Engineering models for refueling protocol development: validation and recommendations – ICHS 2023

Fouad Ammouri[1], Nicola Benvenuti[2], Elena Vyazmina[1], Vincent Ren[1], Guillaume Lodier[1], Quentin Nouvelot[2], Thomas Guewouo[2], Dorine Crouslé[2], Rony Tawk[2], Nick Hart[3], Steve Mathison[4], Taichi Kuroki[5], Spencer Quong[6], Antonio Ruiz[7], Alexander Grab[7], Alexander Kvasnicka[8], Benoit Poulet[9], Christopher Kutz[10], Martin Zerta[10]

[1] Air Liquide Innovation Campus Paris, 1 chemin de la Porte des Loges, 78350 Jouy-en-Josas, France
[2] ENGIE Lab CRIGEN, 4 Rue Joséphine Baker, 93240 Stains, France
[3] ITM Power Plc, 2 Bessemer Park, Sheffield, S9 1DZ, United Kingdom
[4] FirstElement Fuel, Inc. 2549 Eastbluff Drive, #334 Newport Beach, CA 92660, USA
[5] National Renewable Energy Laboratory (NREL), Golden, CO 80401, USA
[6] Quong & Associates, Inc. on behalf of Toyota Motor North America, San Francisco, CA, USA
[7] NIKOLA CORPORATION, 4141 E Broadway Rd, Phoenix, AZ 85040, USA
[8] Zentrum für Brennstoffzellen Technik ZBT GmbH, Carl-Benz-Straße 201 - D-47057 Duisburg, Germany
[9] Shell , Suhrenkamp 71-77, 22335 Hamburg, Germany
[10] Ludwig-Bölkow-Systemtechnik GmbH, Daimlerstr. 15, 85521 Ottobrunn, Germany

Contact e-mail: fouad.ammouri@airliquide.com - nicola.benvenuti@engie.com

Agenda

- Introduction
- Purpose for physical modeling
- Engineering modeling tools used
- Model validation with experiments
  - Hexagon, type 4, H70, 165 L at Nikola
  - Hexagon, type 4, H70, 244 L (at Zentrum für Brennstoffzellen Technik (ZBT))
  - Luxfer, type 3, H35, 322 L (at ZBT)
- Conclusions and recommendations

Introduction

H₂ PRHYDE
Protocol for heavy-duty Hydrogen refuelling

- ***Work done in the frame of PRHYDE - Protocol for heavy-duty hydrogen refuelling (2020 - 2022)***
  Call Identifier FCH-04-2-2019: Refuelling Protocols for Medium and Heavy-Duty Vehicles

- The **PRHYDE project** funded by the Clean Hydrogen partnership aims at developing recommendations for heavy-duty refueling protocols used for future standardization activities for trucks and other heavy duty transport systems applying hydrogen technologies.

Clean Hydrogen Partnership

This project has received funding from the Fuel Cells and Hydrogen 2 Joint Undertaking (now Clean Hydrogen Partnership) under Grant Agreement No 874997. This Joint Undertaking receives support from the European Union's Horizon 2020 Research and Innovation programme, Hydrogen Europe and Hydrogen Europe Research.

Co-funded by the European Union

- We thank all partners of the PRHYDE project (www.prhyde.eu) for their contribution to this work, namely:
  - ✓ Air Liquide, CEA, ENGIE, ITM, NEL, Nikola, Toyota Europe and Toyota North America, Shell, ZBT, and LBST

Purpose for physical modeling

- The objective of physical modeling is to be the basis for defining HD refueling protocols
- It uses 2 approaches:
  - 0D/1D modeling for engineering calculations for refueling protocols
  - Computational Fluid Dynamics (CFD) 3D modeling for detailed calculations on some specific cases with thermal stratifications
- Before using modeling results, need for validation
- Modeling validation using experimental data on different tank sizes and refueling conditions

0D/1D modeling characteristics

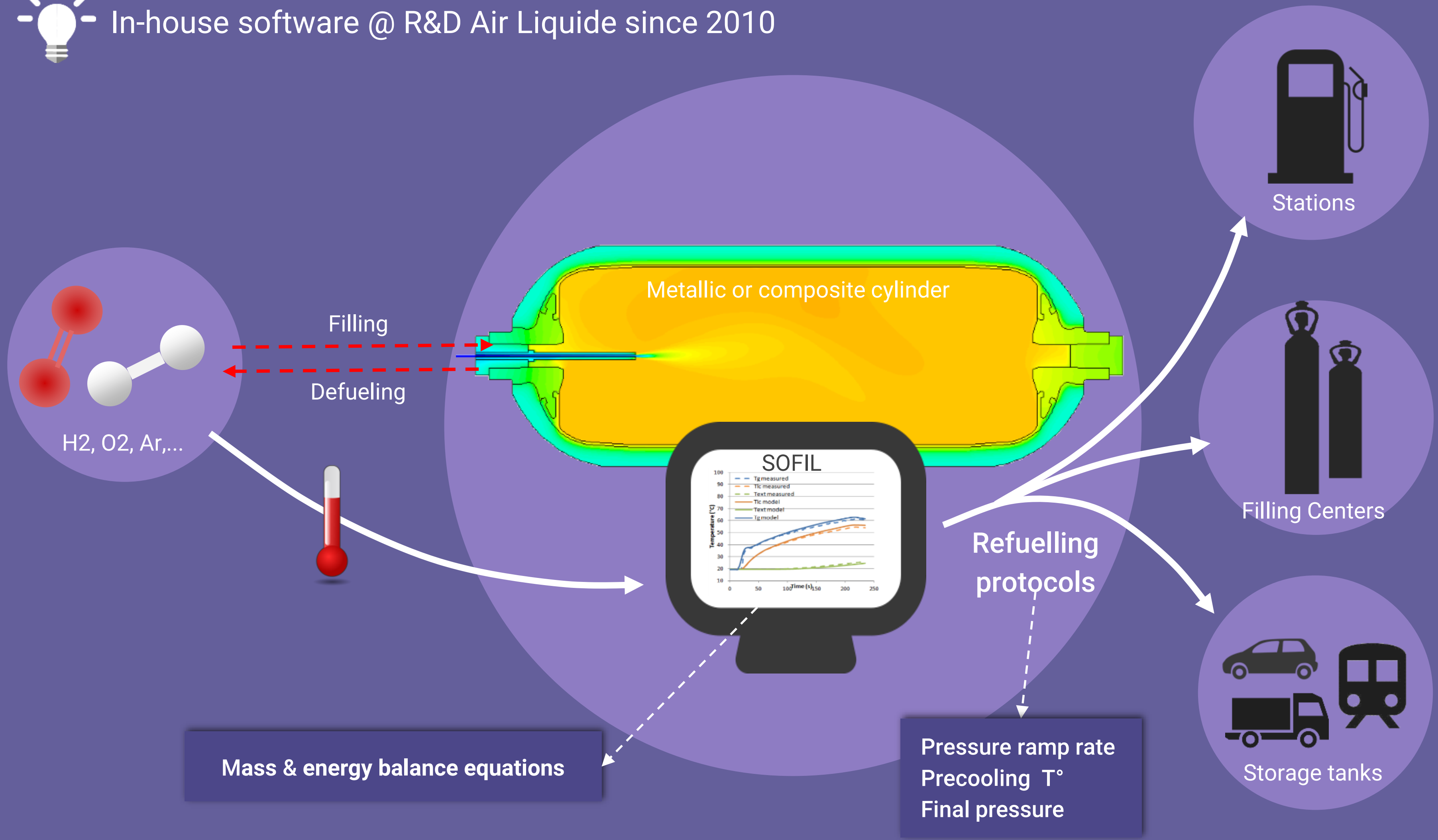
- 0D/1D modeling approach is based on mass and energy balance equations applied on the gas and on tank walls
- 0D modeling for the gas and 1D modeling for the tank walls
- It calculates volume average gas temperature, surface average wall temperature at different thicknesses and gas mass inside the tank in function of time during refueling
- **Its major advantage: computing time = few minutes**
- 0D/1D modeling can be used for parametric study and for defining refueling protocols
- **However, it cannot calculate local variables then cannot be used to estimate maximal local gas and wall temperatures when thermal stratifications occur**

