



Deliverable D4.1

Report on Preliminary Simulations

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R E P O R T

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ACRONYMS AND ABBREVIATIONS

APRR	Average Pressure Ramp Rate
CHSS	Compressed Hydrogen Storage System
H ₂	Hydrogen
NWP	Nominal Working Pressure
MPD	Maximum Pressure Drop
SoC	State of Charge
WP	Work Package

1. INTRODUCTION

This document aims at answering interrogations from PRHYDE Deliverable D3.1¹ that arose from early work on protocol development in Work Package (WP) 3. Several parameters are influencing the fillings, and overheating and/or overfilling can occur. The preliminary simulations run by WP4 will quantify these effects in the configurations chosen by WP3.

In the preliminary simulations, two different simulation models were applied by Air Liquide and Engie. The models were compared and calibrated to the configurations proposed in Deliverable D3.1.

In addition to the 48 scenarios proposed in Deliverable D3.1, further calculations were launched in order to explore a case with a higher ambient temperature.

¹ Deliverable D3.1 “Report on the characteristics of the cases to be studied in the preliminary simulations” is publicly available at the PRHYDE website: <https://prhyde.eu/progress/>.

2. DEFINED PARAMETERS FOR THE PRELIMINARY SIMULATIONS

2.1 Tank characteristics

Tank characteristics necessary to launch preliminary simulations are defined in Deliverable D3.1. The following tables (Table 1 to 4) are directly taken from this report, with the addition of the injection diameter taken as 3 mm.

Table 1: Single Vessel Characteristics – Type III Single Vessel (Small)

Description	H35	H50	H70	Unit
Internal volume	0.050	0.050	0.050	[m ³]
Internal length	0.710	0.710	0.710	[m]
Internal radius	0.150	0.150	0.150	[m]
Liner thickness	0.005	0.005	0.005	[m]
Composite layer thickness	0.010	0.017	0.027	[m]
Liner material density	2700	2700	2700	[kg m ⁻³]
Liner material specific heat capacity	1106	1106	1106	[J kg ⁻¹ K ⁻¹]
Liner material thermal conductivity	164	164	164	[W m ⁻¹ K ⁻¹]
Composite wrapping material density	1494	1494	1494	[kg m ⁻³]
Composite wrapping material specific heat capacity	1120	1120	1120	[J kg ⁻¹ K ⁻¹]
Composite wrapping material conductivity	0.740	0.740	0.740	[W m ⁻¹ K ⁻¹]
Boss material density	-	-	-	[kg m ⁻³]
Boss material specific heat capacity	-	-	-	[J kg ⁻¹ K ⁻¹]
Boss volume	-	-	-	[m ³]
Boss contact surface with hydrogen	-	-	-	[m ²]
Boss contact surface with ambient air	-	-	-	[m ²]
Injection diameter	0.003	0.003	0.003	[m]

Table 2: Single Vessel Characteristics – Type III Single Vessel (Large)

Description	H35	H50	H70	Unit
Internal volume	0.350	0.350	0.350	[m ³]
Internal length	1.240	1.240	1.240	[m]
Internal radius	0.300	0.300	0.300	[m]
Liner thickness	0.005	0.005	0.005	[m]
Composite layer thickness	0.010	0.017	0.027	[m]
Liner material density	2700	2700	2700	[kg m ⁻³]
Liner material specific heat capacity	1106	1106	1106	[J kg ⁻¹ K ⁻¹]
Liner material thermal conductivity	164	164	164	[W m ⁻¹ K ⁻¹]
Composite wrapping material density	1494	1494	1494	[kg m ⁻³]
Composite wrapping material specific heat capacity	1120	1120	1120	[J kg ⁻¹ K ⁻¹]
Composite wrapping material conductivity	0.740	0.740	0.740	[W m ⁻¹ K ⁻¹]
Boss material density	-	-	-	[kg m ⁻³]
Boss material specific heat capacity	-	-	-	[J kg ⁻¹ K ⁻¹]
Boss volume	-	-	-	[m ³]
Boss contact surface with hydrogen	-	-	-	[m ²]
Boss contact surface with ambient air	-	-	-	[m ²]
Injection diameter	0.003	0.003	0.003	[m]

Table 3: Single Vessel Characteristics – Type IV Single Vessel (Small)

Description	H35	H50	H70	Unit
Internal volume	0.050	0.050	0.050	[m ³]
Internal length	0.710	0.710	0.710	[m]
Internal radius	0.150	0.150	0.150	[m]
Liner thickness	0.005	0.005	0.005	[m]
Composite layer thickness	0.015	0.022	0.032	[m]
Liner material density	945	945	945	[kg m ⁻³]
Liner material specific heat capacity	2100	2100	2100	[J kg ⁻¹ K ⁻¹]
Liner material thermal conductivity	0.500	0.500	0.500	[W m ⁻¹ K ⁻¹]
Composite wrapping material density	1494	1494	1494	[kg m ⁻³]
Composite wrapping material specific heat capacity	1120	1120	1120	[J kg ⁻¹ K ⁻¹]
Composite wrapping material conductivity	0.740	0.740	0.740	[W m ⁻¹ K ⁻¹]
Boss material density	7900	7900	7900	[kg m ⁻³]
Boss material specific heat capacity	500	500	500	[J kg ⁻¹ K ⁻¹]
Boss volume	0.002	0.002	0.002	[m ³]
Boss contact surface with hydrogen	0.045	0.045	0.045	[m ²]
Boss contact surface with ambient air	0.047	0.047	0.047	[m ²]
Injection diameter	0.003	0.003	0.003	[m]

Table 4: Single Vessel Characteristics - Type IV Single Vessel (Large)

Description	H35	H50	H70	Unit
Internal volume	0.350	0.350	0.350	[m ³]
Internal length	1.240	1.240	1.240	[m]
Internal radius	0.300	0.300	0.300	[m]
Liner thickness	0.005	0.005	0.005	[m]
Composite layer thickness	0.015	0.022	0.032	[m]
Liner material density	945	945	945	[kg m ⁻³]
Liner material specific heat capacity	2100	2100	2100	[J kg ⁻¹ K ⁻¹]
Liner material thermal conductivity	0.500	0.500	0.500	[W m ⁻¹ K ⁻¹]
Composite wrapping material density	1494	1494	1494	[kg m ⁻³]
Composite wrapping material specific heat capacity	1120	1120	1120	[J kg ⁻¹ K ⁻¹]
Composite wrapping material conductivity	0.740	0.740	0.740	[W m ⁻¹ K ⁻¹]
Boss material density	7900	7900	7900	[kg m ⁻³]
Boss material specific heat capacity	500	500	500	[J kg ⁻¹ K ⁻¹]
Boss volume	0.002	0.002	0.002	[m ³]
Boss contact surface with hydrogen	0.045	0.045	0.045	[m ²]
Boss contact surface with ambient air	0.047	0.047	0.047	[m ²]
Injection diameter	0.003	0.003	0.003	[m]

2.2 Conditions

Deliverable D3.1 also provides filling characteristics, reported in Table 5.

Table 5: Selected characteristic cases for preliminary simulations

Description	H35	H50	H70	Unit
CHSS Tank Type	III IV	III IV	III IV	
CHSS Volume	1400.0	1400.0	1400.0	[L]
Single Vessel (28 vessels)	50.0	50.0	50.0	[L]
Unit (4 vessels)	350.0	350.0	350.0	
Ambient Temperature	15.0	15.0	15.0	[°C]
Initial Pressure	6.0	8.0	10.0	[MPa]
Ref. Pressure Drop	20.0	20.0	20.0	[MPa]
Fuel Delivery Temperature	+15.0 - 20.0	+15.0 - 20.0	+15.0 - 20.0	[°C]
APRR (10 min. fuelling time)	3.78	5.45	7.75	[MPa min ⁻¹]
(15 min. fuelling time)	2.52	3.63	5.17	
Stop criteria	100.0	100.0	100.0	[%]

This leads to 48 cases, whose results will be shown in Chapter 4.

3. DEFINING PIPING k_v / C_v FLOW COEFFICIENTS

3.1 Context

The hardware through which the gas flows from the station to the vehicle compressed hydrogen storage system (CHSS) consists of several components, including a breakaway, hose, nozzle, valves and junctions. Figure 1 shows those different elements that exist between the dispenser and the vehicle CHSS.

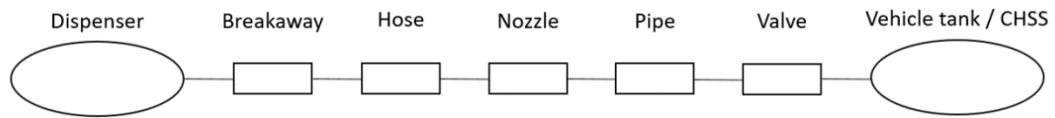


Figure 1: Illustration of different components between dispenser and vehicle tank

All these elements result in a pressure drop. As is shown in Figure 2, they are simulated as a single valve with a k_v / C_v flow coefficient² in order to simplify model and simulations.

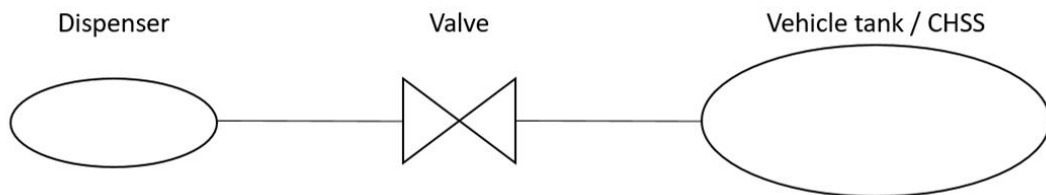


Figure 2: Elements between dispenser and vehicle tank are simulated as an equivalent valve regarding the pressure loss

Heat exchange in the piping between dispenser and vehicle CHSS has been neglected as a hypothesis for the preliminary calculations. This effect will, however, be taken into account in future simulations. For pre-cooled fillings, the heating of the hydrogen before reaching the tank will differ between the cases with 28 x 50 L and 4 x 350 L tanks, as the heat exchanges will be greater for 28 tubes and valves compared to only 4. These effects should be considered for future calculations.

The flow coefficient k_v / C_v is an inherent characteristic of the hardware through which the gas flows. It is linked to the mass flow rate Q via the pressure drop between fuel station (upstream) and vehicle CHSS (downstream). However, the link between these parameters is not fully modelled, and a number of different equations may be used in the simulation software.

² Note: k_v is the flow coefficient in metric units (m^3/h), whereas C_v is the flow coefficient in imperial units (US Gallons per minute, gpm). They are strictly equivalent and can be converted one into the other through the following relations: $k_v = 0.865 C_v$ or $C_v = 1.156 k_v$.

For a given valve, the equations below describe the relationship between the flow coefficient k_v of the valve, the mass flow rate and the pressure. In the simulations, it is assumed that these equations describe the pressure drop between fuel station (dispenser) and vehicle CHSS.

In particular, Air Liquide and Engie have been using in their in-house software the following formulas, where m_g is the mass of gas in the tank (kg), P_1 the upstream pressure (bara) at the dispenser, P_2 the downstream pressure (bara) in the tank, k_v the flow coefficient (m^3/h), ρ_1 the upstream gas density at the temperature T_1 and pressure level P_1 (kg/m^3), N a constant equal to 31.6, ρ_N the gas density at normal conditions $0^\circ C$, 1 atm (kg/Nm^3), Y an adimensional term depending on the pressure levels P_1 and P_2 and a constant $C = 257$.

$$\begin{aligned} \text{Sonic } (P_1 > 2 P_2) \quad \frac{dm_g}{dt} &= C k_v P_1 \sqrt{\frac{\rho_N}{T_1}} \\ \text{Subsonic } (P_1 \leq 2 P_2) \quad \frac{dm_g}{dt} &= 2 C k_v \sqrt{\frac{\rho_N (P_1 - P_2) P_2}{T_1}} \end{aligned}$$

Figure 3: Flow coefficient formula used by Air Liquide

$$\begin{aligned} \text{Sonic } (P_1 > 2 P_2) \quad \frac{dm_g}{dt} &= \rho_1 N k_v Y \sqrt{\frac{P_1}{2 \rho_1}} \\ Y &= \frac{2}{3} \\ \text{Subsonic } (P_1 \leq 2 P_2) \quad \frac{dm_g}{dt} &= \rho_1 N k_v Y \sqrt{\frac{(P_1 - P_2)}{\rho_1}} \\ Y &= 1 - \frac{2 P_1 - P_2}{3 P_1} \end{aligned}$$

Figure 4: Flow coefficient formula used by Engie

3.2 Selecting a value

The flow coefficient used to calculate the mass flow is calibrated from a reference pressure drop situation (approach similar to [SAE J2601 DEC2016] 7.3 and A.3.4). The reference pressure drop situation are defined in Table 6 and are based on 10 minutes fillings of 28 x 50 L tanks, starting at 10 MPa, at $-15^\circ C$ injection temperature and with the approximate maximum pressure drop (MPD) for the respective pressure class:

- H35: MPD of 10 MPa
- H50: MPD of 15 MPa

- H70: MPD of 20 MPa

Table 6: Selected k_v values and related conditions for each case

Parameter	H35	H50	H70	Unit
Pressure level P_1	343.45	431.68	507.63	[bara]
Pressure level P_2	242.98	282.96	314.07	[bara]
Pressure drop ΔP	100.47	148.72	193.56	[bar]
Flow rate Q_{tot}	45.79	65.58	91.96	[g s ⁻¹]
Pre-cooling temperature T_1	-15.0	-15.0	-15.0	[°C]
Flow coefficient k_v (Air Liquide)	0.110	0.120	0.140	[m ³ h ⁻¹]
Flow coefficient k_v (Engie)	0.127	0.143	0.171	[m ³ h ⁻¹]

Please note that the k_v value is relative to the whole system of 28 x 50 L tanks.

