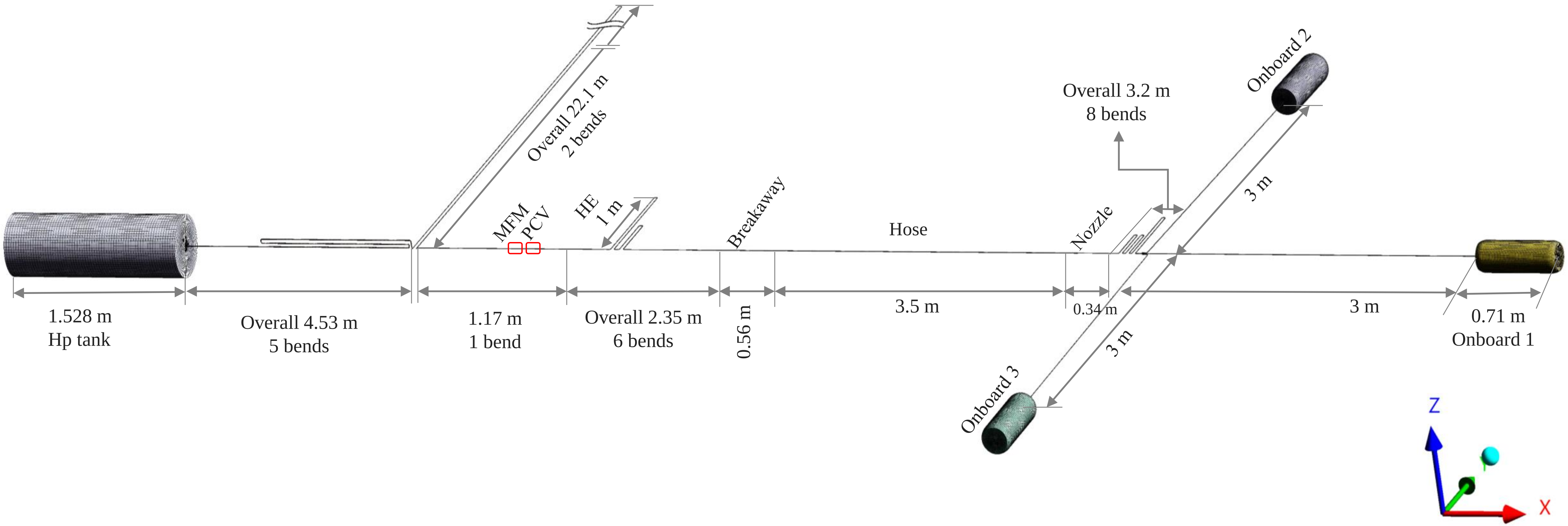
- Conservation equations for mass, momentum, and energy (3D).
- Flow turbulence was modelled using the standard k-ε model.
- Fluent 2020R2 as a CFD engine with NIST real gas equation of state.
- Boundaries of pipes, valves, tanks are modelled as non-slip, impermeable walls.
- Conjugate heat transfer through walls.
- SIMPLE algorithm for pressure-velocity coupling. The first-order upwind scheme for convective terms and the first-order implicit scheme for time marching.
- Valves, including PCV, are modelled as pipe sections with equivalent ID calculated based on flow coefficients. Length is taken as 0.1 m.
- The Fluent fixing the values of variables method is used to control the flow through the PCV and temperature in the HE.

Conclusion: ordinary CFD model (with few know-hows) able to simulate entire HRS.

