Engineering models for refueling protocol development: validation and recommendations.

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Abstract

The **PRHYDE project (PRotocol for heavy duty HYDrogEn refueling)** 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. Development of a protocol requires a validated approach. Due to the limited time and budget, the experimental data cannot cover the whole possible ranges of protocol parameters such as initial vehicle pressure and temperature, ambient and precooling temperatures, pressure ramp, refueling time, hardware specifications etc. Hence, a validated numerical tool is essential for a safe and efficient protocol development. For this purpose, engineering tools are used. They give good results in a very reasonable computation time of several seconds or minutes. These tools provide the heat parameters estimation in the gas (volume average temperature) and 1D temperature distribution in the tank wall. The following models were used SOFIL (Air Liquide tool), HyFill (by ENGIE) and H2Fills (open access code by NREL). The comparison of modelling results and experimental data demonstrated a good capability of codes to predict the evolution of average gas temperature in function of time. Some recommendations on model validation for the future protocol development are given.

Keywords: *Engineering models, refueling protocol, modelling, validation, recommendations*

Introduction

The emission of global transport greenhouse gases accounts for over one fifth of global emissions [1]. The objective of the European Union is to reduce the heavy-duty transport emission of 90% by 2040 [2]. The most promising technology to overtake the market of heavy-duty transport (trucks, buses, trains, boats) is hydrogen fuel cell technology. But to reach this ambitious goal, it is necessary that along the development of the vehicles there is a correspondent effort in the advance of hydrogen refueling infrastructure and the associated protocols.

Hydrogen refueling stations (HRS) are needed to be safe, easy-to-use, and fast. The PRHYDE project [3] focused on the definition and development of new and advanced refueling protocols for heavy duty transports. Such protocols, like the one developed by the SAE, referenced J2601 [4], detail process control requirements for the station to respect limits on gas or tank wall temperature, and gas density.

By controlling the gas delivery temperature as well as the pressure ramp rate, thus the filling time, it is possible to regulate the gas temperature and density inside the tank. This regulation aims to avoid the occurrences of over-heating (exceeding gas or wall temperature limits) or over-filling (exceeding density limit) that lead to tanks degradation or even to a one-time failure. Hence predicting as precisely as possible the temperature and the gas density increase inside the tank is critical to achieve the best operational conditions.

Nowadays, HRS's design is based on the protocol used. Protocol development is a long and complicated process to be followed, which requires modelling tools and experimental validation. This can take up to 3 or 4 years, as in the HyTransfer project [5], which also makes the development of a standard protocol very expensive. The usage of validated modelling tools can significantly accelerate the protocol development and reduce its cost with limited experimental campaign. To achieve this target only validated models should be used. Several models have already been developed and detailed. Johnson et al. [6], Galassi et al. [7], Bourgeois et al. [8], Melideo and Baraldi [9] and Melideo et al. [10] compared experimental data with Computational Fluid Dynamics (CFD) results and predictions from one-dimensional modelling for hydrogen fast fillings. Average gas properties could be predicted reasonably well with simple models, and CFD computations allowed to understand more thoroughly all underlying phenomena.

The current paper is dedicated to show the comparison of the data collected during PRHYDE experimental campaign with the simulation performed with the codes for modelling of tank refueling. The three codes used in this article are SOFIL by Air Liquide, HyFill by ENGIE, H2FillS by NREL.

Modelling tools

Air Liquide's SOFIL

The SOFIL model assumes homogeneous gas temperature and pressure in the tank (0D), and 1D temperature evolution in the tank wall. The model accounts for the unsteady state behaviour of temperature and pressure inside the tank during the different phases of gas transfer (refueling and defueling). The 0D-gas/1D-wall approach has been found in comparison to experiments to be predictive, allowing to estimate the gas as well as the tank wall temperature accurately [8][9][10][11].

The model solves mass and energy balance equations to estimate gas temperature and pressure, and tank wall temperature in function of time and along the wall thickness. A real gas equation with the gas compressibility factor is used for the gas equation of state. The model considers, if present, the tank bosses. The piping, from dispenser to FCV tank, can be modelled through a lumped thermal mass or a more precise 2D (radially and longitudinally) discretization.