This approach allows to calibrate the k_v value despite slightly different flow coefficient formulas. Exact pressure drop values are close but not strictly equal to the aim mentioned earlier, which isn't an issue as long as all simulations carried are consistent with each other.

Graphs and detailed characteristics corresponding to these simulations can be found in Annex A.

4. SIMULATION RESULTS

4.1 Three benchmark cases

Three cases have been defined as benchmark cases and have been simulated several times for comparison. The simulations consider a 50 L tank configuration, with injection diameter of 3 mm, with a 10 minutes filling pre-cooled at -20°C:

- H35, Type III, with initial pressure at 6 MPa,
- H50, Type IV, with initial pressure at 8 MPa, and
- H70, Type IV, with initial pressure at 10 MPa.

k_v values for each case have been selected according to Table 6.

Graphs showing temperature and pressure evolutions for each case can be found in Annex B.

Table 7 summarises the conditions reached at the end of each filling for the selected benchmark cases, run by Air Liquide and Engie.

Air Liquide uses in-house SOFIL code (Software for Filling) [Bourgeois et al. 2017]. Engie uses in-house HyFill code. Both software are based on a 0D (0-dimensional) gas - 1D (1-dimensional) wall model.

Table 7: Conditions reached at the end of filling for the 3 benchmark cases

		ΔP max (bar)	Tg end (°C)	Pg end (bara)	End-of-fill time (s)	End-of-fill SoC (%)
H35	AL	141.1	38.3	310.3	600	84.6
	Engie	140.6	36.5	307.3	600	85.0
H50	AL	168.2	51.0	510.0	600	92.5
	Engie	164.4	48.3	502.7	600	93.0
H70	AL	189.2	60.6	814.1	595	100
	Engie	182.5	56.8	794.7	590	100

“Tg end” and “Pg end” represent the gas temperature and pressure, respectively, at the end of filling, at 10 minutes or SoC = 1, if it is reached before the end of the 10 minutes.

A maximum difference of about 4°C is present between Air Liquide and Engie results, which is in line with the level of accuracy of such models.

4.2 Preliminary H35 simulations

Table 8 presents results for the 16 cases with H35. Graphs are available in the Annex C for each of the simulations. Results come from Air Liquide simulations with SOFIL.

The first four columns indicate the parameters for each simulation. APRR is not a numerical value, but indicates whether the pressure ramp rate was made to fill in 10 minutes (“1”) or 15 minutes (“2”). Table 5 provides the actual numerical value for the pressure ramp rate in each case.

“T inlet” is the inlet temperature into the equivalent valve (see Figure 2), “Tg” the tank gas temperature, “Tw int” the wall temperature at the gas-liner interface, “Tw LC” the wall temperature at the liner-composite interface, “Tw ext” the external wall temperature.

“Q Max (CHSS)” is the maximum flow rate for all tanks (1400 L in total) and “ΔP max” the MPD between dispenser and tank. Both values are not necessarily reached at the end of fill. Graphs available in the Annex C can indicate when the MPD is reached.

The fillings last 10 or 15 minutes but can be stopped before that time in case the SoC reaches 100%. The “Time” column in the table indicates the duration of the actual filling (in seconds).

Table 8: H35 results at end of fill

Type	Volume [L]	APRR*	T inlet [°C]	Tg [°C]	Tw int [°C]	Tw LC [°C]	Tw ext [°C]	Time [s]	SoC [%]	Q Max (CHSS) [g/s]	ΔP max [bar]
III	50	1	15	49.2	42.4	42.3	34.4	600.0	78.9	55.1	151.0
			-20	37.8	33.4	33.4	28.1	600.0	82.7	58.2	147.0
	350	2	15	53.7	48.1	48.1	41.9	900.0	97.9	40.1	94.0
			-20	40.3	36.7	36.6	32.5	882.0	99.9	41.9	91.1
	350	1	15	62.6	58.1	58.0	46.5	600.0	78.6	53.9	143.8
			-20	46.8	43.9	43.8	36.1	600.0	82.4	57.2	142.2
IV	50	2	15	68.4	64.9	64.8	56.4	900.0	95.9	38.4	89.5
			-20	50.5	48.1	48.1	42.5	895.0	100.0	40.7	88.2
	50	1	15	54.9	49.7	35.8	25.1	600.0	78.8	54.6	146.8
			-20	41.7	38.3	28.9	21.7	600.0	82.5	57.8	144.2
	350	2	15	56.4	51.5	41.0	31.6	900.0	97.3	39.6	91.5
			-20	42.3	39.1	32.0	25.7	886.0	100.0	41.6	89.5
	350	1	15	71.4	67.7	47.6	31.3	600.0	78.3	53.0	137.9
			-20	52.6	50.2	36.6	25.7	600.0	82.2	56.6	138.1
	350	2	15	73.5	70.1	55.2	41.3	900.0	95.0	37.7	85.8
			-20	54.1	51.8	41.7	32.4	900.0	99.8	40.2	85.7

*APRR is not a numerical value but indicates whether the pressure ramp rate was made to fill in 10 minutes (“1”) or 15 minutes (“2”).

Under the conditions chosen for this study, H35 fillings do not result in overheating (defined as a tank gas temperature Tg over 85 °C).

15 minutes fillings (grey rows) reach a relatively high SoC of at least 95%, even without pre-cooling. In case, pre-cooling is applied, the SoC reaches values close to 100%. 10 minutes fillings (white rows) lead to incomplete fillings, since the SoC doesn’t reach 100%. This consideration on limited SoC are dependent on the k_v value chosen and it may be worth to further refine these simulations in the project when pressure drop and k_v value will have been adjusted with operational feedbacks.

In general, Type III tanks lead to a lower end-of-fill temperature of the gas (“Tg”) compared to Type IV tanks, all other parameters being equal.

The configurations with 50 L tanks reach significantly lower temperatures, about 10°C, compared to the configuration with 350 L tanks. This is due to a higher heat exchange external surface for the same total volume.

4.3 Preliminary H50 simulations

Table 9 presents the results for the 16 cases with H50. Graphical simulation results are available in Annex D for each simulation. Results come from Engie simulations with HyFill.

For a description of the different parameters, please see Chapter 4.2.

Table 9: H50 results at end of fill

Type	Volume [L]	APRR*	T inlet [°C]	Tg [°C]	Tw int [°C]	Tw LC [°C]	Tw ext [°C]	Time [s]	SoC [%]	Q Max (CHSS) [g/s]	ΔP max [bar]
III	50	1	15	56.6	53.4	51.9	30.2	600.0	89.9	75.9	172.9
			-20	43.5	41.3	40.2	25.2	600.0	93.4	78.8	169.8
	50	2	15	56.3	53.9	52.9	36.1	856.5	100.0	54.0	103.9
			-20	42.3	40.6	39.8	28.3	821.3	100.0	56.1	101.3
	350	1	15	73.9	71.5	69.4	39.0	600.0	88.9	72.7	162.3
			-20	55.2	53.5	52.0	31.1	600.0	92.6	76.5	162.6
IV	50	1	15	62.7	57.2	38.7	20.8	600.0	89.4	74.7	165.6
			-20	48.3	44.1	31.1	18.8	600.0	93.0	77.9	164.4
	50	2	15	58.1	54.3	41.0	25.0	856.5	100.0	53.2	99.4
			-20	44.4	41.4	32.0	21.1	821.3	100.0	55.4	98.0
	350	1	15	85.3	79.6	52.4	24.6	600.0	87.9	70.7	152.3
			-20	63.1	59.1	40.1	21.3	600.0	91.9	75.0	155.5
	350	2	15	82.5	77.6	57.9	32.8	900.0	98.8	50.0	90.8
			-20	60.5	56.7	42.8	25.8	858.1	100.0	53.2	92.4

In red the filling where the gas temperature exceeds 85°C.

*APRR is not a numerical value but indicates whether the pressure ramp rate was made to fill in 10 minutes ("1") or 15 minutes ("2").

H50 fillings do not result in overheating, except for one case (Type IV, 350 L, 10 minutes, without pre-cooling). Pre-cooling to -20 °C only slightly improves the final SoC. In all cases, no complete filling is possible with 10 minutes fillings (white rows), as the SoC is between 87.9 and 93.4%.

As already described in Chapter 4.2, end-of-fill gas and wall temperatures are lower for 50 L tank configurations compared to 350 L. Same applies for Type III tanks, where the end-of-fill temperatures are lower compared to Type IV tanks.

4.4 Preliminary H70 simulations

Table 10 presents results for the 16 cases with H70. Graphical simulation results are available in Annex E for each simulation. Results come from Air Liquide simulations with SOFIL.

For a description of the different parameters, please see Chapter 4.2.

Note: Simulations were run with Type III and Type IV tanks. However, at the date of writing, Type III tanks are not recommended at H70. Therefore, the results shown below are only informative with regard to Type III tanks.

Table 10: H70 results at end of fill

Type	Volume [L]	APRR*	T inlet [°C]	Tg [°C]	Tw int [°C]	Tw LC [°C]	Tw ext [°C]	Time [s]	SoC [%]	Q Max (CHSS) [g/s]	ΔP max [bar]
III**	50	1	15	70.5	63.5	63.4	22.9	600.0	96.7	101.8	207.5
			-20	54.3	49.2	49.2	20.3	594.0	99.9	106.7	203.3
	50	2	15	65.2	58.9	58.8	28.8	862.0	100.0	71.8	129.7
			-20	49.5	44.9	44.9	23.5	818.0	100.0	75.2	126.7
	350	1	15	87.8	83.4	83.3	27.6	600.0	94.6	97.9	197.1
			-20	66.7	63.5	63.4	23.7	600.0	99.1	103.8	196.1
IV	50	2	15	83.0	79.0	78.9	38.2	900.0	99.4	68.9	123.0
			-20	61.7	58.7	58.7	29.4	849.0	100.0	73.0	122.2
	50	1	15	79.3	74.1	51.2	18.1	600.0	95.5	99.3	198.7
			-20	60.8	57.0	40.5	17.1	600.0	99.8	104.8	197.2
	350	2	15	71.9	66.6	51.1	22.2	880.0	100.0	70.0	124.1
			-20	54.4	50.6	39.3	19.2	831.0	100.0	73.9	122.9
	350	1	15	99.3	95.9	65.8	19.8	600.0	93.0	94.9	186.4
			-20	74.8	72.4	50.7	18.2	600.0	97.8	101.4	188.6
	350	2	15	92.4	88.8	67.7	26.6	900.0	97.6	66.7	116.0
			-20	68.8	66.2	51.0	22.3	868.0	100.0	71.4	117.3

In red the three fillings where the gas temperature exceeds 85°C.

*APRR is not a numerical value but indicates whether the pressure ramp rate was made to fill in 10 minutes ("1") or 15 minutes ("2").

** Only informative here since Type III tanks are currently not recommended to be used at H70.

H70 fillings have three conditions that lead to overheating. Pre-cooling allows these fillings to stay in the tolerated temperature range below 85°C. The SoC at end-of-fill is at least 93% for H70 cases.

Again, lower end-of-fill gas and wall temperatures are reached for 50 L tank configuration compared to 350 L tank configurations. Type IV 350 L configuration lead to overheating without pre-cooling, independently of the applied APRR.

4.5 H35 simulations with ambient temperature of 40°C

Given the results in previous sections which are based on the assumption of a relatively low ambient temperature of 15°C, another set of simulations was launched. Especially the rather low end-of-fill gas temperatures listed in Table 8 show, that higher ambient temperatures could be applied for H35 without overheating. It was deemed feasible to aim for non-pre-cooled fillings for all ambient temperatures. Therefore, it was decided to launch six cases at 40°C, without pre-cooling.