0D/1D modeling tools used

- SOFIL (Air Liquide)
- HyFill (Engie)
- H2FillS (NREL)

SOFIL: software to estimate gas temperature & mass when filling / defueling gas tanks for **safety & energy optimization**

In-house software @ R&D Air Liquide since 2010



H2, O2, Ar,...

Filling

Defueling

Metallic or composite cylinder

SOFIL

Refuelling protocols

Stations

Filling Centers

Storage tanks

Mass & energy balance equations

Pressure ramp rate
Precooling T°
Final pressure

Validated during HyTransfer project

- On experimental fillings and CFD results
- For horizontal tanks type III/IV

Major benefits

- Quick computations (~ min)
- Precise

Simulation assumptions

- 0D-gas
- 1D-wall
- 2D-piping discretization

0D/1D models used: HyFill (Engie)

- HyFill developed on Matlab/Simulink allows to simulate the fast filling and emptying of hydrogen tanks in order to predict the final temperature reached by the hydrogen. HyFill is a pseudo-1D model. It considers that the gas temperature is uniform at each instant in the tank. The heat transfer between the gas and the outside is modeled by the unsteady 1D cylindrical conduction equation.
- Mass and energy balance equations (0D):
- $$\begin{cases} \frac{dm}{dt} = \dot{m}_{in} - \dot{m}_{out} \\ \frac{dmu}{dt} = \dot{m}_{in} h_{in} - \dot{m}_{out} h_{out} - Q_{gas-wall} \\ \frac{P}{\rho} = ZRT \end{cases}$$
- Unsteady state 1D conduction equation for the heat in the tank walls

0D/1D models used: H2FillS (NREL)

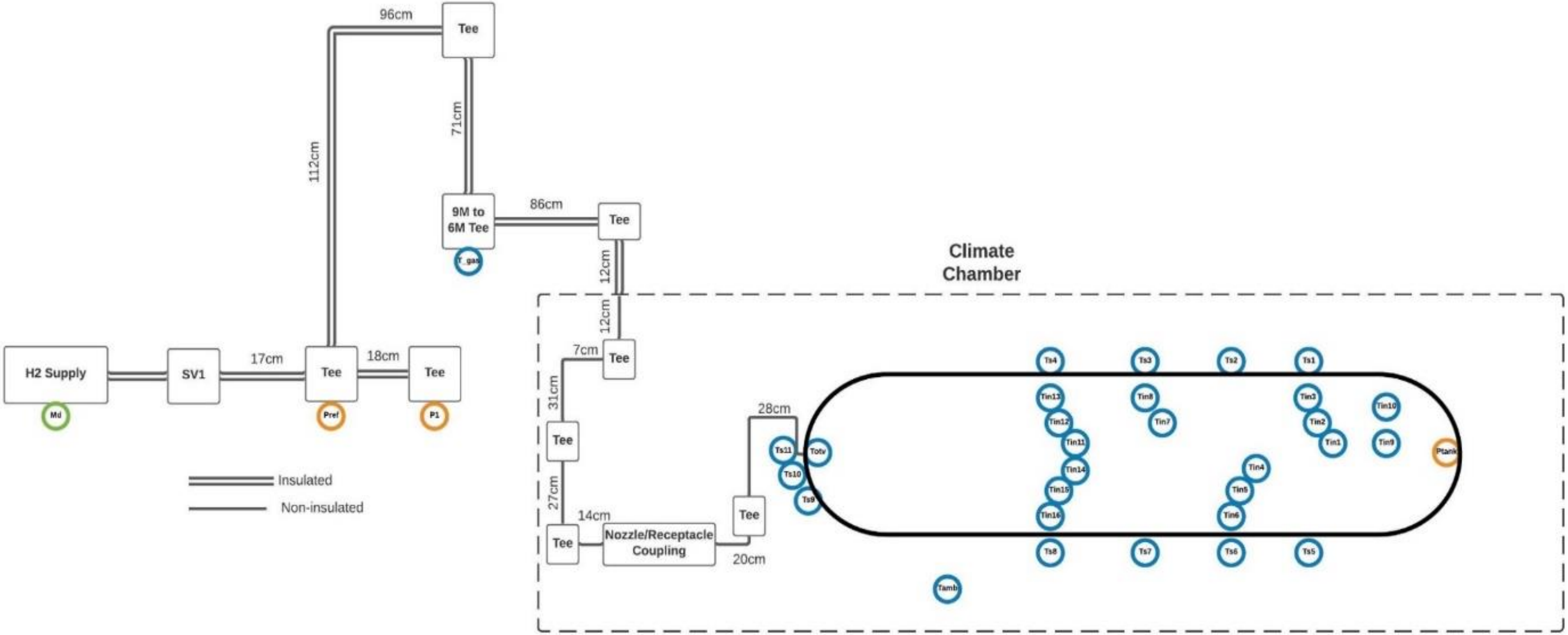
- Mass and energy balances are calculated with the assumption that tank volume does not increase with the pressure rise. The governing equations for the mass and energy balances:
- $\frac{d}{dt}(m) = \dot{m}_{in}$
- $\frac{d}{dt}(mu) = \dot{m}_{in}h_{in} + A_{wall}\alpha_{in}(T_{wall}|_{x=0} - T)$
- Unsteady heat conduction equation and boundary conditions are applied to obtain the temperature distribution in the wall:
- $\frac{\partial T_{wall}}{\partial t} = a_{wall}\frac{\partial^2 T_{wall}}{\partial x^2}$
- $-\lambda_{wall}\frac{\partial T_{wall}}{\partial x}\Big|_{x=0} = \alpha_{in}(T - T_{wall}|_{x=0})$
- $-\lambda_{wall}\frac{\partial T_{wall}}{\partial x}\Big|_{x=l} = \alpha_{out}(T_{wall}|_{x=l} - T_{amb})$