The pressure drop formula used to determine the mass flow into the tank is presented in Equation (1) for the sonic ($P_1 > 2\ P_2$) and subsonic ($P_1 \leqslant 2\ P_2$) conditions:

$$\frac{dm_g}{dt} = \begin{cases} C\ k_v P_1 \sqrt{\dfrac{\rho_N}{T_1}} & if\ P_1\ >\ 2\ P_2 \\ 2\ C\ k_v \sqrt{\dfrac{\rho_N\ (P_1 -\ P_2)P_2}{T_1}} & if\ P_1 \leqslant 2\ P_2 \end{cases} \qquad 1$$

where m_g is the gas mass in the tank (kg), C a constant equal to 257, k_v the equivalent flow coefficient (m^3/h) which represents a virtual valve that has the same flow coefficient as the whole piping system and different elements between dispenser and tank vehicle, P_1 the upstream pressure (bara) at the dispenser, P_2 the downstream pressure ρ_N the gas density (kg/Nm^3) at normal conditions (0°C, 1 atm) and T_1 the upstream temperature (K).

ENGIE's HyFill

To contribute to the reflection on hydrogen mobility and more particularly on hydrogen refueling stations, the ENGIE Lab CRIGEN has initiated the development of a tool called HyFill. HyFill is developed on MATLAB/Simulink and allows to simulate the fast filling of hydrogen tanks from the dispenser to inside tank 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 one-dimensional radial heat conduction equation. To have access to the temperature, mass, and pressure of the gas in the tank, a system of three equations is solved at each time step during the whole filling or emptying simulation; these are the mass rate balance, the energy rate balance for a control volume and the equation of state here given by [12]:

$$\begin{cases} \dfrac{dm}{dt} = \dot{m}_{in} - \dot{m}_{out} \\ \dfrac{dmu}{dt} = \dot{m}_{in}h_{in} - \dot{m}_{out}h_{out} - Q_{gas-wall} \\ \dfrac{P}{\rho} = ZRT \end{cases} \tag{2}$$

In this equation system, m is the hydrogen mass in the tank, $\dot{m}_{in}$ and $\dot{m}_{out}$ are the inlet and outlet mass flow rate respectively, u is the specific internal energy, h is the specific enthalpy, P, T and ρ are hydrogen pressure, temperature and density respectively, Z is the hydrogen compressibility factor, R is the gas constant. The hydrogen compressibility factor as well as all other thermodynamic properties of hydrogen are calculated in HyFill using the GERG-2008 equation of state [13]. The heat flow from the gas to the tank wall is given by Equation (3):

$$Q_{gas-wall} = S_{in}H_{in}\left(T - T_{wall_{r=r_{in}}}\right) \tag{3}$$

Where S_{in} is the inner wall surface of the tank, H_{in} is the inner film heat transfer coefficient determined from the correlation for internal turbulent flow [14], $T_{wall_{r=r_{in}}}$ is the temperature of the inner wall of the tank. It is obtained by solving the unsteady one-dimensional radial heat conduction equation (assuming azimuthal symmetry as the tank wall temperature is the same along its entire length for a given radius) given by [16], in Equation (4):

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\lambda}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) \tag{4}$$

The boundary conditions necessary to solve this equation being the heat flow from gas to the inner tank wall ($Q_{gas-wall}$) and the heat flow from the outer tank wall to the ambient air:

$$Q_{wall-air} = S_{out}H_{out}\left(T_{wall_{r=r_{out}}} - T_{amb}\right) + \varepsilon_{wall}\sigma S_{out}\left(T^4_{wall_{r=r_{out}}} - T^4_{amb}\right) \tag{5}$$

where H_{out} is the outer film heat transfer coefficient kept constant (natural convection assumption), S_{out} is the outer wall surface of the tank, $T_{wall_{r=r_{out}}}$ is the temperature of the outer wall of the tank, T_{amb} is the ambient temperature, ε_{wall} is the emissivity of the external wall of the tank, σ is the Stefan-Boltzmann constant.

HyFill considers that the fueling line composed of stainless-steel pipe, breakaway, hose, nozzle, receptacle, on-tank valve (OTV), is modeled as a cylindrical pipe. The geometric model of the pipe conserves the fueling line thermal mass.