Table 11 presents the results for the 6 cases with H35 and ambient temperature of 40°C. Graphs are available in Annex F for each simulation. Results come from Air Liquide simulations with SOFIL.

For a description of the different parameters, please see Chapter 4.2.

Table 11: H35 results, ambient temperature = 40 °C, at end of fill

Type	Volume [L]	APRR*	T inlet [°C]	Tg [°C]	Tw int [°C]	Tw LC [°C]	Tw ext [°C]	Time [s]	SoC [%]	Q Max (CHSS) [g/s]	ΔP max [bar]
III	50	1	40	76.3	69.2	69.2	60.9	600.0	76.5	53.2	140.8
		2	40	80.3	74.6	74.5	68.4	900.0	93.3	37.8	87.1
	350	1	40	90.8	86.1	86.1	74.0	600.0	76.1	51.8	134.2
		2	40	96.1	92.4	92.3	83.8	900.0	91.2	36.3	83.0
IV	50	2	40	83.0	77.9	67.2	57.6	900.0	92.8	37.4	84.7
	350	2	40	101.3	97.7	82.5	68.1	900.0	90.3	35.6	79.5

In red the three fillings where the gas temperature exceeds 85°C.

*APRR is not a numerical value but indicates whether the pressure ramp rate was made to fill in 10 minutes ("1") or 15 minutes ("2").

The results show that no overheating is reached for the 50 L tank configuration, but only incomplete fillings of up to 92.8% can be achieved.

With a 350 L tank configuration, the simulations show that filling in less than 15 minutes without precooling in hot summer day with 40°C ambient temperature leads to tank overheating. Additional simulations are needed to determine the adequate filling time for those cases.

10 minutes fillings (white rows) are too short for a complete filling, independently of the configuration, since the SoC at end-of-fill is only about 76%.

For 50 L tank configuration, these results confirm our earlier assumptions that at H35, non-pre-cooled fillings can be applied for all ambient temperatures. For 350 L tank configuration, with an ambient temperature of 40°C, pre-cooling seems to be necessary to avoid overheating.

5. CONCLUSIONS

The simulation results presented in this report are consistent with the knowledge and intuition of the authors:

- Type IV tanks do not dissipate as much heat as Type III tanks do and have therefore a higher end-of-fill temperature, in the gas as well as in the tank wall.
- The tank configuration with 28 x 50 L tanks, compared to 4 x 350 L tanks, have a lower end-of-fill temperature as there is, for the same volume of gas, a higher heat exchange surface.
- Shorter fillings, in this case 10 minutes fillings compared to 15 minutes fillings, lead to higher end-of-fill temperature or a much lower SoC, which describes an incomplete filling.

For each pressure class, H35, H50 and H70, k_v values were chosen to simulate the pressure drop between station dispenser and vehicle CHSS. All results and the conclusions presented here are therefore highly dependent on these assumed values.

Results for H35 show there is no need for pre-cooling with an ambient temperature of 15°C to avoid overheating, but 10 minutes fillings are too short to lead to a SoC of 100%. This consideration on limited SoC are dependent on the k_v value chosen and it may be worth to further refine these simulations in the project when pressure drop and k_v value have been adjusted based on operational feedbacks. Simulations with an ambient temperature of 40°C show that it should be possible to develop a refuelling protocol without pre-cooling, as the 50 L configurations do not cause any overheating, even with Type IV tanks. For the 350 L configurations, our preliminary calculations show overheating in the situation with a high ambient temperature of 40°C.

Results for H50 show that there is no overheating with an ambient temperature of 15°C. In case of 10 minutes fillings, it is not possible to reach a SoC of 100%, in contrast to 15 minutes. As one configuration (Type IV 350 L tanks) leads to temperatures approaching 85°C, a large increase of ambient temperature above 15°C will result in overheating. It may therefore be necessary to install pre-cooling hardware in H50 stations.

In case of H70 simulations, the results indicate overheating in several cases, especially for 350 L tank configurations. As these simulations were run with an ambient temperature of 15 °C, which could easily be higher in reality, pre-cooling will be necessary for a H70 protocol. 10 minutes fillings lead to a relatively high SoC (above 93%), and 15 minutes fillings with the same conditions allow to reach an almost complete fill, of at least 97.6 %. Simulations were run with Type III tanks as well as with Type IV tanks, even if there is currently no H70 Type III tank: the simulations are meant to be informative.

6. REFERENCES

- [SAE J2601-1 DEC2016] SAE J2601 - Fueling Protocols for Light Duty Gaseous Hydrogen Surface Vehicles, Revised 2016-12
https://www.sae.org/standards/content/j2601_201612/
- [Bourgeois et al. 2017] Bourgeois T, Brachmann T, Barth F, Ammouri F, Baraldi D, Melideo D, Acosta-Iborra B, Zaepffel D, Saury D, and Lemonnier D. 2017. Optimization of hydrogen vehicle refuelling requirements. International Journal of Hydrogen Energy 42:13789–809

ANNEX: GRAPHICAL SIMULATION RESULTS

A. K_v SELECTION SIMULATIONS

Simulations launched to determine the correct k_v value used these conditions:

- for 28 x 50 L tanks:
 - Type III, H35,
 - Type IV, H50,
 - Type IV, H70,
- initial pressure in tank: 100 bar,
- constant pressure ramp rate, from 100 bar to 1.25 x NWP (350, 500, 700 bar),
- 10 minutes of filling,
- ambient temperature = initial gas temperature = 15°C,
- inlet temperature = -15°C,
- no heat exchange in inlet piping,
- pressure drop in piping modelled via k_v .

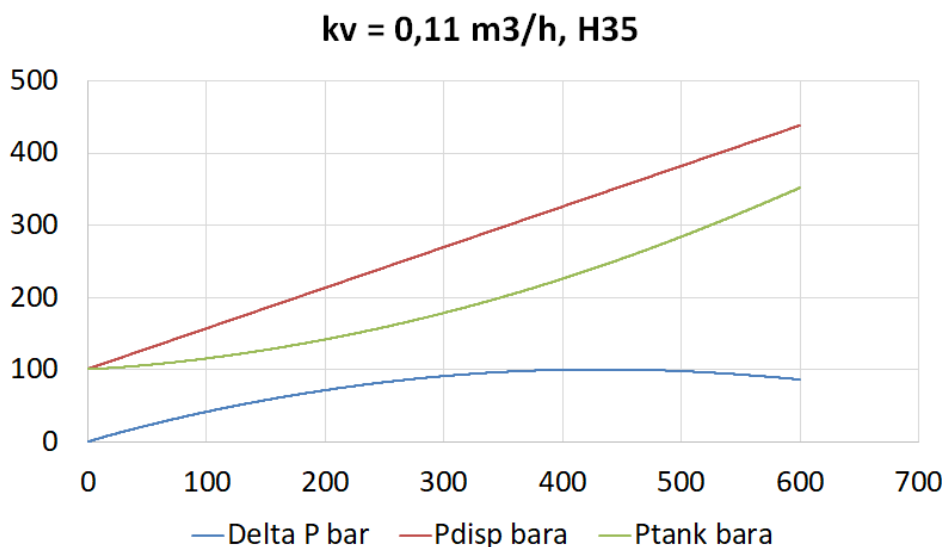


Figure A-1: Simulation of filling for NWP = 35 MPa, with $k_v = 0.11 \text{ m}^3/\text{h}$

$k_v = 0,12 \text{ m}^3/\text{h}$, H50

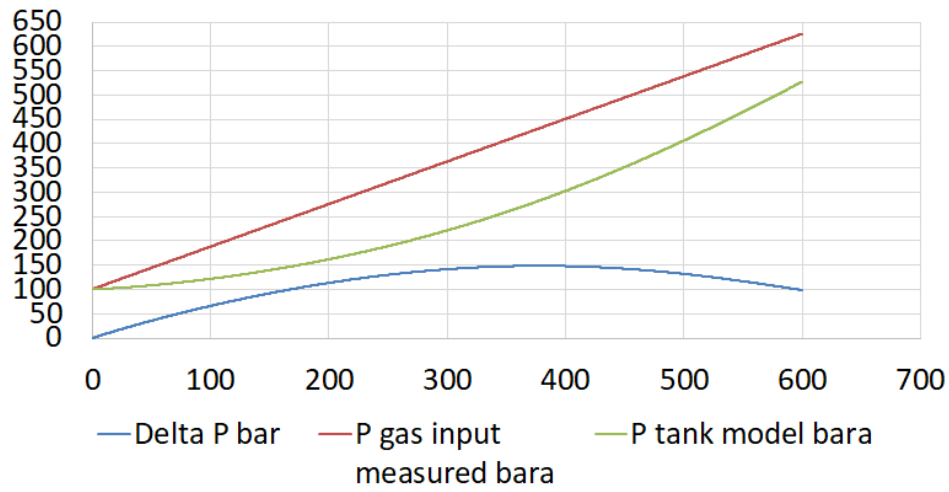


Figure A-2: Simulation of filling for NWP = 50 MPa, with $k_v = 0.12 \text{ m}^3/\text{h}$

$k_v = 0,14 \text{ m}^3/\text{h}$, H70

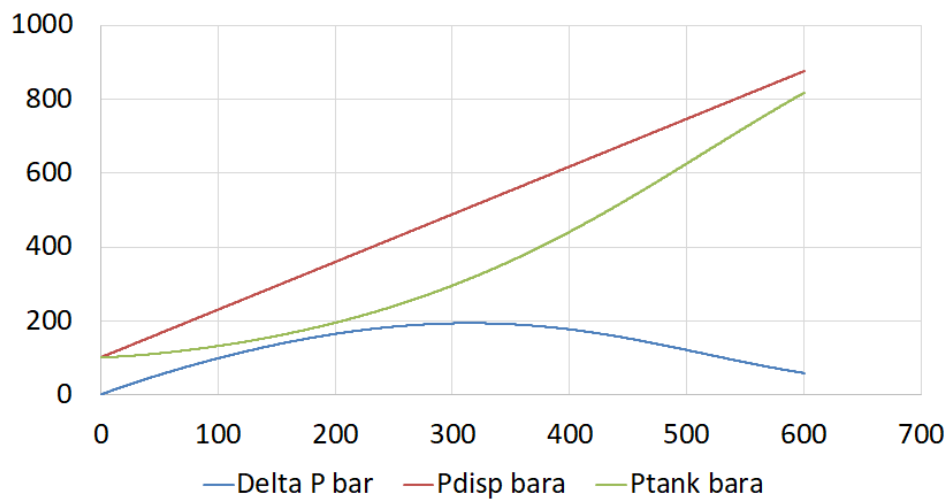


Figure A-3: Simulation of filling for NWP = 70 MPa, with $k_v = 0.14 \text{ m}^3/\text{h}$

B. BENCHMARK CASES SIMULATIONS

Figures B.1-6 show the evolution of gas and wall temperatures, as well as pressure in the dispenser and the tank and their difference, for the three benchmark cases, for simulations by Engie and Air Liquide.