Validation for 0D/1D models

- Validation for different tank sizes and refueling conditions:
  - 165 L type IV H70 tank at Nikola
  - 244 L type IV H70 tank at ZBT
  - 322 L type III H35 tank at ZBT

Validation for 0D/1D models: 165 L type IV H70 tank at Nikola – Experimental setup

PRHYDE
Protocol for heavy-duty Hydrogen refuelling



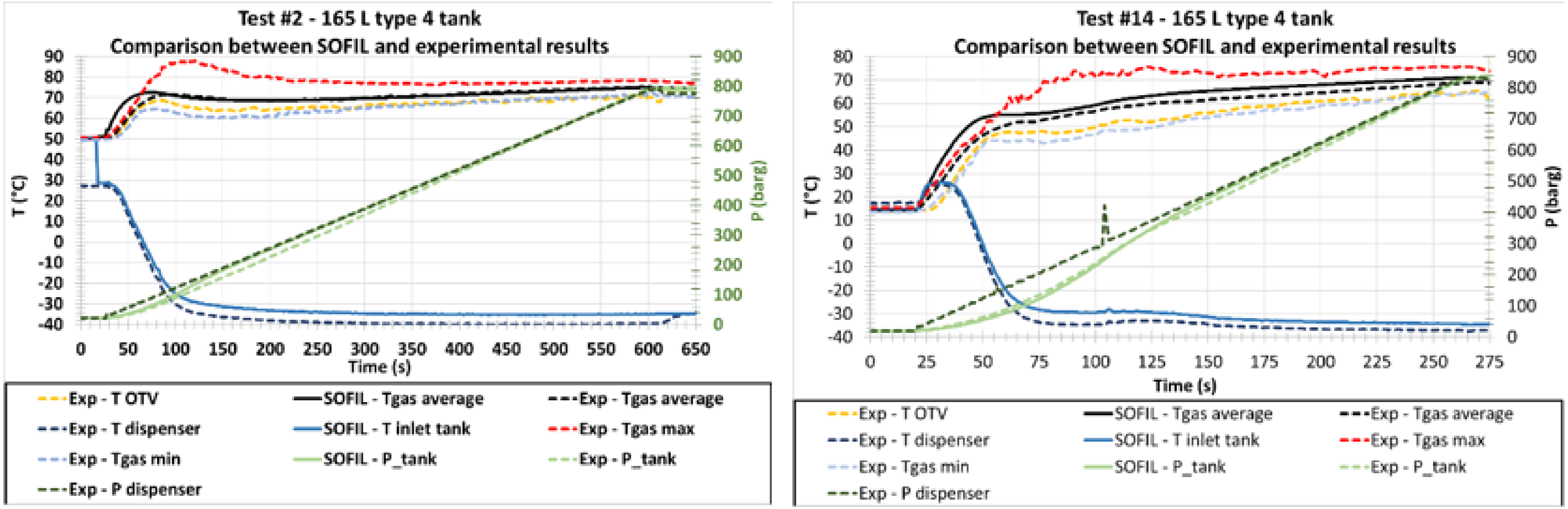
Validation for 0D/1D models: 165 L type IV H70 tank at Nikola – Test matrix

PRHYDE
Protocol for heavy-duty Hydrogen refuelling

Test matrix for H70 165 L type IV tank at Nikola

Test Number	Ambient Temperature (°C)	Initial P (bar)	Dispenser Temperature Profile (°C)	Dispenser Pressure Profile
1	15	20	-40	Constant PRR 8 MPa/min
2	50	20	-40	Constant PRR 8 MPa/min
3	40	20	-40	Constant PRR 8 MPa/min
4	-30	20	-40	Constant PRR 8 MPa/min
5	-15	20	-40	Constant PRR 8 MPa/min
6	0	20	-40	Constant PRR 8 MPa/min
7	15	20	-33	Constant PRR 8 MPa/min
8	15	20	-26	Constant PRR 8 MPa/min
9	15	20	-17.5	Constant PRR 8 MPa/min
10	15	50	-40	Constant PRR 8 MPa/min
11	15	250	-40	Constant PRR 8 MPa/min
12	15	20	-40	Constant PRR 5 MPa/min
13	15	20	-40	Constant PRR 16 MPa/min
14	15	20	-40	Constant PRR 20 MPa/min
15	15	20	-40	20 MPa/min for 3.85 min, transition to 1 MPa/min
16	15	20	-40	20 MPa/min for 3.85 min, transition to 3 MPa/min
17	15	20	-40	20 MPa/min for 3.33 min, transition to 1 MPa/min with pulse of 8 MPa/min for 10s every 30s
18	40	20	-17.5	Constant PRR 8 MPa/min

Validation for 0D/1D models: 165 L type IV H70 tank at Nikola – Comparison between modeling results and experiments