The CFD model

Calculation domain

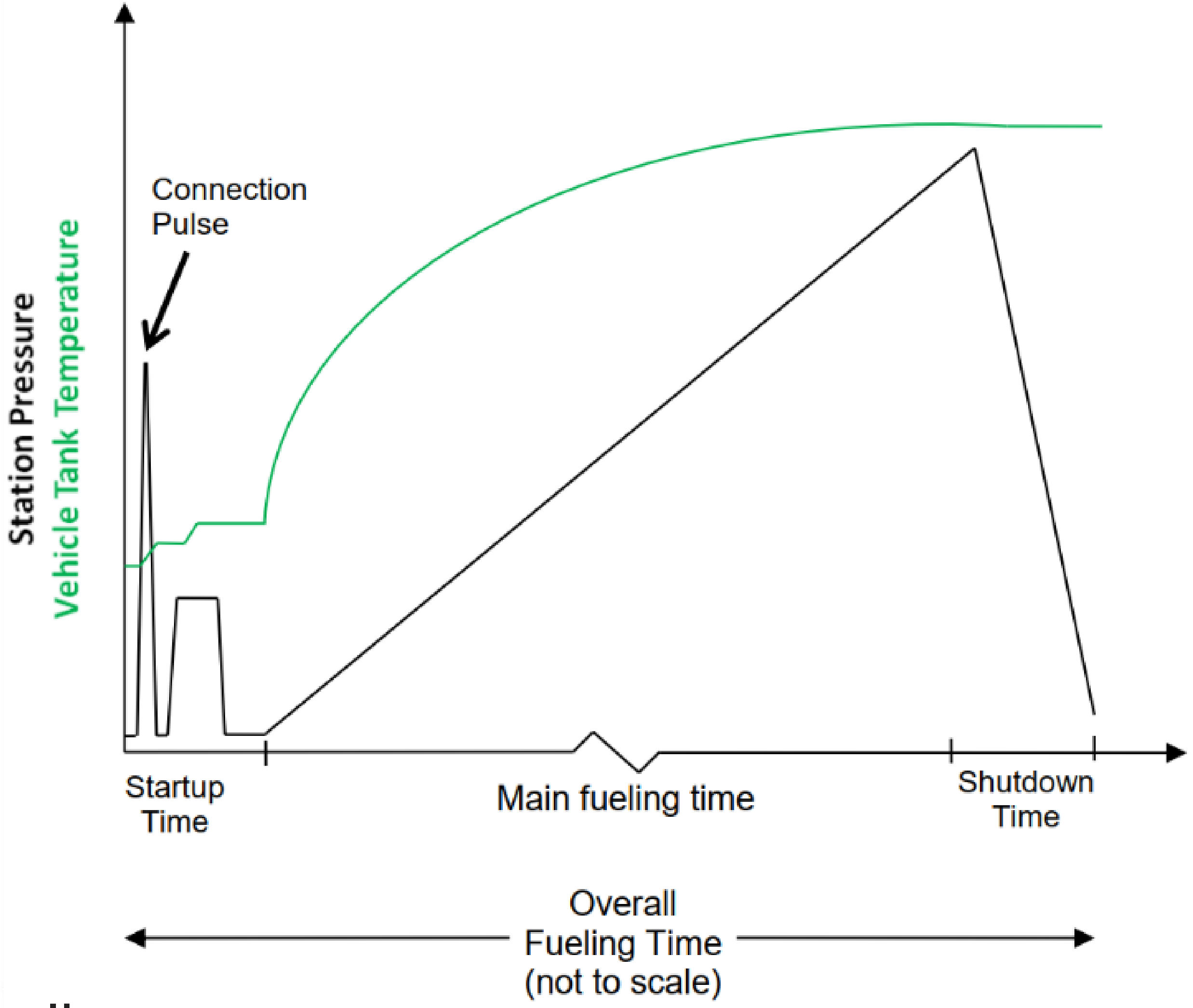
- Entire HRS components (slide 4) are included into the computational domain.
- The computational domain is meshed with 207,252 control volumes.
- The minimum orthogonal quality is 0.7 with an average of 0.97.



Simulations versus experiment

Start-up phase: SAE J2601

- SAE J2601 specifies the start-up phase as a period which begins when the user starts fuelling for a short period called start-up time and finishes when hydrogen flow through the dispenser to the vehicle tanks.
- This start-up period includes a connection pulse, determination of vehicle tank capacity category, and a leak check. The connection pulse starts when a nozzle is connected to the receptacle. This stage measures any decrease in pressure in the fuelling line.