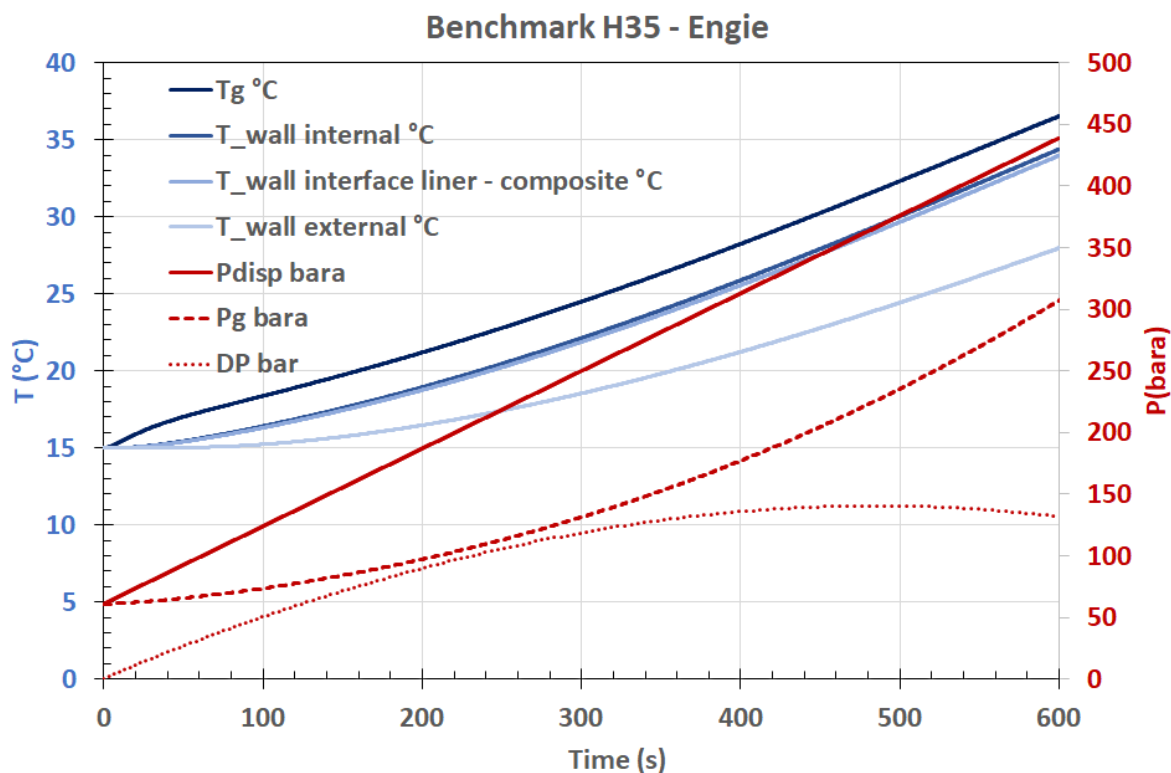


Figure B-1: Simulation of filling for NWP = 35 MPa, by Engie

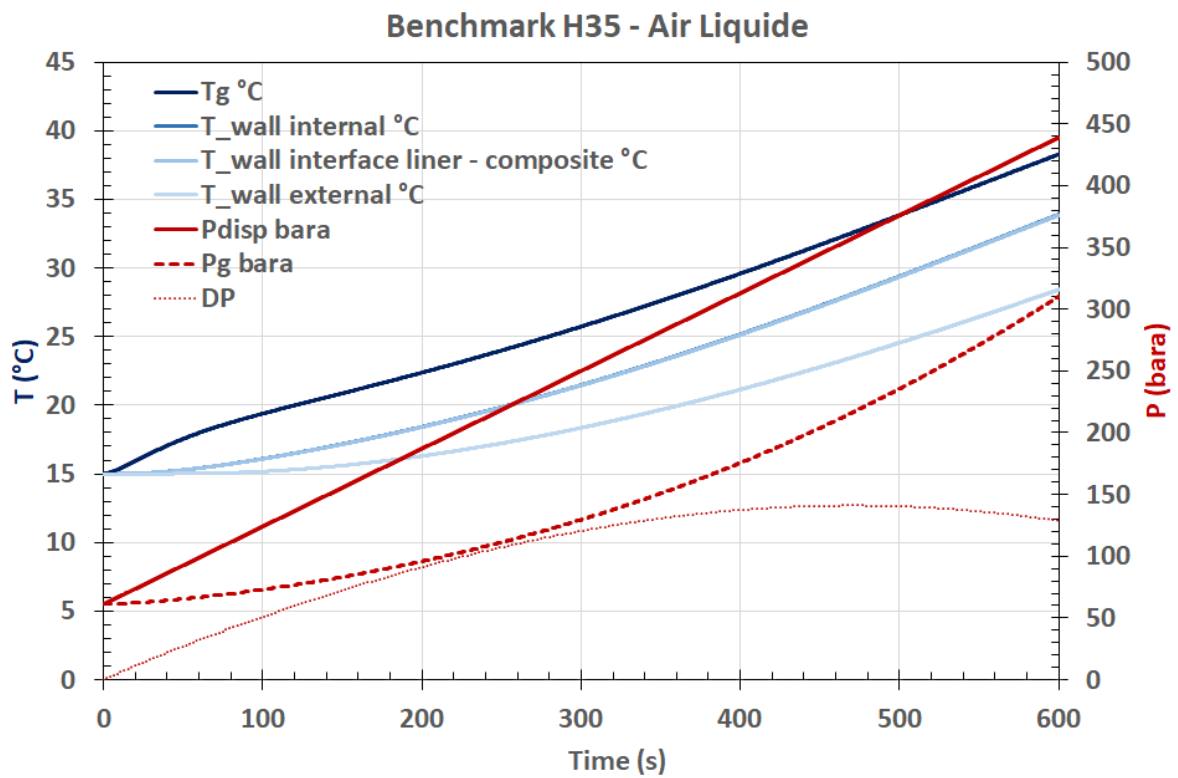


Figure B-2: Simulation of filling for NWP = 35 MPa, by Air Liquide

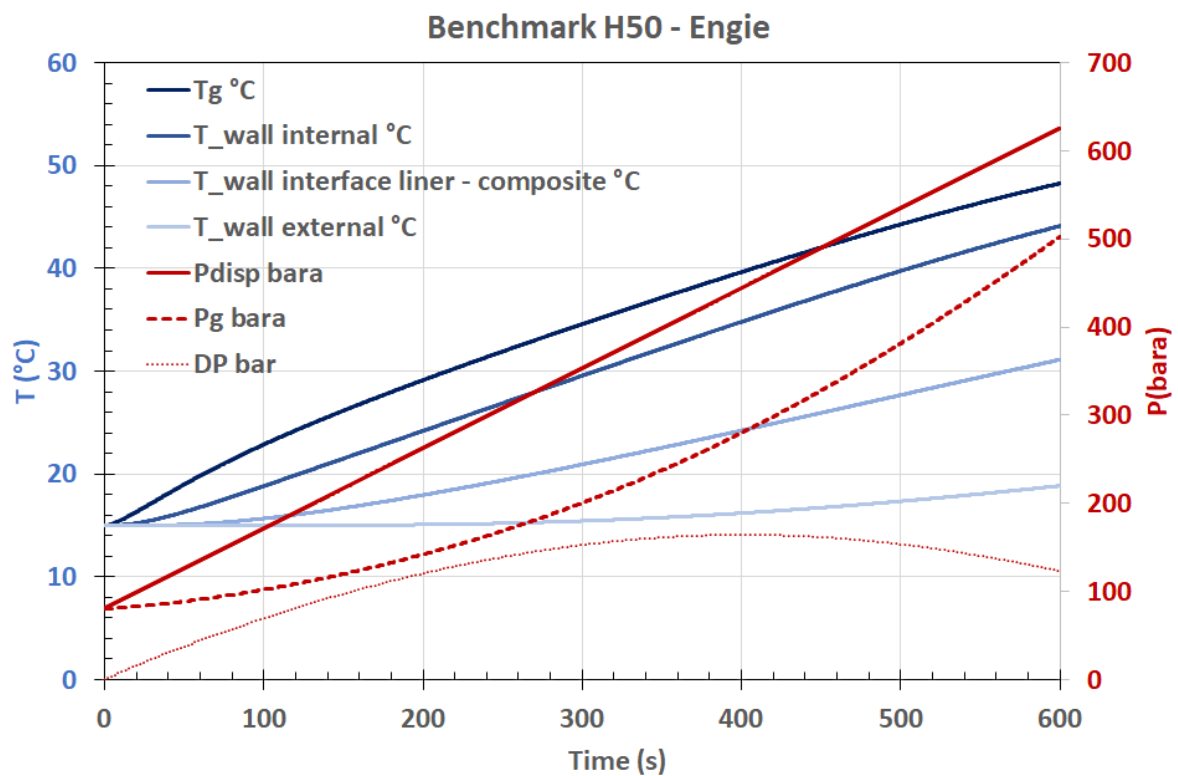


Figure B-3: Simulation of filling for NWP = 50 MPa, by Engie

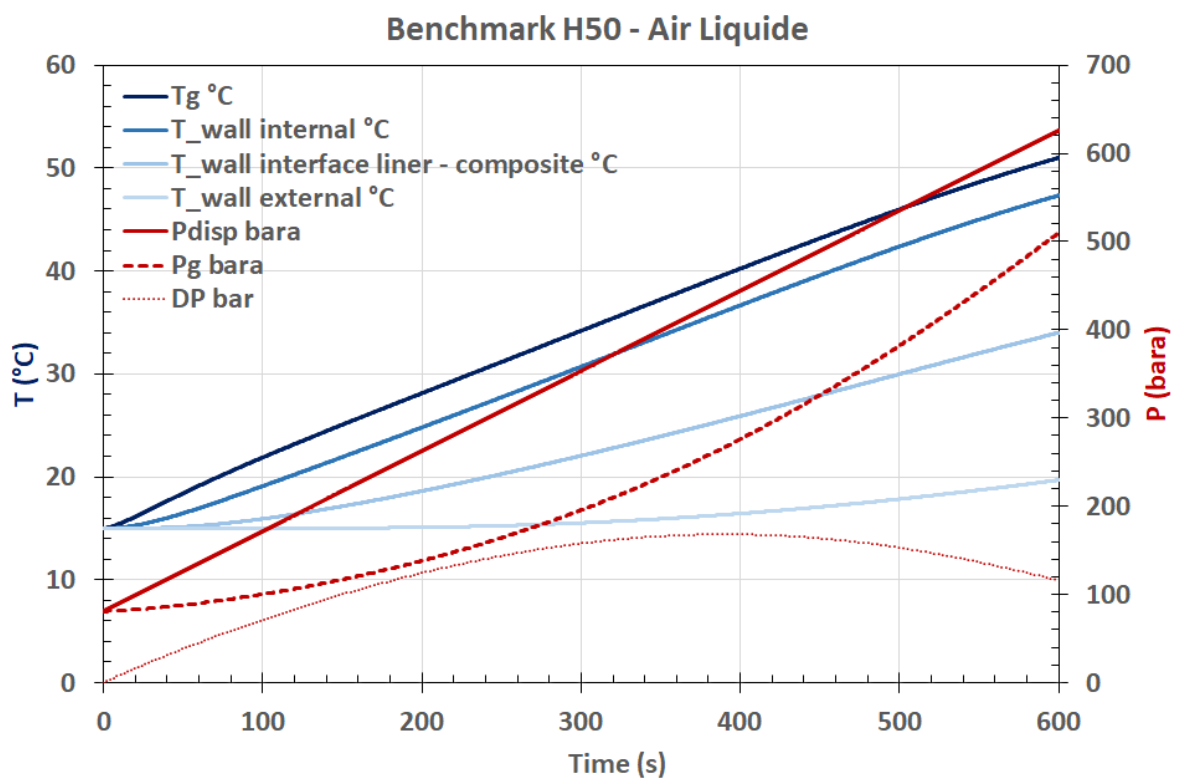


Figure B-4: Simulation of filling for NWP = 50 MPa, by Air Liquide

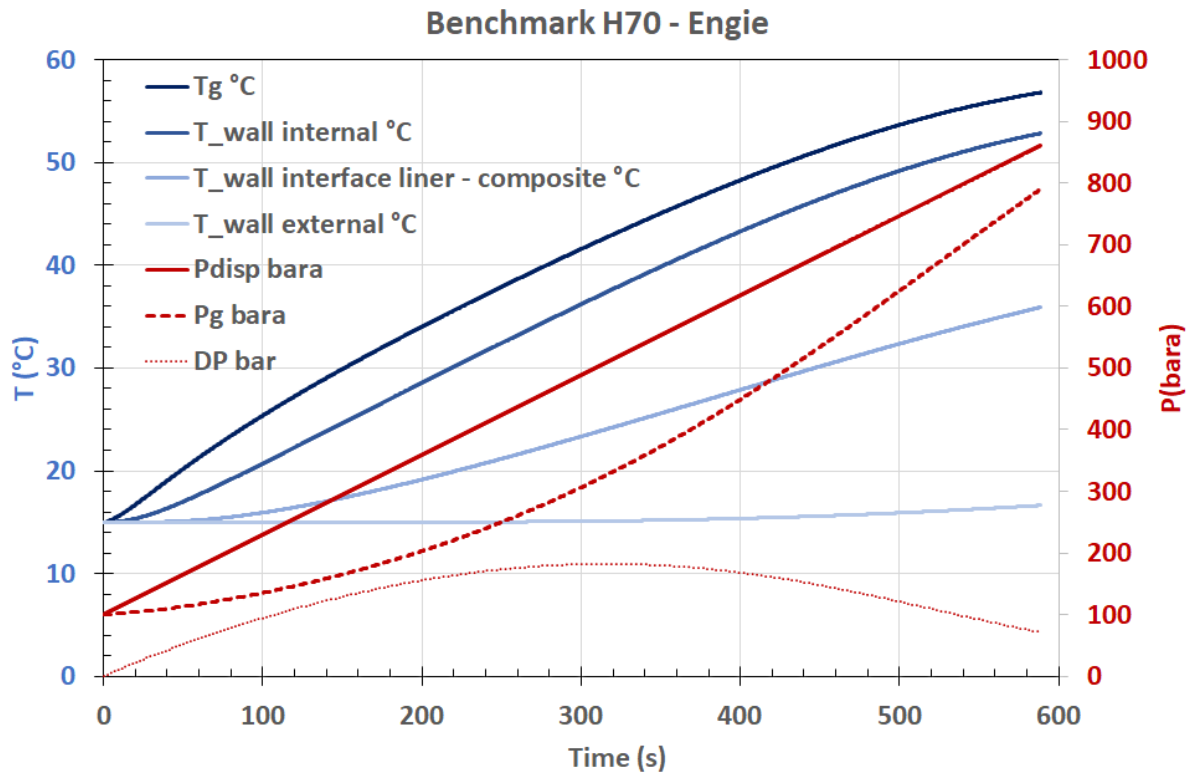


Figure B-5: Simulation of filling for NWP = 70 MPa, by Engie

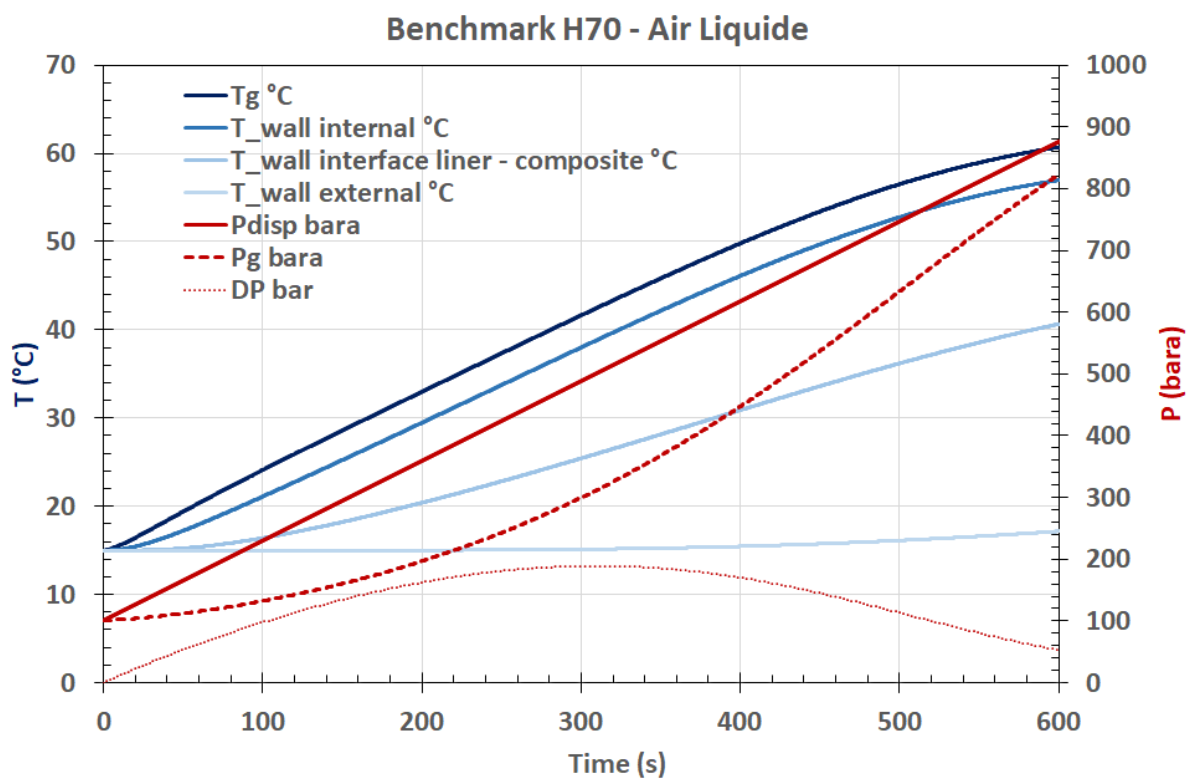


Figure B-6: Simulation of filling for NWP = 70 MPa, by Air Liquide

C. H35 SIMULATIONS

Figures C.1-16 show the evolution of gas and wall temperatures, as well as pressure in the dispenser and the tank and their difference, for the sixteen H35 cases.