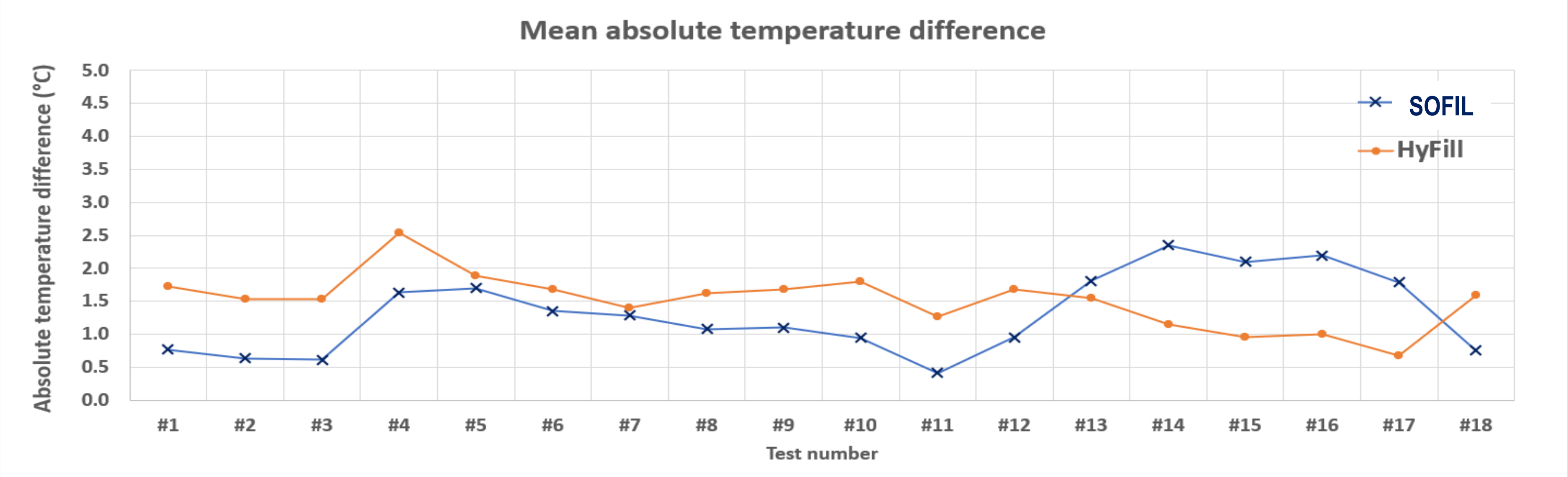


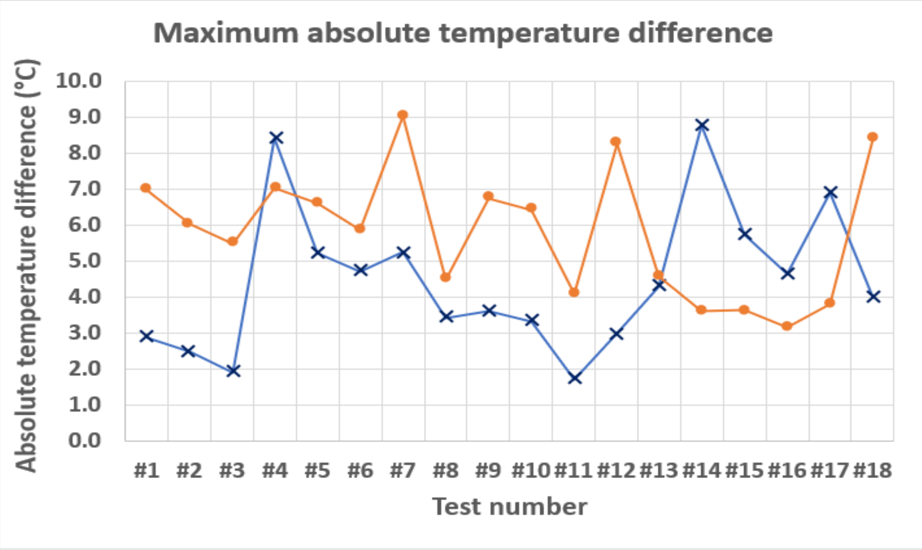
(a)

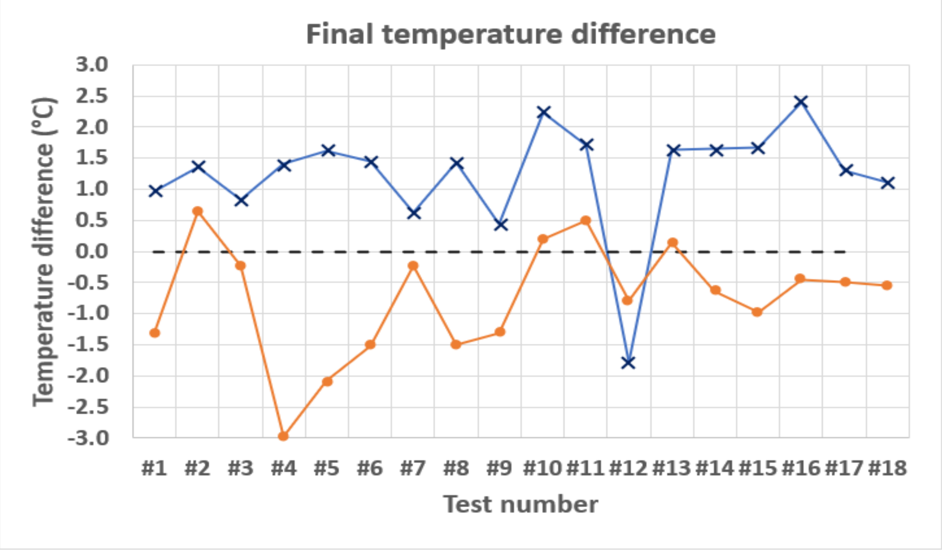
(b)

Figure 2 – Comparison between the simulation results and the experimental data for the refueling tests #2 (a) and #14 (b) of H70 165 L type IV tank performed at Nikola