The pipe is then discretized longitudinally. In each longitudinal cell the following energy balance between the gas and the wall is solved.

$$\begin{cases} \dfrac{dm}{dt} = 0 = \dot{m}_{in} - \dot{m}_{out} \\ \dfrac{dmu}{dt} = 0 = \dot{m}_{in}\left(h_{g,out} - h_{g,in}\right) + \dot{Q}_{gas-wall} \\ \dot{Q}_{gas-wall} = -H_{int}\, S_{int}(T_{g,in} - T_{wall,r=r_{in}}) \end{cases} \tag{6}$$

Where S_{int} is the inner wall surface of the pipe, H_{int} is the inner film heat transfer coefficient determined from the correlation for internal turbulent flow [15], $T_{wall_{r=r_{in}}}$ is the temperature of the inner wall of the pipe. The thermal balance between the wall and the ambient is solved with the same method presented for the tank wall.

The flow equation used to determine the mass flow into the tank is derived from IEC 60534 standard [17] presented in Equation (7) for the sonic conditions ($P_1 > 2P_2$) and for the subsonic conditions ($P_1 \leqslant 2P_2$):

$$\frac{dm_g}{dt} = \begin{cases} \rho_1 N k_{v,eq} \frac{2}{3}\sqrt{\frac{P_1}{2\rho_1}} & if\ P_1 > 2\,P_2 \\ \rho_1 N k_{v,eq}\left(1 - \frac{2}{3}\frac{P_1 - P_2}{P_1}\right)\sqrt{\frac{(P_1 - P_2)}{\rho_1}} & if\ P_1 \leqslant 2\,P_2 \end{cases} \quad 7$$

where mg is the mass of gas in the tank (kg), ρ_1 the upstream gas density (kg/m³), N a constant equal to 31.6, P_1 the upstream gas pressure (bara) at the dispenser, P_2 the downstream gas pressure (bara) in the tank. $k_{v,eq}$ is the equivalent flow coefficient (m³/h) of fueling line from the dispenser to the tank.

NREL's H2FillS

The tank model described in [18], [19] has been implemented in the H2FillS software. Initially, the FCEV tank is given a pressure, temperature, internal volume, internal surface area, internal diameter, and the thermal properties of the liner and carbon fiber reinforced polymer (CFRP). After the values are set to the tank model, the mass and energy balances are calculated with the assumption that the tank volume does not increase with the pressure rise. The governing equations for the mass and energy balances are shown as follows:

$$\begin{cases} \frac{d}{dt}(m) = \dot{m}_{in} \\ \frac{d}{dt}(mu) = \dot{m}_{in}h_{in} + A_{wall}\alpha_{in}(T_{wall}|_{x=0} - T) \end{cases} \quad 8$$

Where m is the hydrogen mass, u is the specific internal energy, $\dot{m}_{in}$ is the mass flow rate, $h_{in}$is the specific enthalpy, A_{wall} is the inner surface area in the tank a_{in} the heat transfer coefficient at the inner surface, T is the hydrogen temperature, $T_{wall}|_{x=0}$ is the inner surface wall temperature, dt is the time step, and t is the time. When the energy and mass balances are solved by the equations, the state inside the tank is assumed to be a lumped model; thus, the acquired temperature and pressure are treated as mean values calculated by the bulk specific internal energy and density. The heat conduction in the wall is assumed to be one-dimensional. It is assumed that the tank wall is a flat plate, even though the tank shape is cylindrical. This is because the curvature radius of the tank is large compared to the wall thickness. (The effectiveness of this assumption has been examined.) Hence, the following unsteady heat conduction equation and boundary conditions are applied to obtain the temperature distribution in the wall:

$$\begin{cases} \frac{\partial T_{wall}}{\partial t} = a_{wall}\frac{\partial^2 T_{wall}}{\partial x^2} \\ -\lambda_{wall}\frac{\partial T_{wall}}{\partial x}\Big|_{x=0} = \alpha_{in}(T - T_{wall}|_{x=0}) \\ -\lambda_{wall}\frac{\partial T_{wall}}{\partial x}\Big|_{x=l} = \alpha_{out}(T_{wall}|_{x=l} - T_{amb}) \end{cases} \quad 9$$

where a_{wall} is the thermal diffusivity, x is the position at which $x = 0$ is the inner wall surface and $x = l$ is the total thickness of the wall, λ_{wall} is the thermal conductivity, a_{out} is the heat transfer coefficient at the outer surface, and T_{amb} is the ambient temperature. The value of a_{out} was set to 8.0 W/(K·m^2). The value of a_{in} was derived from a Nusselt number correlation based on the Reynolds number at the tank inlet and Rayleigh number inside the tank.