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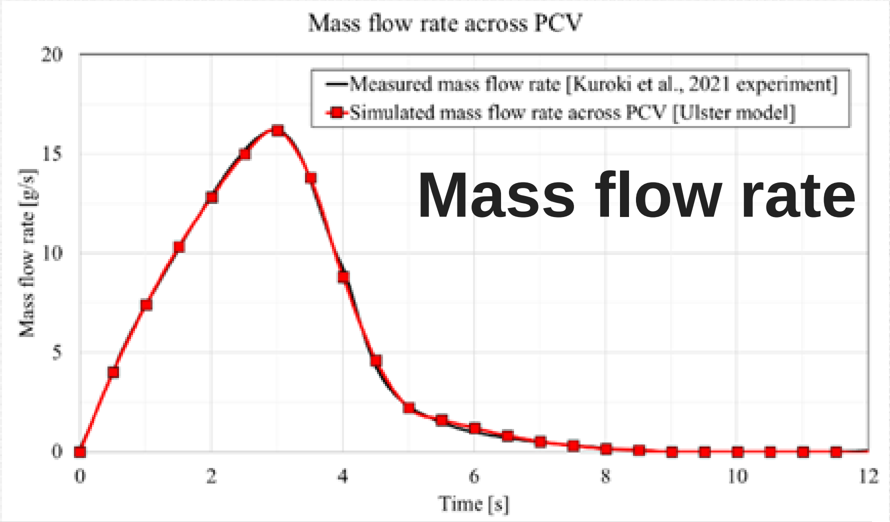
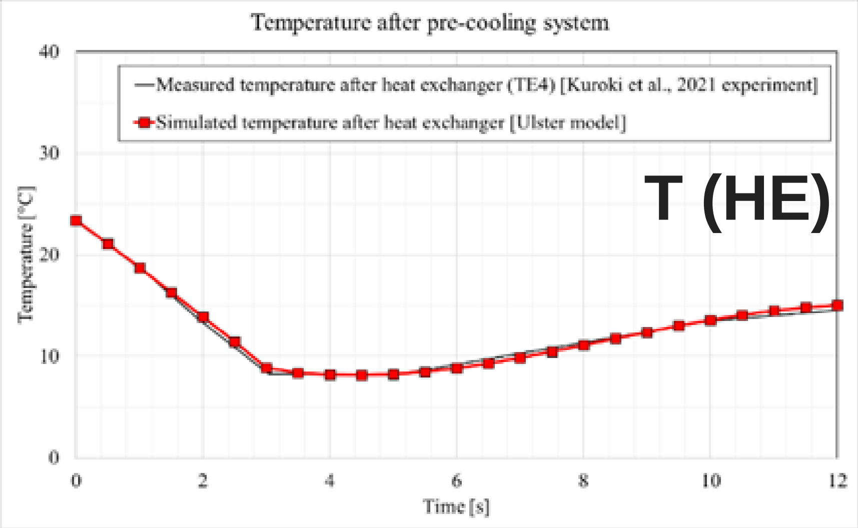