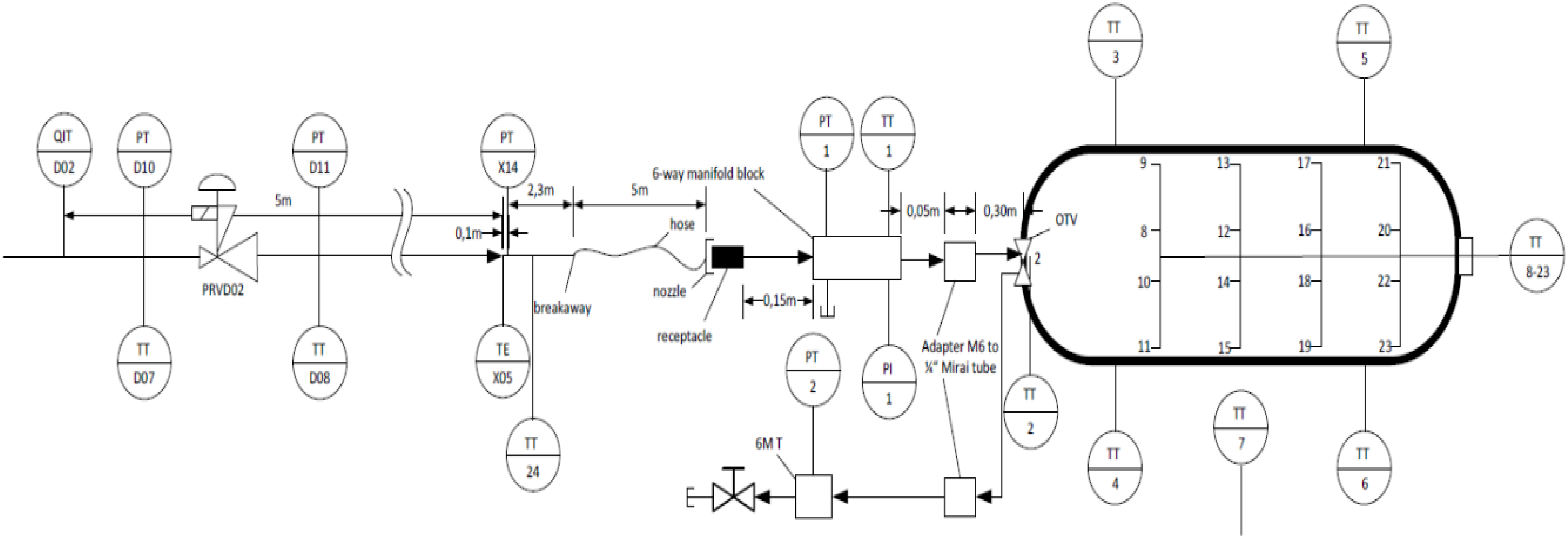
Validation for 0D/1D models: 165 L type IV H70 tank at Nikola – Comparison between modeling results and experiments


Mean absolute temperature difference


Maximum absolute temperature difference


Final temperature difference

Validation for 0D/1D models: 244 L type IV H70 tank at ZBT – Experimental setup



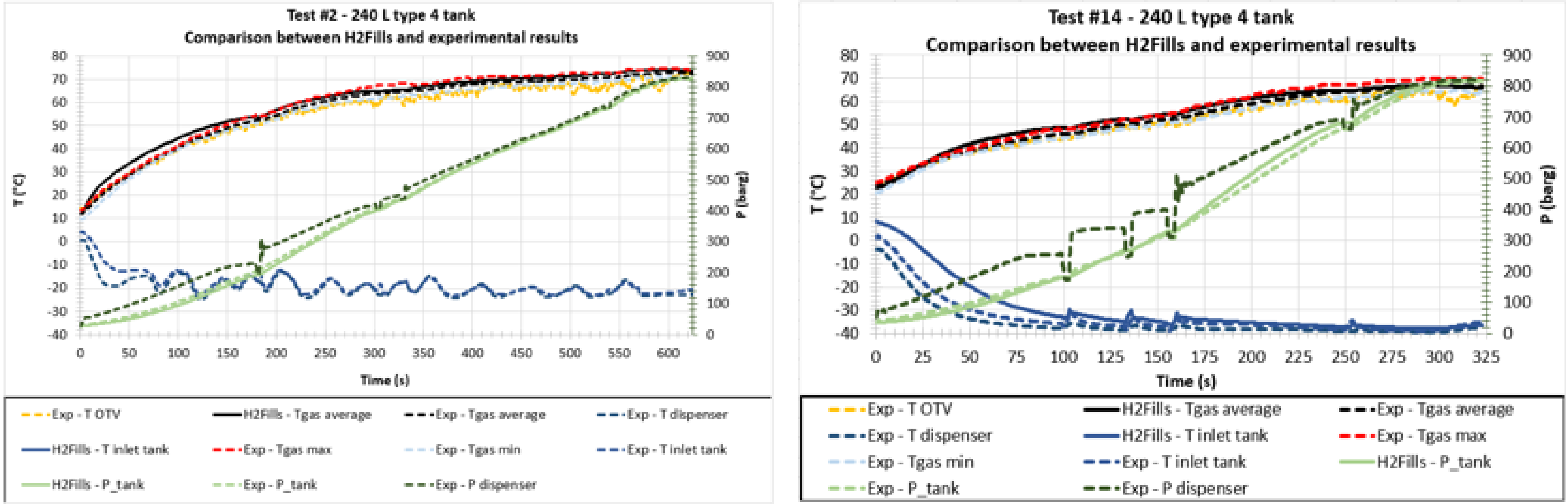
Validation for 0D/1D models: 244 L type IV H70 tank at ZBT – Test matrix

PRHYDE
Protocol for heavy-duty Hydrogen refuelling

Test matrix for H70 244 L type IV tank at ZBT

Test Number	Initial P (bar)	Dispenser Temperature Profile	Dispenser Pressure Profile
#1 (ref)	20	-40°C	Constant PRR 8 MPa/min
#2	20	-20°C	Constant PRR 8 MPa/min
#3	20	-10°C	Constant PRR 8 MPa/min
#4	20	0°C	Constant PRR 8 MPa/min
#5	20	-40°C for 5 min, then no cooling	Constant PRR 8 MPa/min
#6	20	No cooling for 4 min 30, then -40°C	Constant PRR 8 MPa/min
#7	20	-40°C for 5 min, then -20°C	Constant PRR 8 MPa/min
#8	70	-40°C	Constant PRR 8 MPa/min
#9	350	-40°C	Constant PRR 8 MPa/min
#10	20	-40°C	Constant PRR 5 MPa/min
#10bis	20	-40°C	Constant PRR 1 MPa/min
#11	20	-40°C	16 MPa/min for 3.85 min, transitions to 1 MPa/min
#12	20	-40°C	16 MPa/min for 3.85 min, transitions to 3 MPa/min
#13	20	-40°C	Constant PRR 3 MPa/min
#14	20	-40°C	Constant PRR 16 MPa/min
#17 (ref)	20	-40°C	Constant PRR 8 MPa/min