The equations implemented in the model for the mass flow calculation are based on two steps:

1. Volumetric flow rate (m³/h) calculation calculates the volumetric flow rate based on the differential pressure at the inlet and outlet of the valve (P_{in} and P_{out}), temperature at the inlet of the valve T_{in}, and specific gravity to air G.

$$\dot{V} = \begin{cases} 2930\, C_v \sqrt{\dfrac{(P_{in} - P_{out})(P_{in} + P_{out})}{P_{in} G T_{out}}} & if\ P_{in} \leq 2P_{out}\ \text{(non} - \text{choked flow)} \\ 2538 C_v \dfrac{P_{in}}{G T_{in}} & if\ P_{in} > 2P_{out}\ \text{(choked flow)} \end{cases} \quad 10$$

2. Conversion to mass flow rate (kg/s): Converts the volumetric flow rate (m³/h) to the mass flow rate (kg/s) using density at 0.1 MPa and 15.6°C and a coefficient β, developed to handle the unsteady flow during the fueling process:

$$\dot{m} = \frac{\beta \rho \dot{V}}{3600} \quad 11$$

Model validation with experiments

HyFill and SOFIL were validated by using the experimental data collected during the test campaign performed for the European Project PRHYDE. The refueling tests were performed at the Nikola facility and at the *Zentrum für BrennstoffzellenTechnik* (ZBT) facility in Duisburg, Germany, using three experimental rigs with three different tanks. The properties of the fueling lines are reported in Table 1 and the corresponding tanks in Table 2.

Table 1 - List of geometric and thermal characteristics of the fueling lines at ZBT and Nikola.

Fueling line	Unit	ZBT H70	ZBT H35	NIKOLA
Length	[m]	8.0	8.5	2.4
Internal Diameter	[mm]	5.16	5.16	5.16
Thermal Mass	[kJ/K]	5.7	6.2	4.6
Kv equivalent	[m^3/h]	0.095	0.124	0.110

Table 2 - List of geometric and thermal characteristics of the tanks tested at ZBT and Nikola.

Tank specifications	Unit	ZBT H70	ZBT H35	NIKOLA
Type	-	Type IV	Type III	Type IV
Tank volume	[l]	244	322	164.8
Nominal Working Pressure	[bar]	700	350	700
Diameter internal	[m]	0.4	0.4	0.3
Length internal	[m]	1.8	3.6	2.2
Thermal Mass Liner	[kJ/K]	37	40	40
Thermal Mass Composite	[kJ/K]	169	107.	122
Thermal Mass Boss	[kJ/K]	3	-	5

For the tests conducted at Nikola the testing rig consisted of a dispenser and a climatic chamber able to simulate different ambient temperatures around the tank, but the fueling line does not include the breakaway and the hose as it consists of only stainless-steel piping. At ZBT it was not possible to control the ambient temperature, but the tests were effectuated with the fueling lines used in refueling stations.

The measured data used for the validation are:

- the mass flow rate flowing from the dispenser to the tank,
- the dispenser temperature and pressure (T dispenser and P dispenser),
- the injection temperature (T inlet tank),
- the gas pressure in the tank (P tank),

- the average gas temperature in the tank, which is calculated as the average value of the thermocouples equally distributed inside the tank to compensate the effect of horizontal and vertical stratification (Tgas average). Along with the average temperature the maximum (Tgas max), minimum (Tgas min), and OTV (T OTV) temperature are also traced. The accuracy for each thermocouple measured value is estimated to +/- 1°C. When making the average for the sixteen thermocouples in the gas volume, the accuracy on the measured volume average gas temperature would reach +/- 3°C.

Hexagon, type 4, H70, 165 L at Nikola

The P&ID of the experimental test rig including the tank is shown in Figure 1.