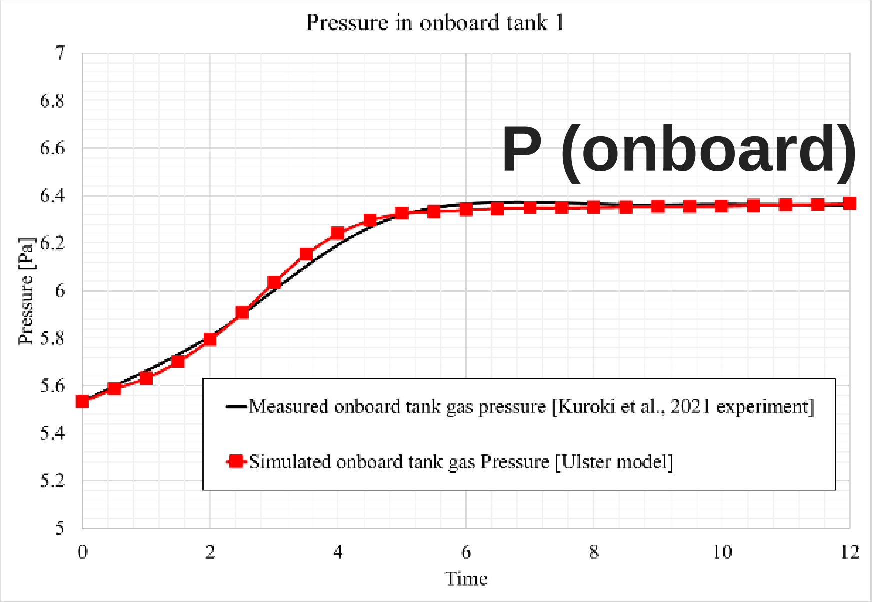
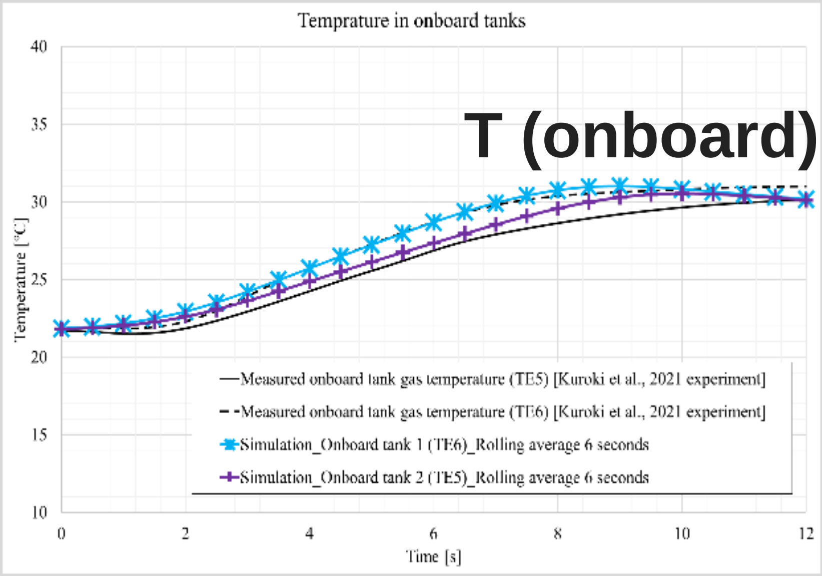
Simulations versus experiment