Note: three simulations in Table 8 reached 100% SOC before the end of the filling. The graphs in Annex C show results until the end of simulation, even if the filling could have in practice been stopped earlier.

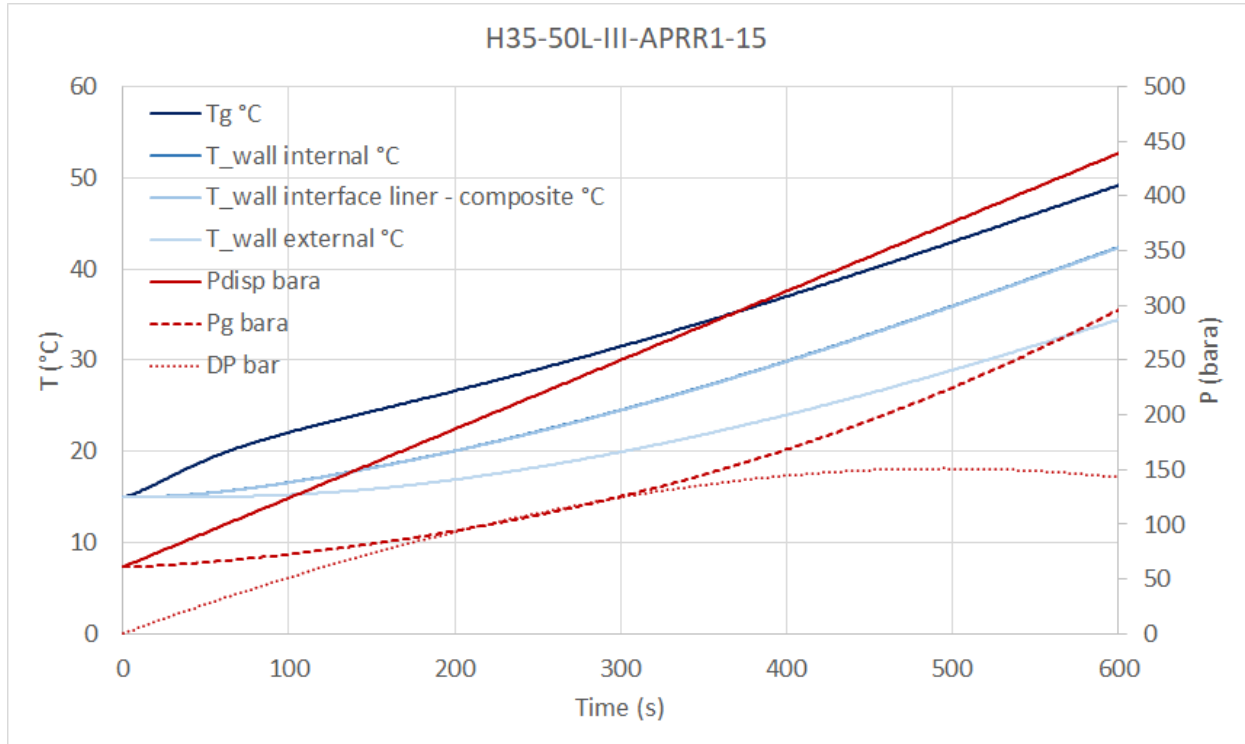


Figure C-1: Simulation of 10 minutes filling for NWP = 35 MPa, Type III 50 L tank, inlet temperature = 15°C

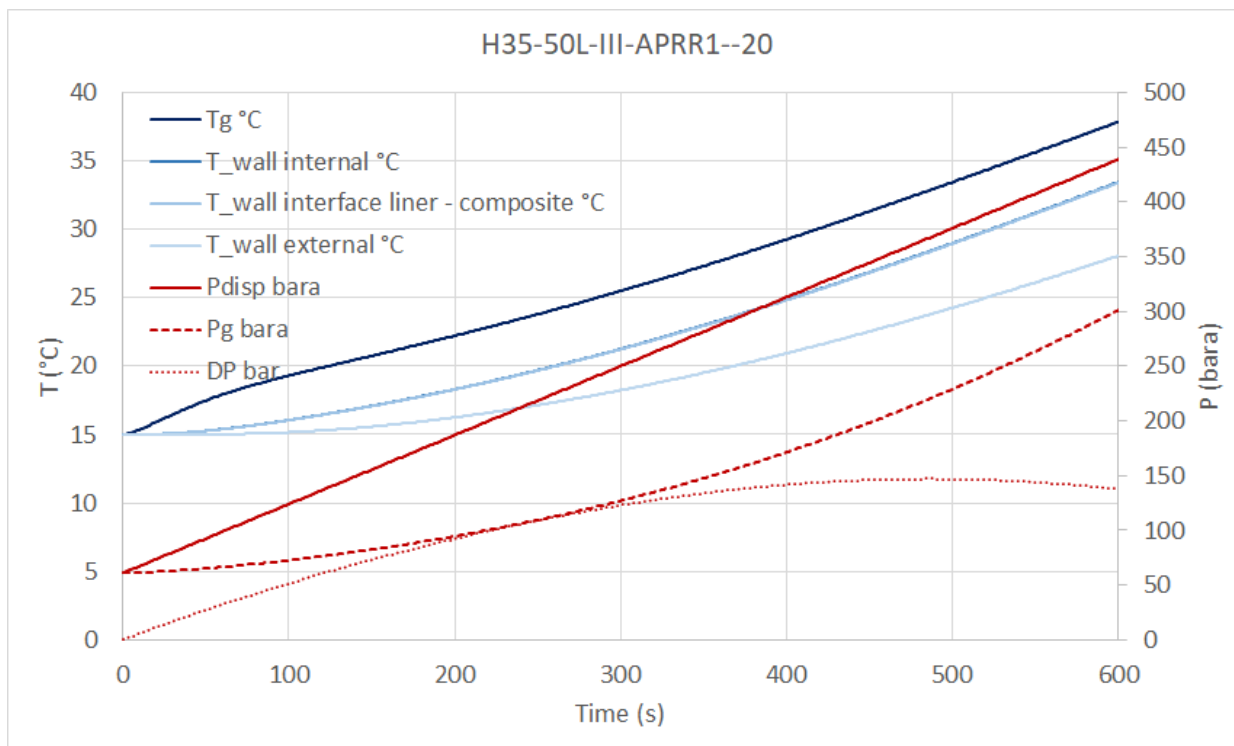


Figure C-2: Simulation of 10 minutes filling for NWP = 35 MPa, Type III 50 L tank, inlet temperature = -20°C

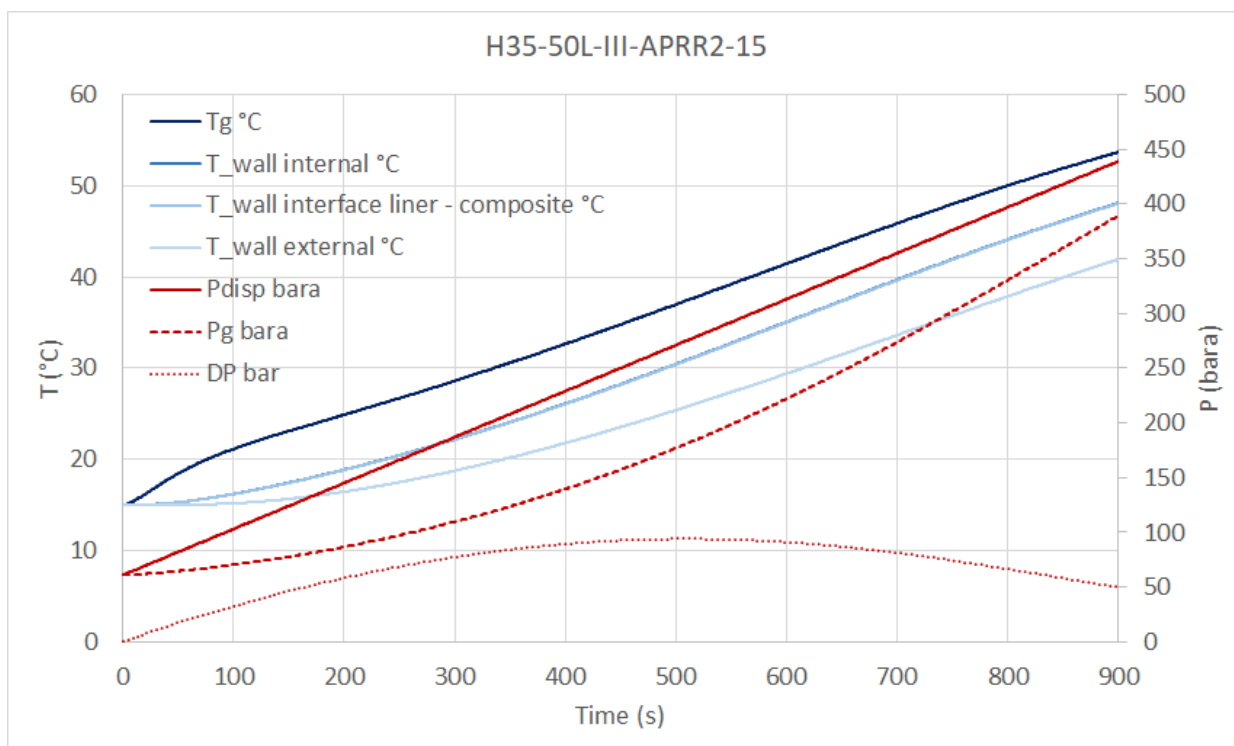


Figure C-3: Simulation of 15 minutes filling for NWP = 35 MPa, Type III 50 L tank, inlet temperature = 15°C