Validation for 0D/1D models: 244 L type IV H70 tank at ZBT – Comparison between modeling results and experiments

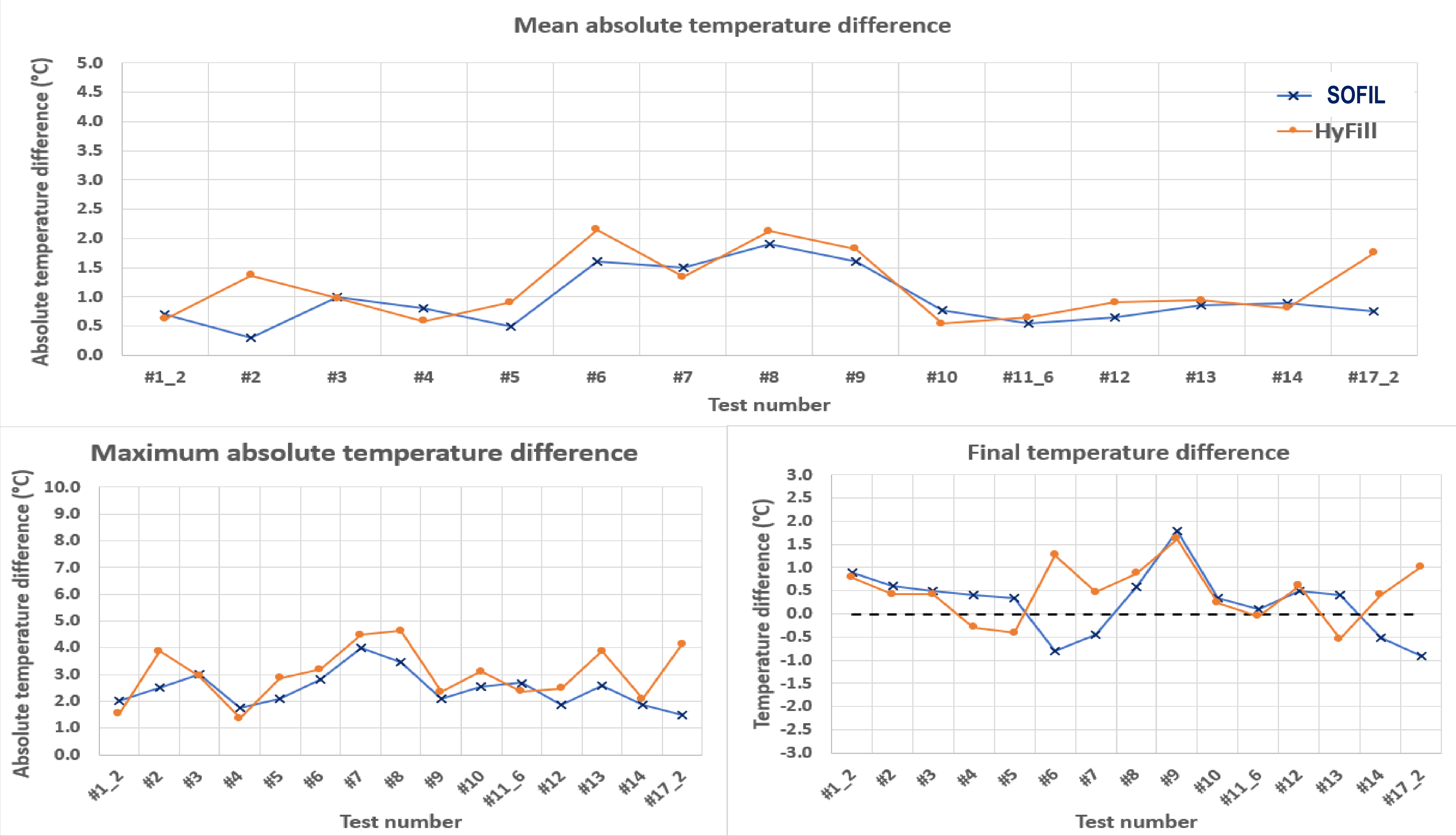


(a) *(b)*

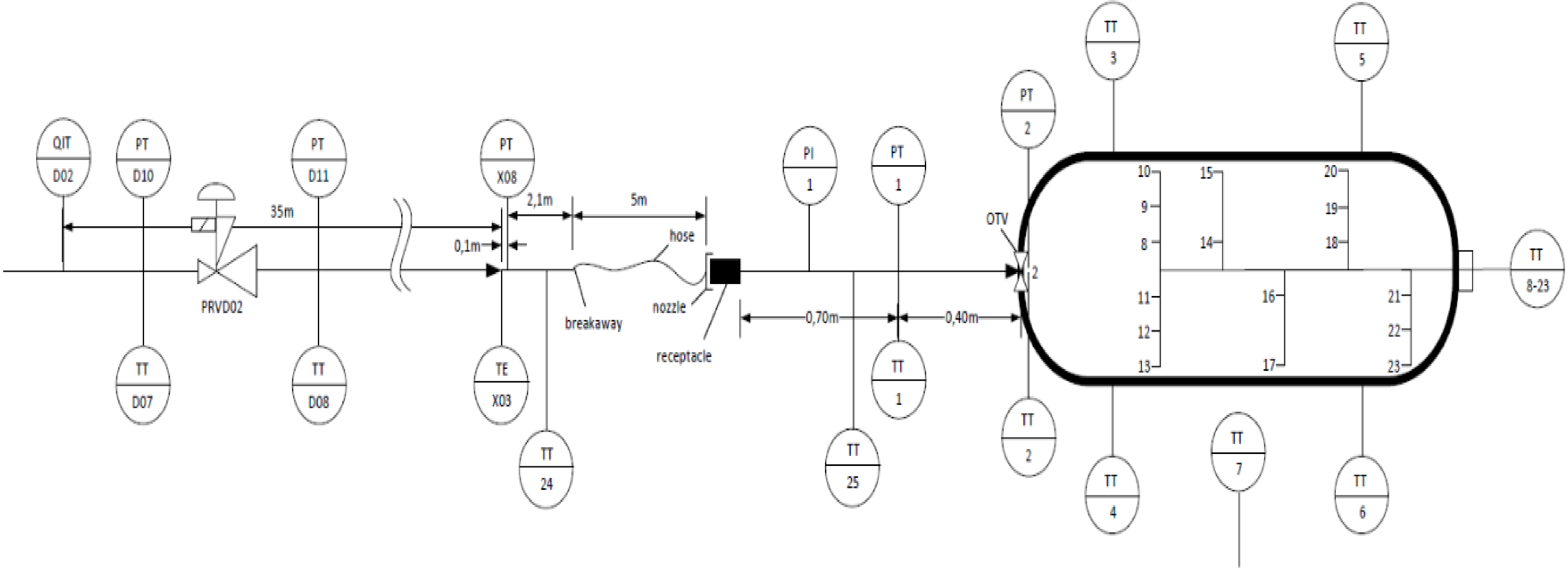
Figure 5 - Comparison between the simulation results of H2Fills and the experimental data for the refueling test #2 (a) and #14 (b) of 244 L type IV tank performed at ZBT