Start-up phase (12 s): simulation time is about 1 hour









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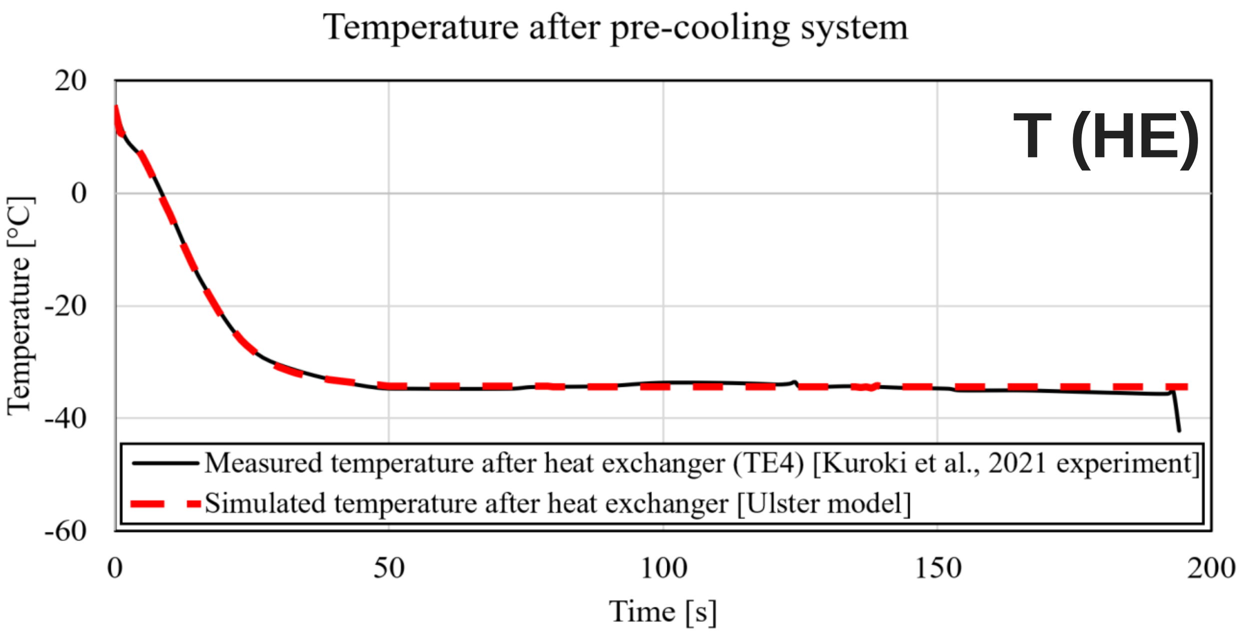
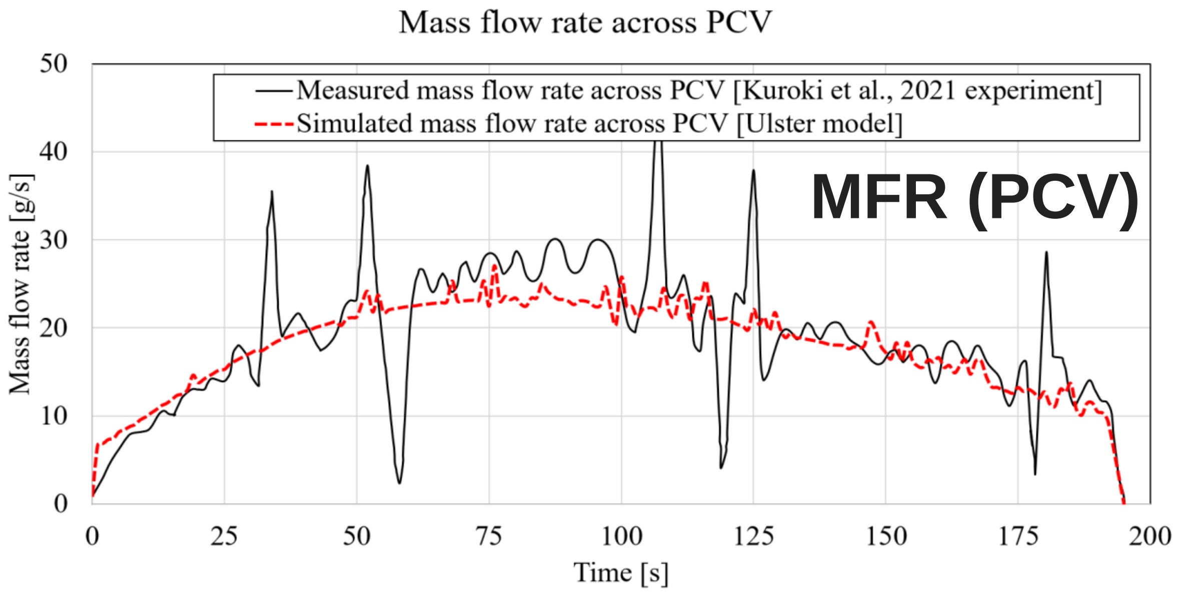
Simulations versus experiment

Entire refuelling process: simulation time is about 1 day

In-house UDF for simulation of Heat Exchanger (HE) and Pressure Control Valve (PCV).