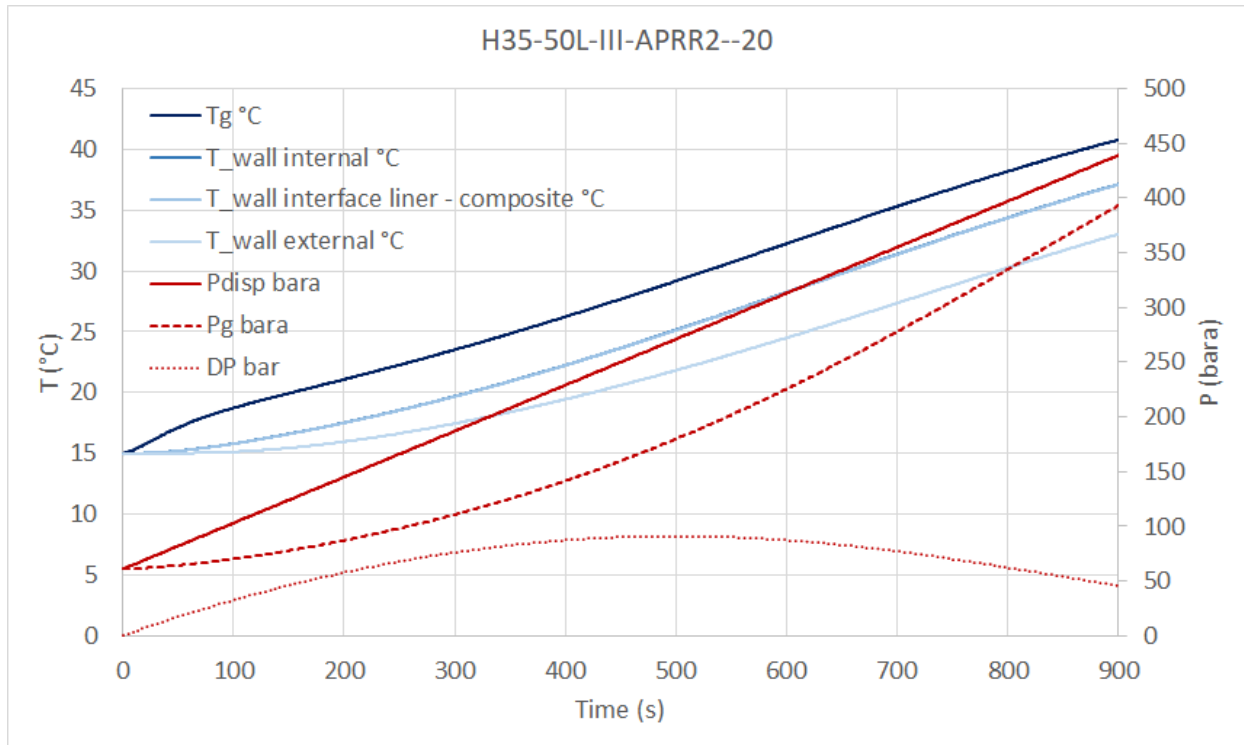


Figure C-4: Simulation of 15 minutes filling for NWP = 35 MPa, Type III 50 L tank, inlet temperature = -20 $^{\circ}\text{C}$

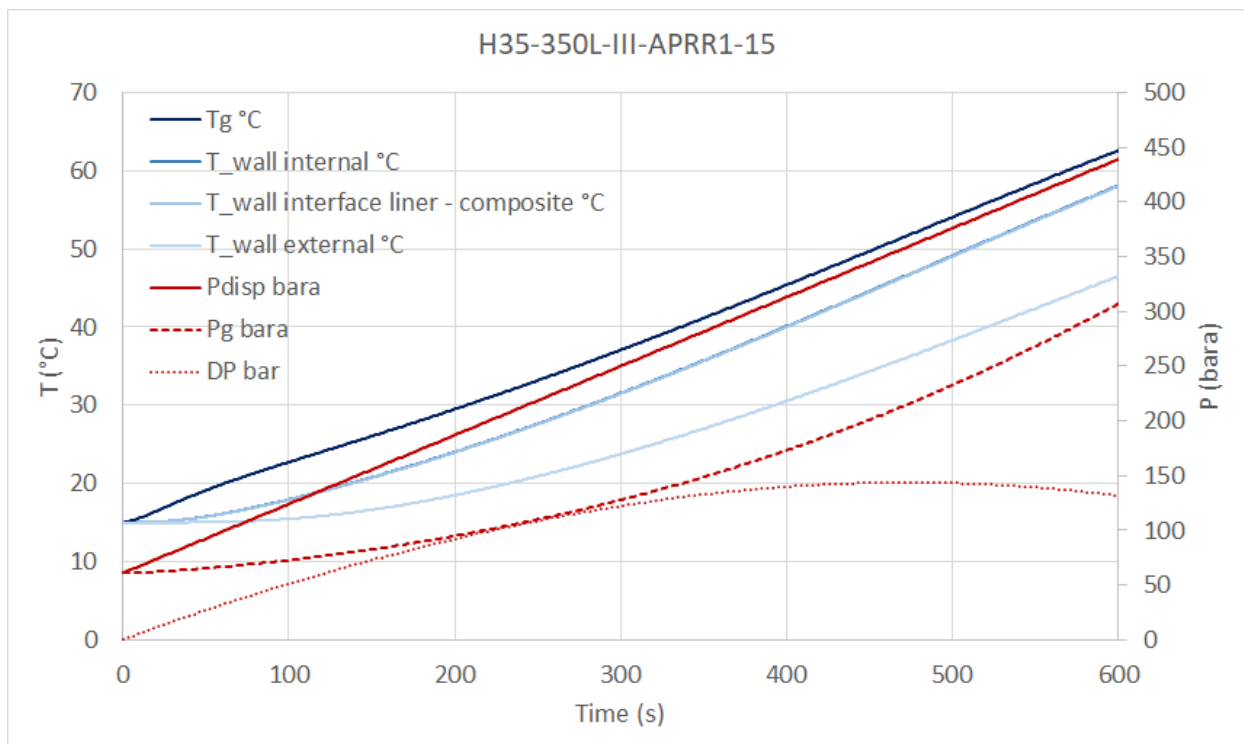


Figure C-5: Simulation of 10 minutes filling for NWP = 35 MPa, Type III 350 L tank, inlet temperature = 15 $^{\circ}\text{C}$

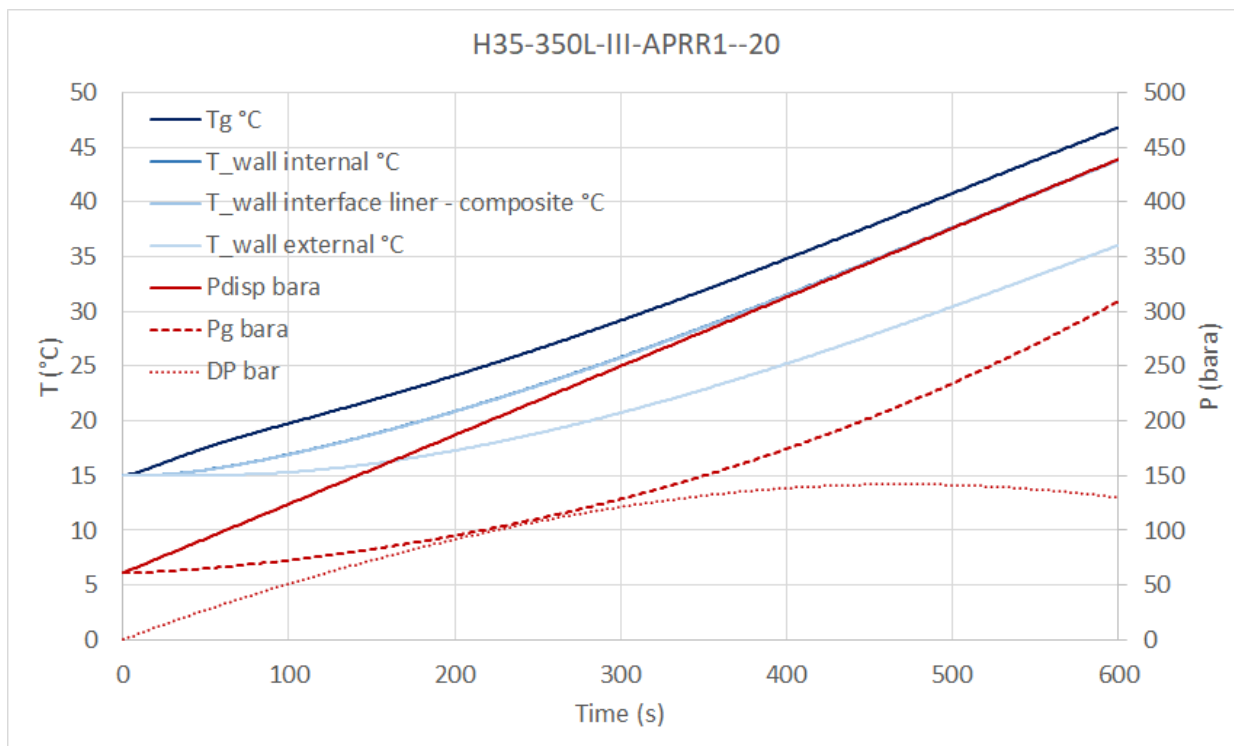


Figure C-6: Simulation of 10 minutes filling for NWP = 35 MPa, Type III 350 L tank, inlet temperature = -20°C

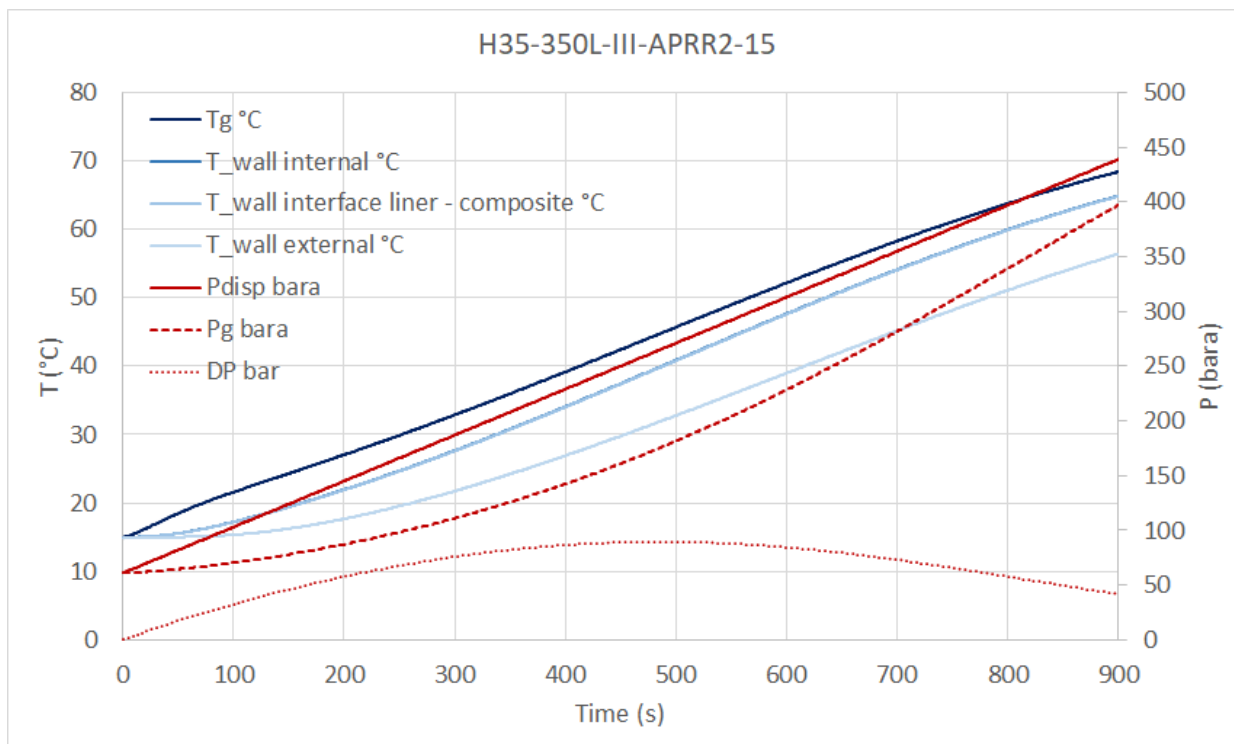


Figure C-7: Simulation of 15 minutes filling for NWP = 35 MPa, Type III 350 L tank, inlet temperature = 15°C