Validation for 0D/1D models: 244 L type IV H70 tank at ZBT – Comparison between modeling results and experiments

PRHYDE
Protocol for heavy-duty Hydrogen refuelling



Validation for 0D/1D models: 322 L type III H35 tank at ZBT – Experimental setup



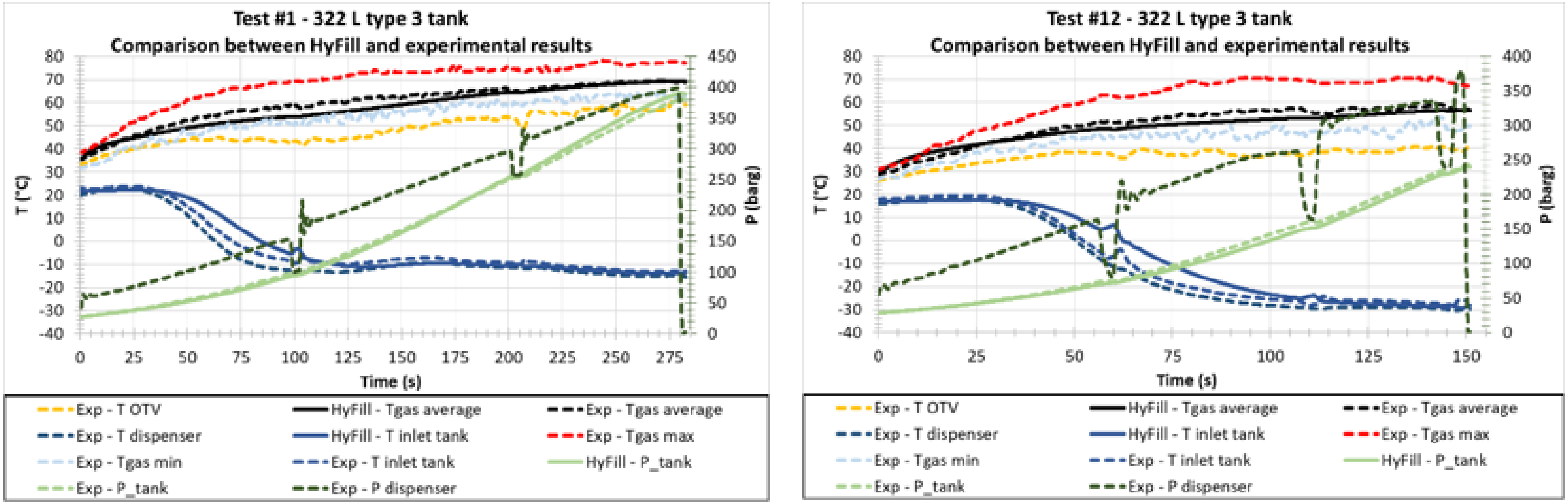
Validation for 0D/1D models: 322 L type III H35 tank at ZBT – Test matrix

Test matrix for 322 L type III tank at ZBT

Test Number	Initial P (bar)	Dispenser Temperature Profile	Dispenser Pressure Profile
#1 (ref)	20	-20°C	Constant PRR 8 MPa/min
#2	20	-40°C	Constant PRR 8 MPa/min
#3	20	-10°C	Constant PRR 8 MPa/min
#4	20	0°C	Constant PRR 8 MPa/min
#5	20	no cooling	Constant PRR 8 MPa/min
#6	20	-40°C for 5 min, then no cooling	Constant PRR 8 MPa/min
#8	70	-20°C	Constant PRR 8 MPa/min
#9	150	-20°C	Constant PRR 8 MPa/min
#10	20	-20°C	Constant PRR 4 MPa/min
#11	20	-20°C	Constant PRR 3 MPa/min
#12	20	-20°C	Constant PRR 14 MPa/min
#13	20	-20°C	PRR 14 MPa/min for 2.75 min, then 1 MPa/min
#14	20	-20°C	PRR 14 MPa/min for 2.5 min, then 3 MPa/min
#15	20	-20°C	Simulate Tgas Throttle with initial PRR 12 MPa/min
#16	20	-20°C	Simulate Tgas Throttle with initial PRR 10 MPa/min
#17	20	-20°C	Simulate Tgas Throttle with initial PRR 8 MPa/min
#18 (ref)	20	-20°C	Constant PRR 8 MPa/min

Validation for 0D/1D models: 322 L type III H35 tank at ZBT – Comparison between modeling results and experiments