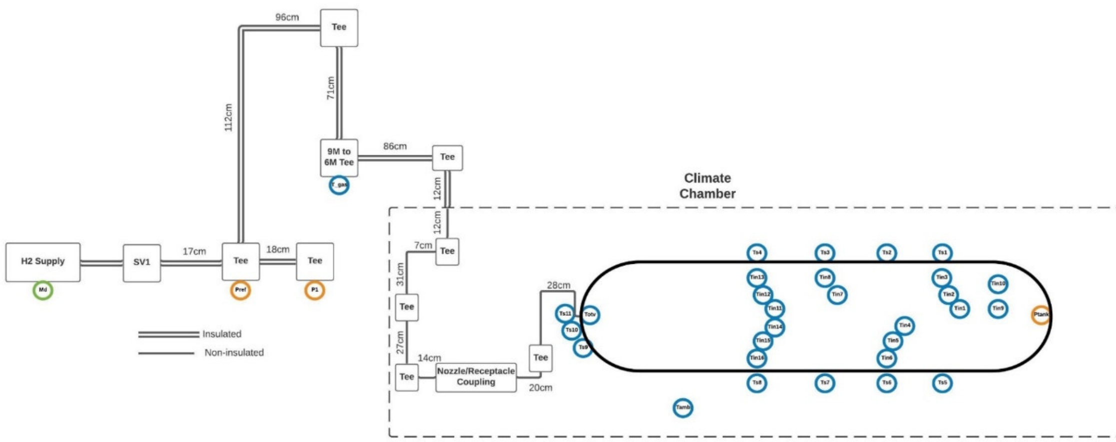


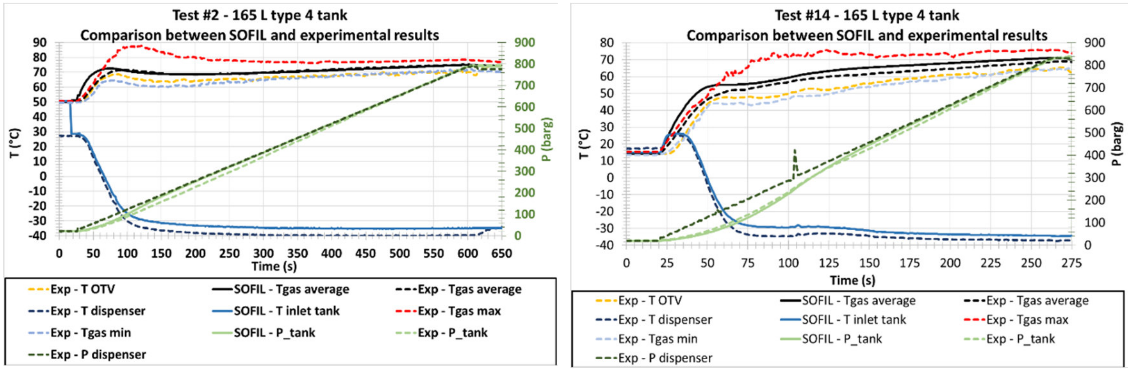
Figure 1 - P&ID of the experimental setup for the H70 165 L type IV tank at Nikola

The tests performed at Nikola are summarized in Table 3. During the tests, it was possible to change ambient temperature, initial pressure of the tank, dispenser temperature and pressure profile.

Table 3 - 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

The results for simulation using SOFIL software for filling tests #2 and #14 done at Nikola with the 165 L type IV tank are compared with the experimental in Figure 2 (a) and (b).



(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

The results for simulation using SOFIL and HyFill codes for the 18 filling tests done with the 165 L type IV tank are summarized in Figure 3.