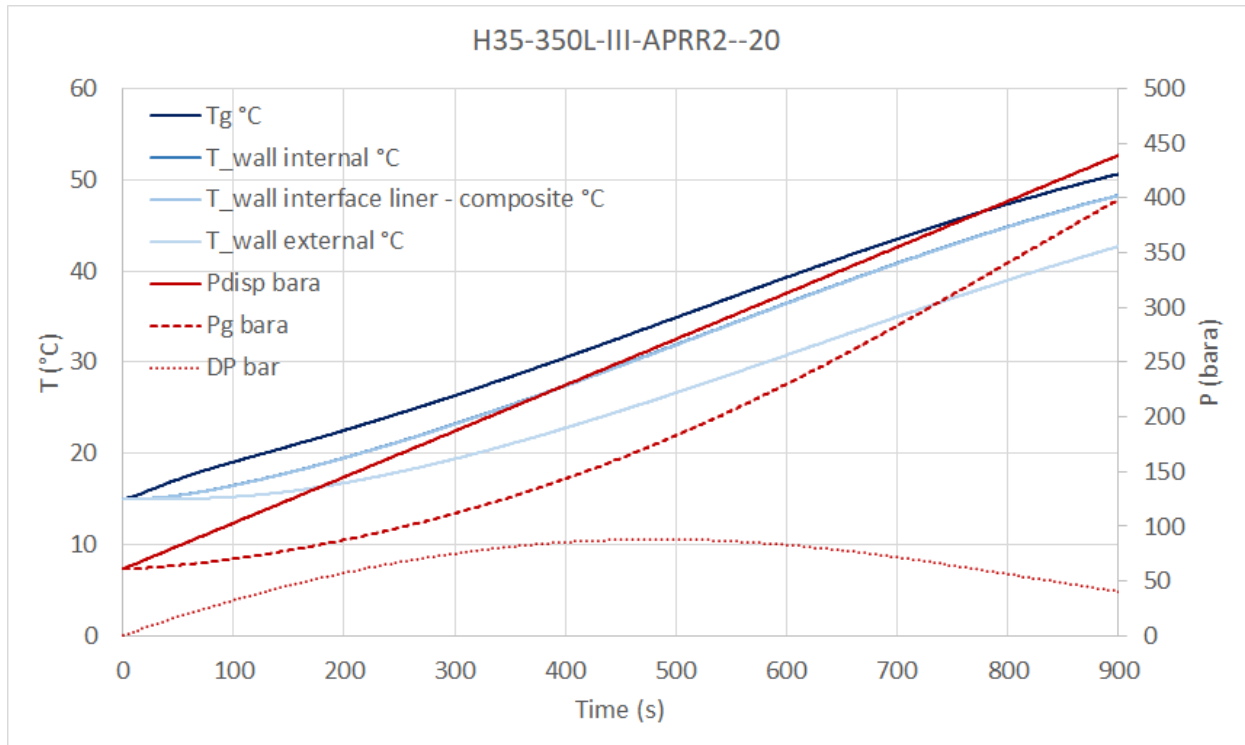


Figure C-8: Simulation of 15 minutes filling for NWP = 35 MPa, Type III 350 L tank, inlet temperature = -20°C

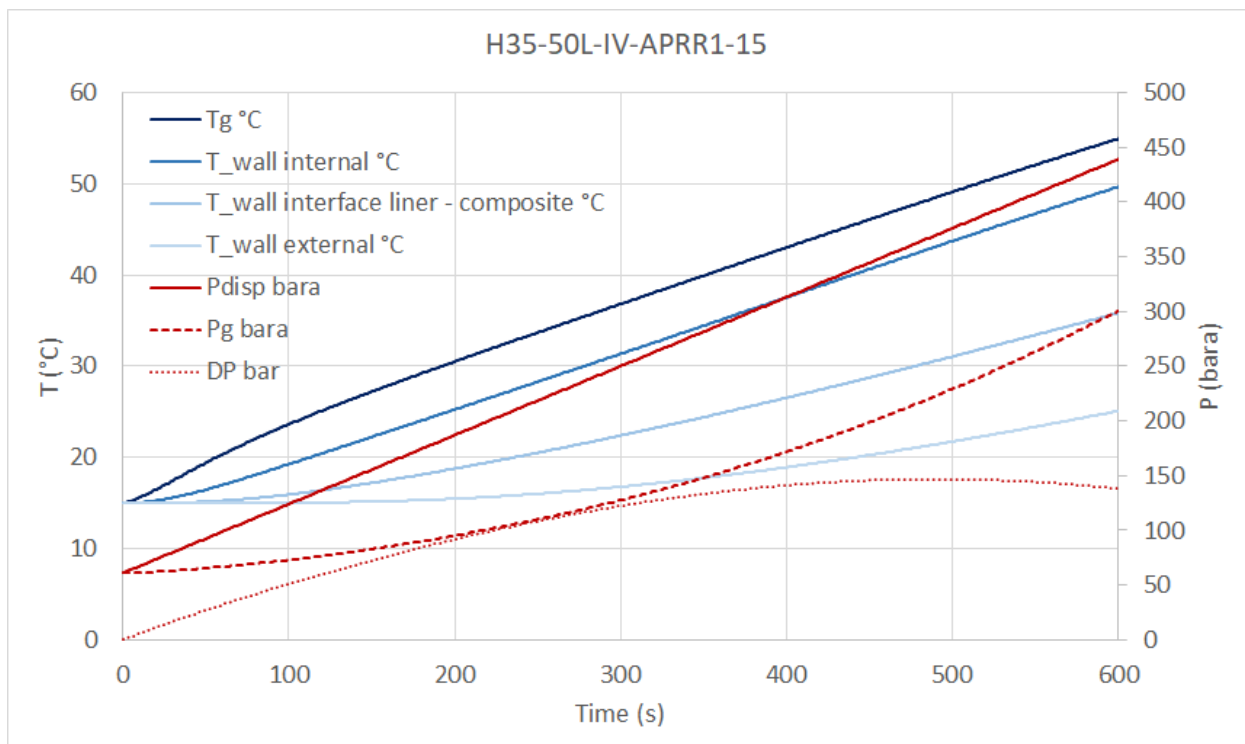


Figure C-9: Simulation of 10 minutes filling for NWP = 35 MPa, Type IV 50 L tank, inlet temperature = 15°C

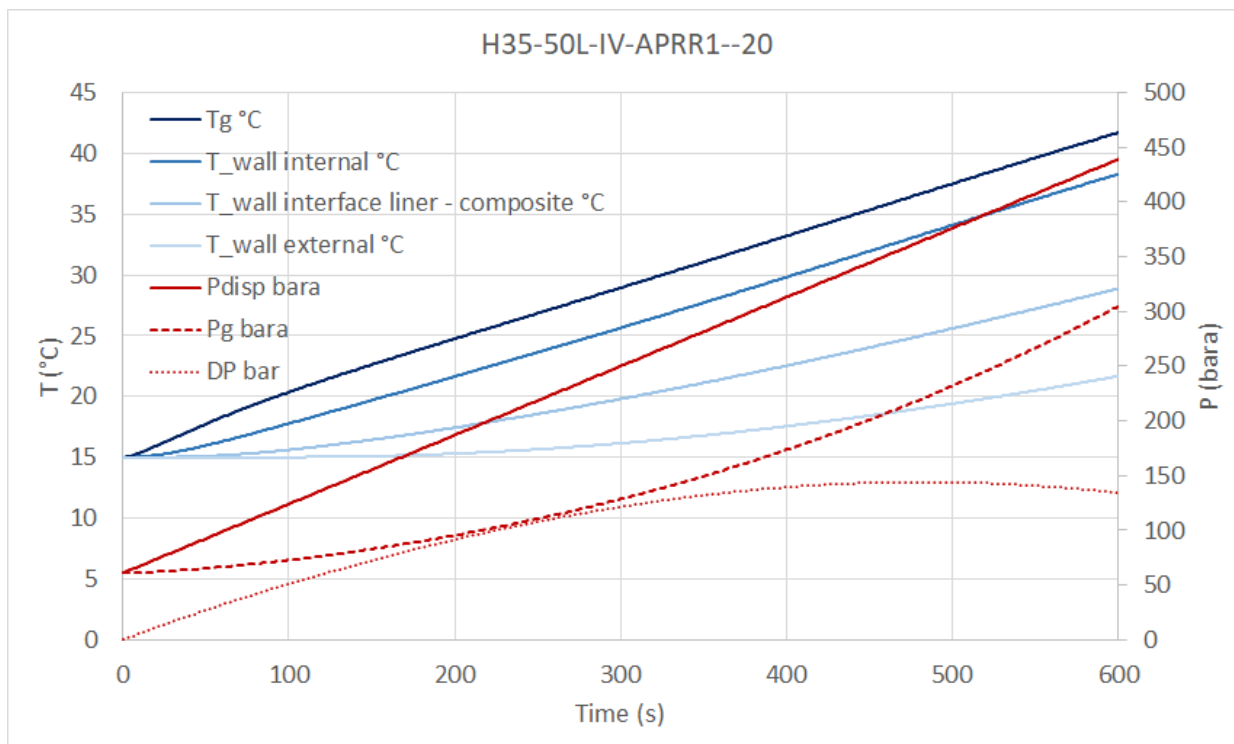


Figure C-10: Simulation of 10 minutes filling for NWP = 35 MPa, Type IV 50 L tank, inlet temperature = -20°C

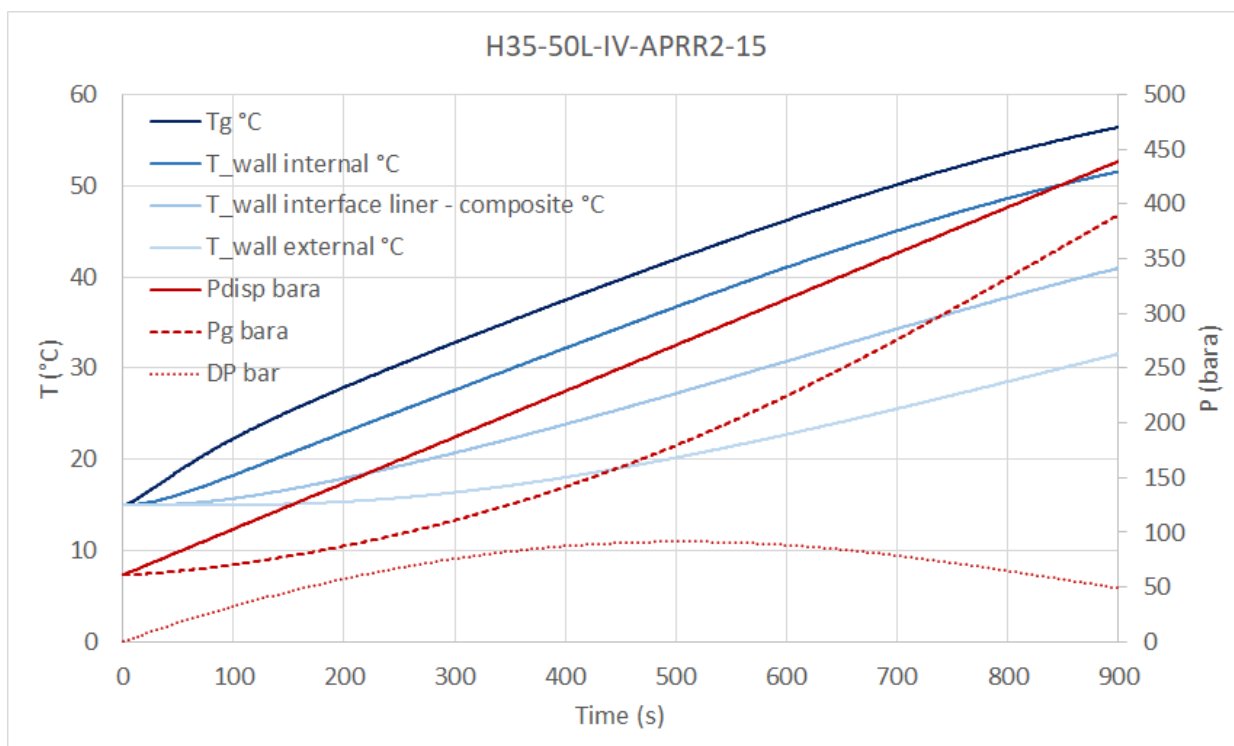


Figure C-11: Simulation of 15 minutes filling for NWP = 35 MPa, Type IV 50 L tank, inlet temperature = 15°C