H2 PRHYDE
Protocol for heavy-duty Hydrogen refuelling

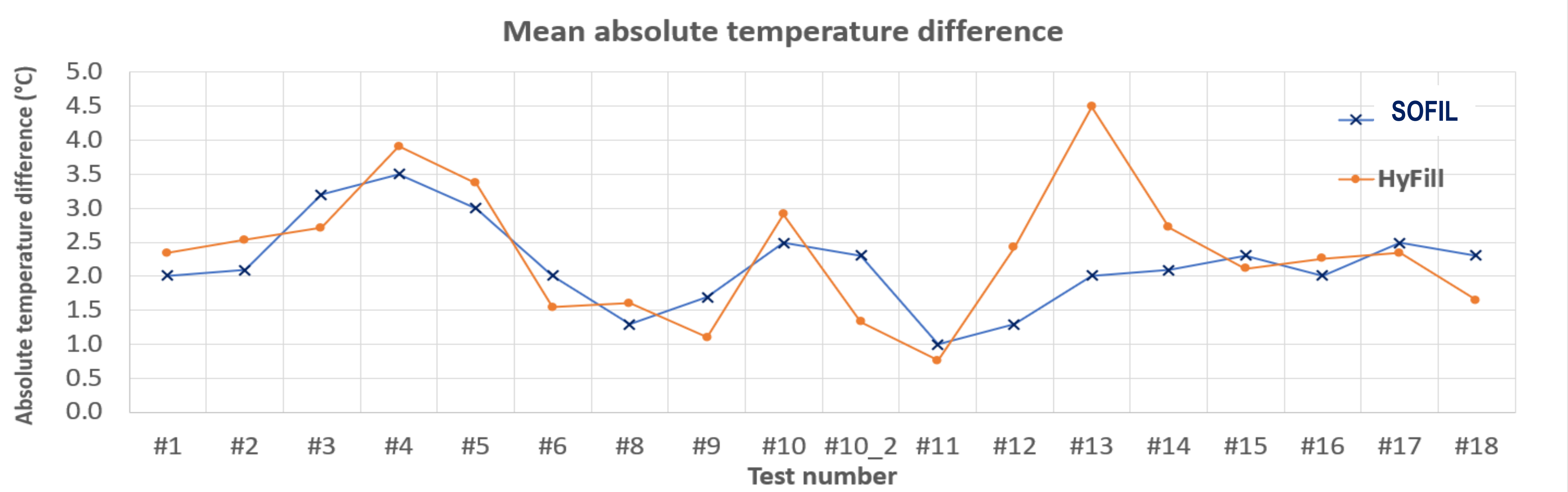


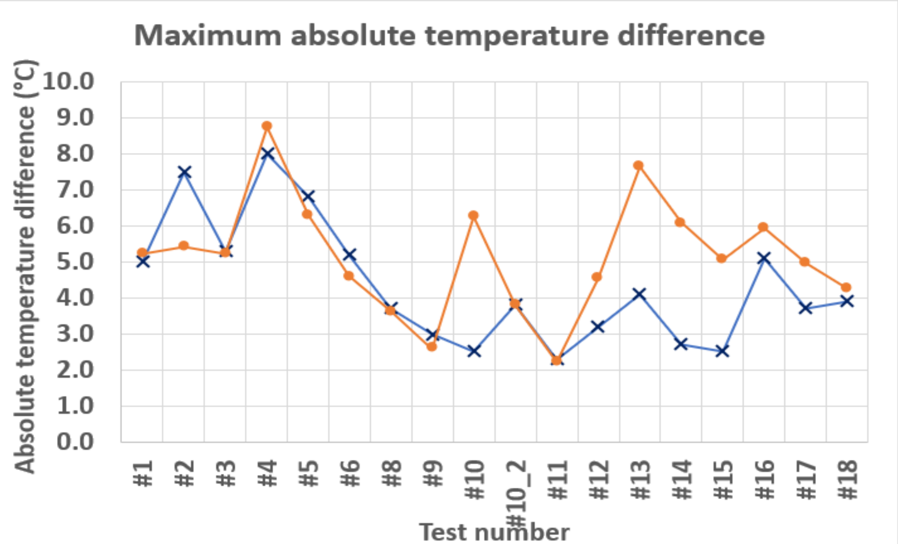
(a) *(b)*

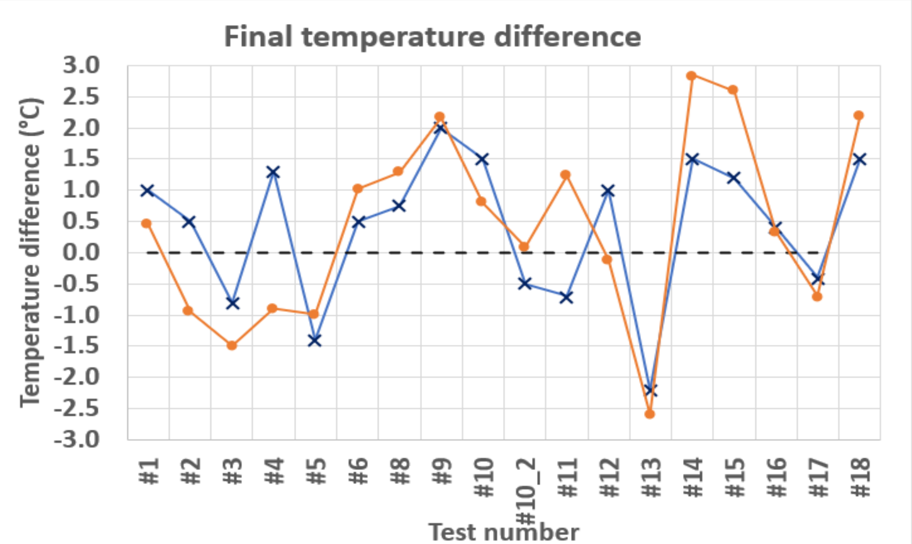
Figure 8 - Comparison between the simulation results and the experimental data for the refueling test #1 and #12 of 322 L type III tank performed at ZBT

Validation for 0D/1D models: 322 L type III H35 tank at ZBT – Comparison between modeling results and experiments

H_2 PRHYDE
Protocol for heavy-duty Hydrogen refuelling


Mean absolute temperature difference


Maximum absolute temperature difference


Final temperature difference

Conclusions and recommendations

- 0D/1D models once validated are very useful to define gas refueling protocols for different vehicle sizes and potentially could replace experimental systematic approach
- SOFIL, HyFill and H2FillS after validation were used to select the better approach for HD refueling protocol
- These models can estimate volume average gas temperature and surface average wall temperature for different refueling conditions within +/-3°C of uncertainty
- Nowadays 0D/1D models are not able to calculate the maximum local temperature once thermal stratification occurs during filling
- These models indicate the appearance of thermal stratification for axial injection. For non axial injections, experimental or CFD approach is still needed