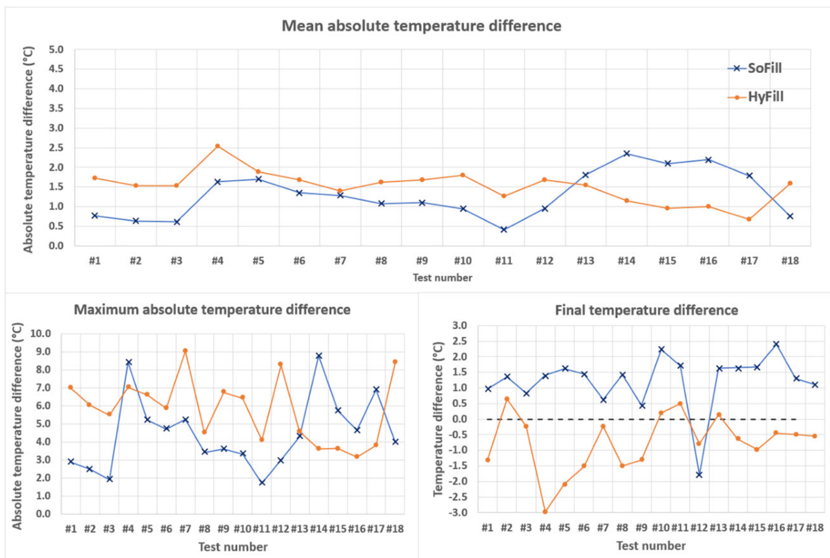


Figure 3 – Comparison between experimental temperature and the calculated temperature from SOFIL and HyFill for eighteen filling tests on H70 165 L type IV tank at Nikola

The mean absolute gas temperature difference is less than 2.5°C for all the tests as well as the gas temperature at the filling end. Consequently, the agreement between the modelling results from the two codes, SOFIL and HyFill, and the experiments for gas temperature is good for the 165 L tank.

Hexagon, type 4, H70, 244 L (at ZBT)

The P&ID of the experimental test rig at ZBT including the tank is shown in Figure 4.

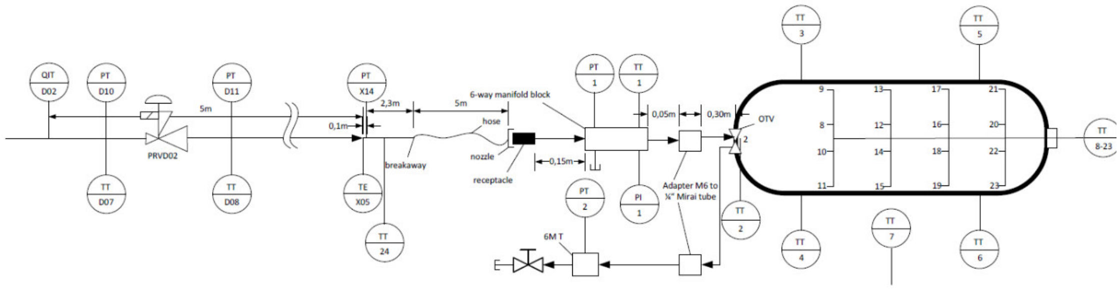


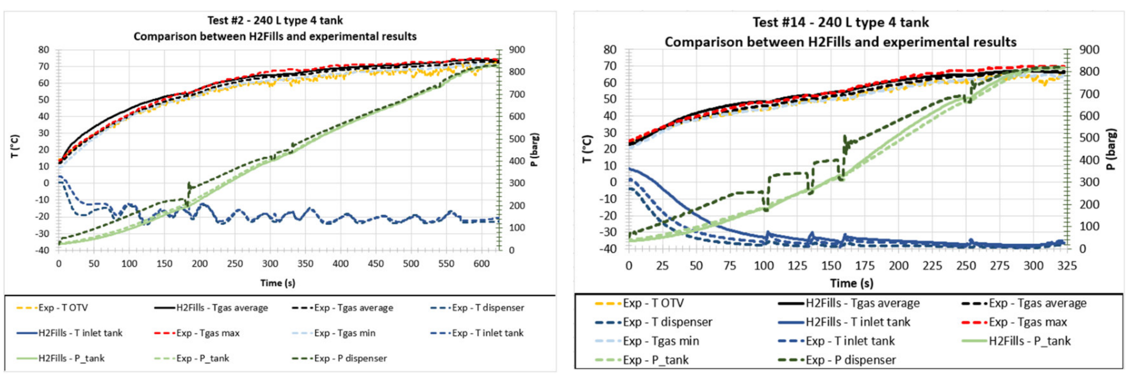
Figure 4 - P&ID of the experimental setup for the H70 244 L type IV tank at ZBT

The tests performed at ZBT on the H70 244 L type IV tank are summarized in Table 4. During the tests it was possible to change the initial pressure of the tank, dispenser temperature and pressure profile.