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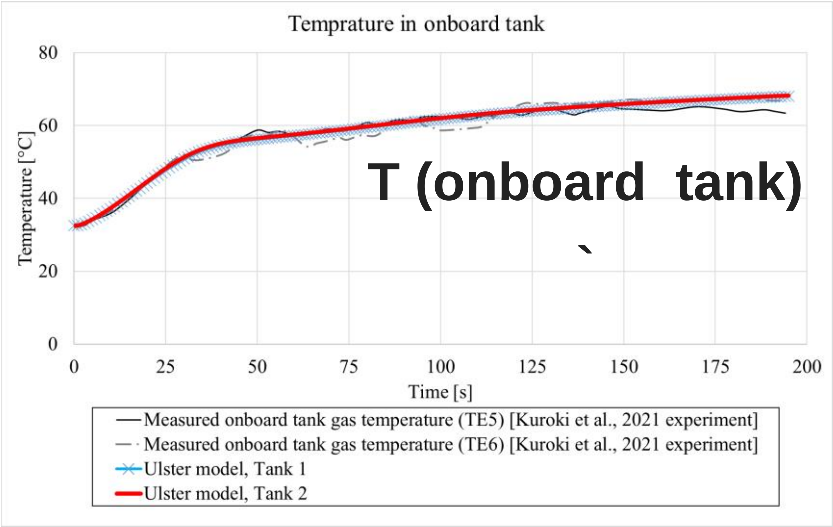
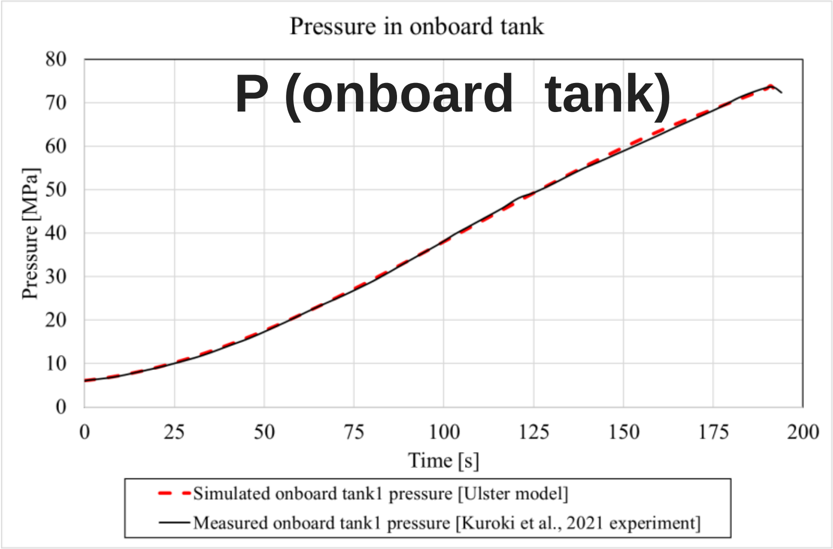
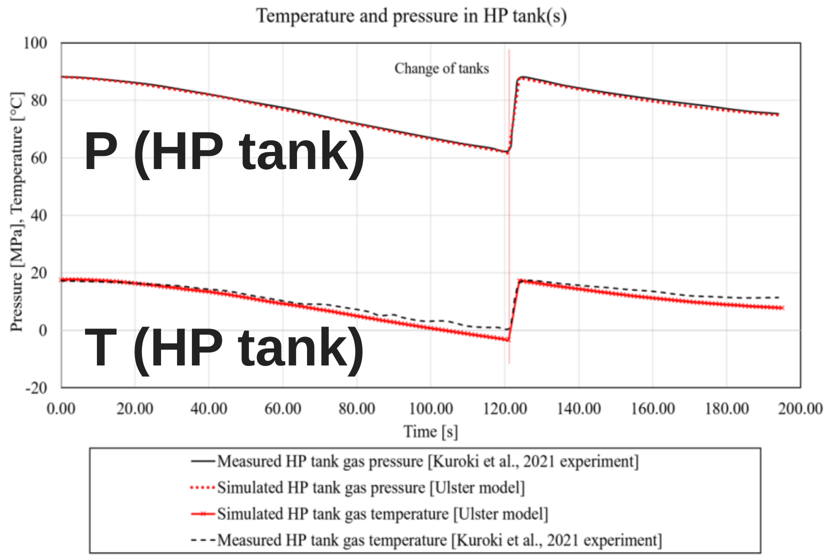
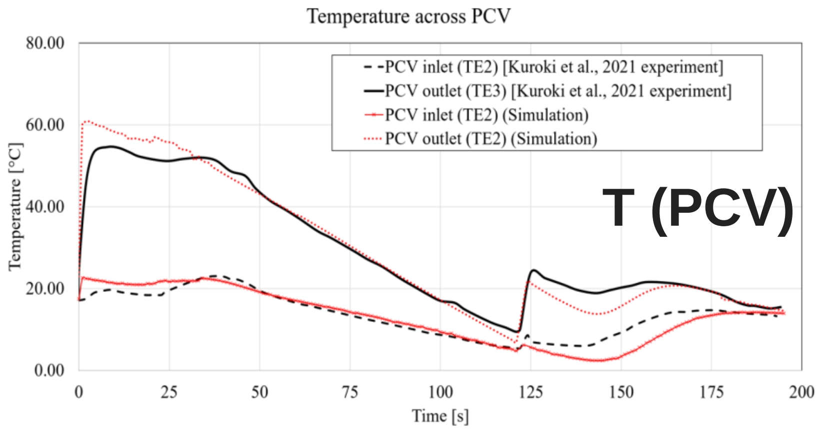
Simulations versus experiment

Entire refuelling process: simulation time is about 1 day









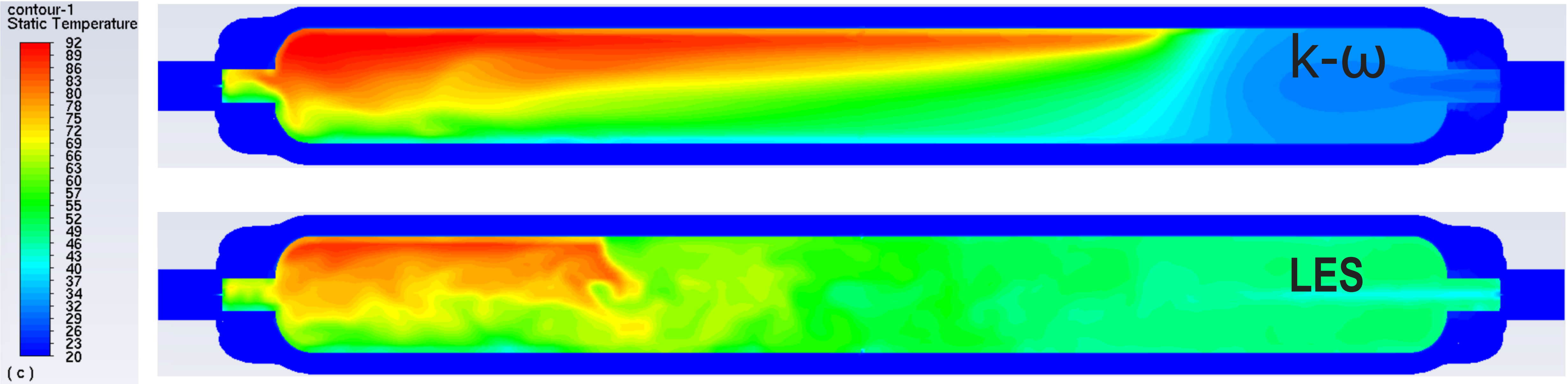
Joule-Thompson effect is reproduced

Temperature non-uniformity in onboard tank

Regulated limit 85 C: for bulk or localised temperature?

CFD simulations of large L/D tanks in the SH2APED project (after first 10 s):

- While bulk temperature is below 85ºC, the local is above 85ºC just 10 s after the start.
- Initial hydrogen pressure 2 MPa and temperature 20°C.
- Mass flow rate $\dot{m}$=2.4 g/s (targeted fuelling time 180 s), no pre-cooling (inlet T=20°C).



Question to be answered by forthcoming research: RANS or LES to simulate reality?

Concluding remarks

- The developed CFD model **reproduced experimentally measured pressure and temperature through the entire equipment of HRS**, including the start-up phase. The advanced modelling of performance of the key HRS components, i.e. the PCV and the HE, is carried out using an **in-house UDFs.**
- The CFD model is a **computationally affordable** contemporary tool for **designing of fuelling protocols** for the whole range of HRS equipment and hydrogen-powered vehicles for road, rail, marine, and aeronautical applications.
- Unlike the reduced models inherently simplifying the refuelling process, the CFD model is capable to provide insight into the underlying physical phenomena of **heat and mass transfer between hydrogen, HRS equipment, onboard vehicle tanks, and the surrounding atmosphere.** This includes reproduction of the **Joule-Thompson effect at PVC**.
- One of the key advantages of the CFD model over reduced models is the capability to predict **temperature non-uniformity** in onboard tanks. This is essential for the prevention of tank failure, especially in tanks with large L/D ratios like in **conformable tanks**.

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Thank you

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