Table 4 - 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

The results for simulation using H2Fills software for filling tests #2 and #14 done at ZBT with the 244 L type IV tank are compared with the experimental in Figure 5 (a) and (b).



(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

The results for simulation using SOFIL and HyFill codes for the 15 filling tests done with the 244 L type IV tank are summarized in Figure 6.

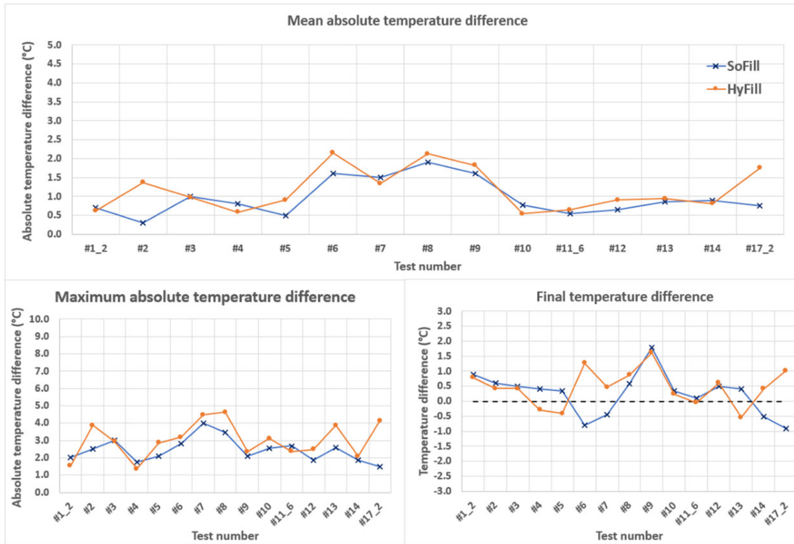


Figure 6 - Comparison between experimental temperature and the calculated temperature from SOFIL and HyFill for fifteen filling tests on 244 L type IV tank at ZBT

HyFill and SOFIL give very accurate results when reproducing the ZBT experiments on 244 L type IV tank: the mean absolute temperature difference between the experiments and the model is inferior to 2.5°C for all experiments, and the final temperature is predicted with +/- 2°C accuracy.

Luxfer, type 3, H35, 322 L (at ZBT)

The P&ID of the experimental test rig including the tank is shown in Figure 7.

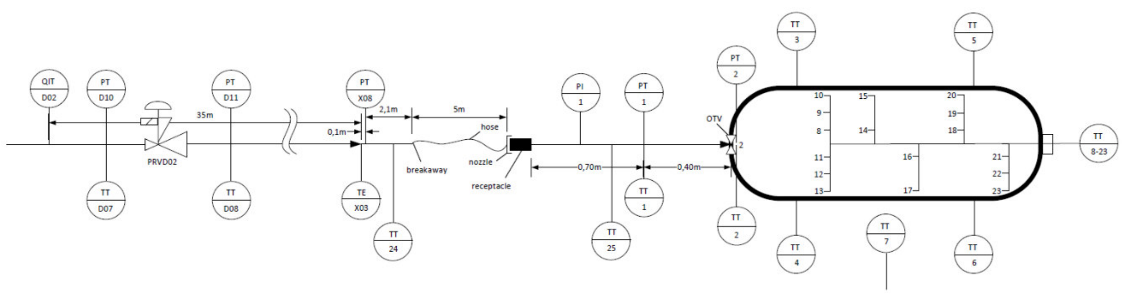


Figure 7 - P&ID of the experimental setup for the H35 322 L type III tank at ZBT

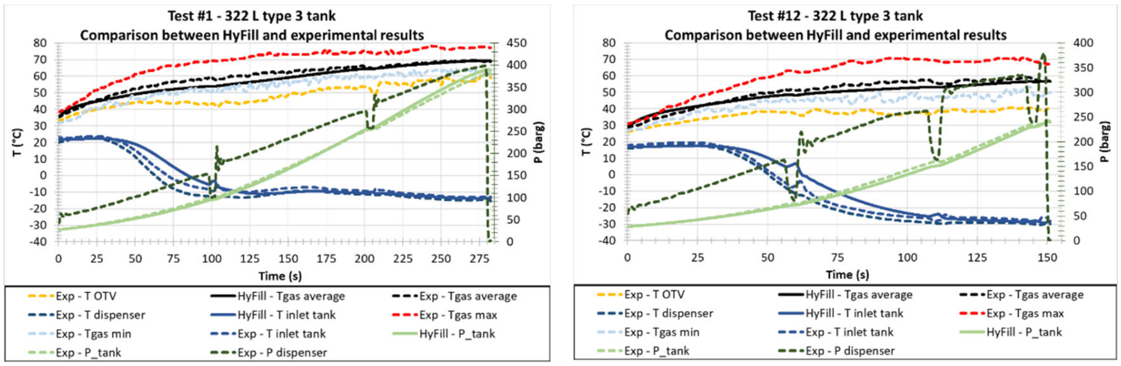
The tests performed at ZBT on the H35 322 L type III tank are summarized in Table 5. During the tests it was possible to change the initial pressure of the tank, dispenser temperature and pressure profile.

Table 5 - 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

The results for simulation using HyFill software for filling tests #1 and #12 done at ZBT with the 322 L type III tank are compared with the experimental in Figure 8 (a) and (b).



(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

The results for simulation using SOFIL and HyFill codes for the 18 filling tests done with the 322 L type IV tank are summarized in Figure 9.

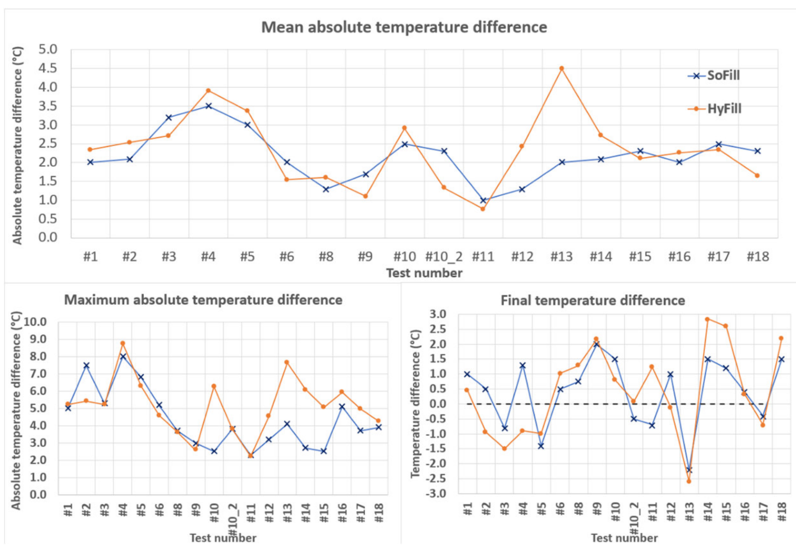


Figure 9 - Comparison between experimental temperature and the calculated temperature from SOFIL and HyFill for eighteen filling tests on 322 L type III tank at ZBT

HyFill and SOFIL give accurate results when reproducing the ZBT experiments on 322 L type III tank: the mean absolute temperature difference between the experiments and the model is inferior to 4.5°C for all experiments, and the final temperature is predicted with +/- 3°C accuracy.

Conclusions and recommendations

Engineering models such as SOFIL, HyFill and H2Fills reach an accuracy of +/- 3°C for the estimation of the volume average gas during filling of hydrogen tanks. This error is within the accuracy of the measured volume average gas temperature of +/- 4°C. These models run in a few minutes, as they have a much lower computational cost than CFD models. Nevertheless, they cannot represent/evaluate the presence of thermal gradient inside the tank volume. However, they can be used to develop refueling protocols when thermal stratifications are well mitigated by tank/OTV design or considered with additional margin [20].

These models can suggest that thermal stratification is possible by estimating the gas velocity at the inlet. According to previous studies [21] with axial injections in horizontal tanks, potential appearance of thermal stratification occurs when injection velocities are below 5 m/s.

For the development of future protocols, numerical tools such as engineering models as well as CFD can be used. However, these models should be further validated using experimental data in different tank refueling conditions.

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