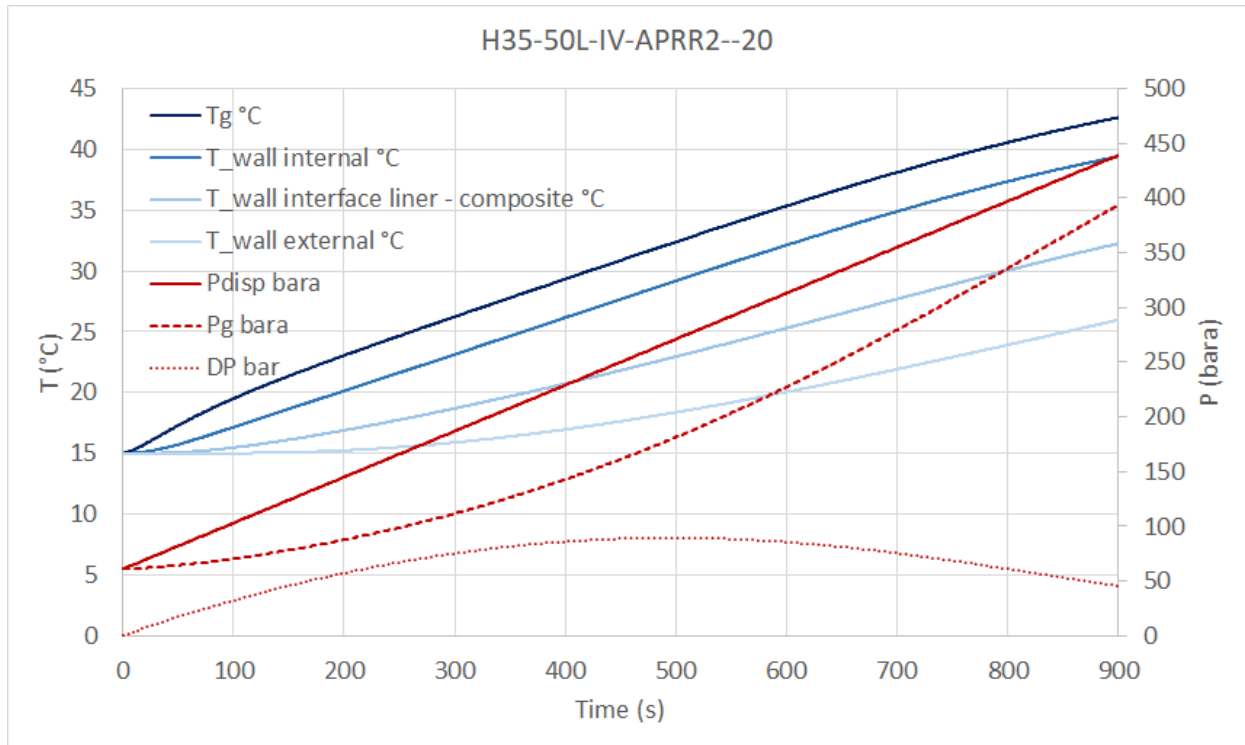


Figure C-12: Simulation of 15 minutes filling for NWP = 35 MPa, Type IV 50 L tank, inlet temperature = -20°C

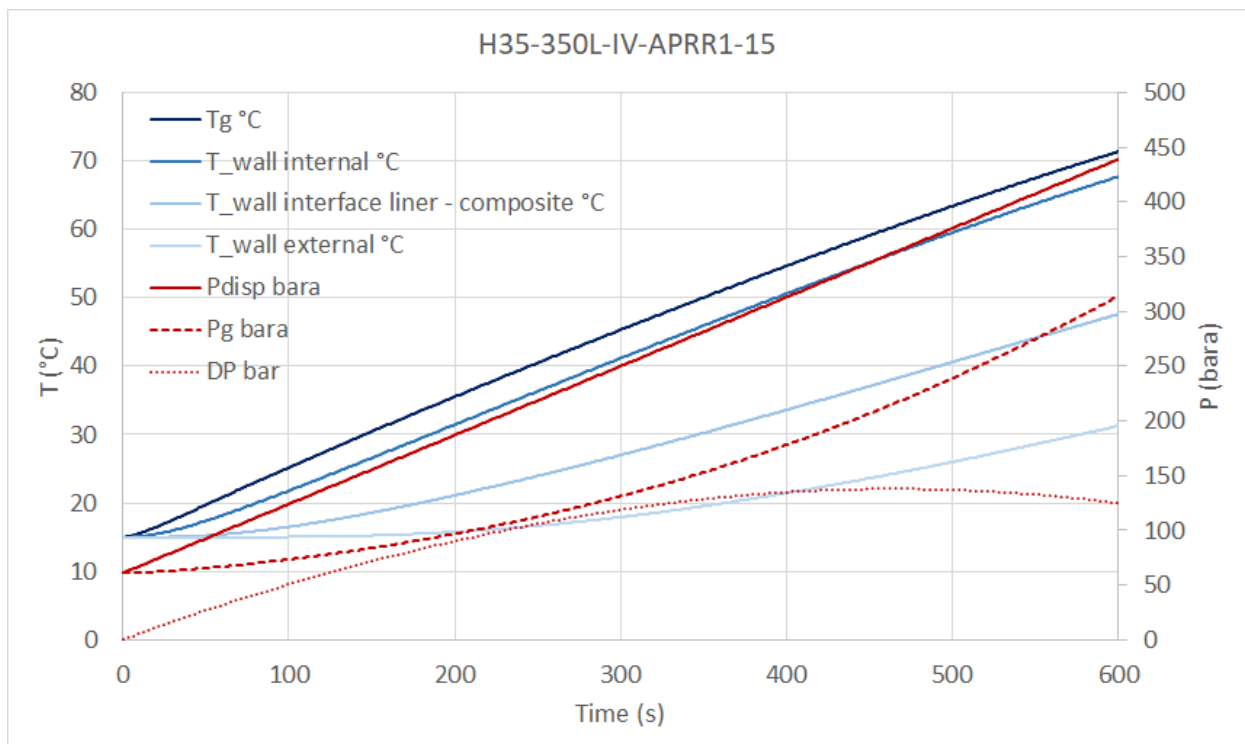


Figure C-13: Simulation of 10 minutes filling for NWP = 35 MPa, Type IV 350 L tank, inlet temperature = 15°C

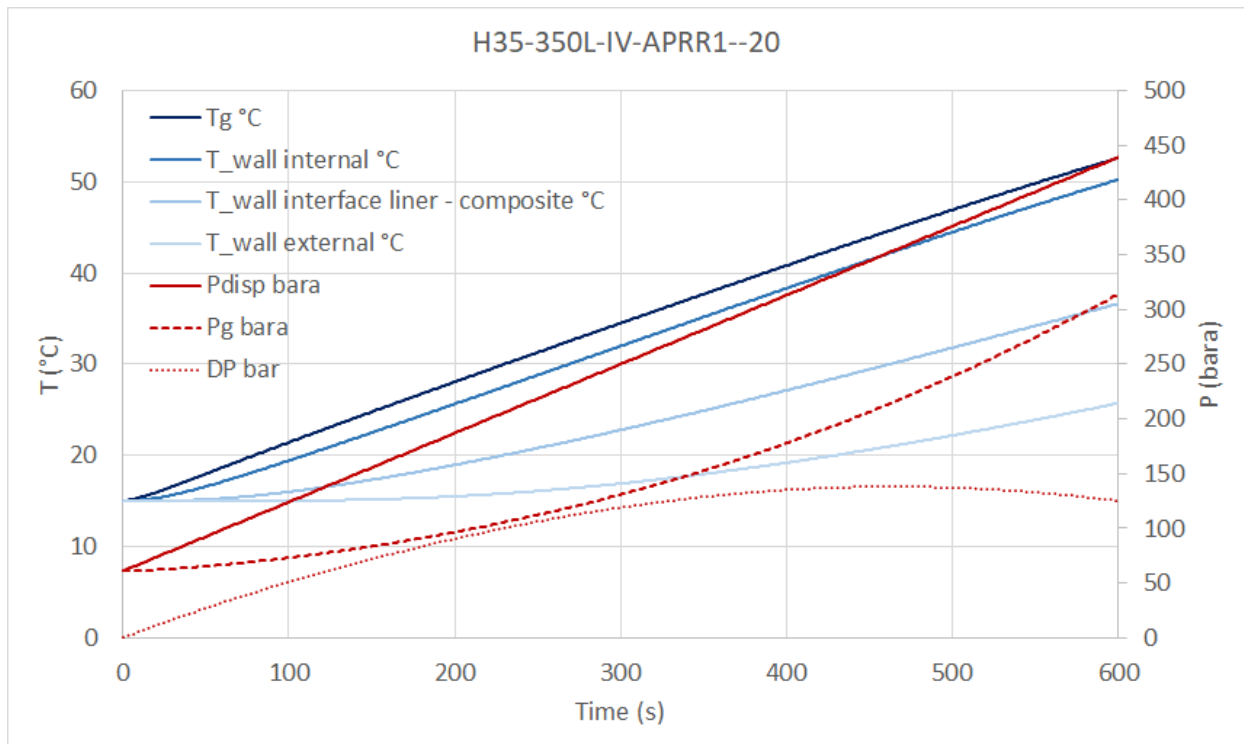


Figure C-14: Simulation of 10 minutes filling for NWP = 35 MPa, Type IV 350 L tank, inlet temperature = -20°C

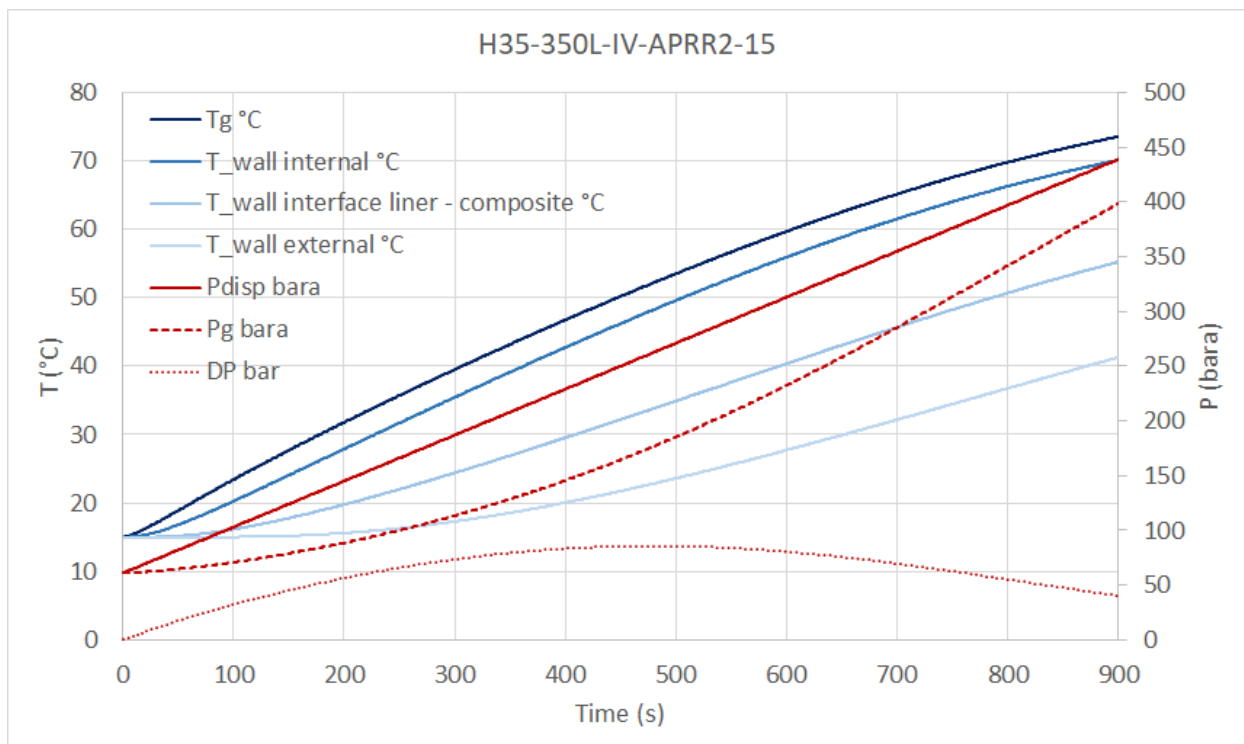


Figure C-15: Simulation of 15 minutes filling for NWP = 35 MPa, Type IV 350 L tank, inlet temperature = 15°C

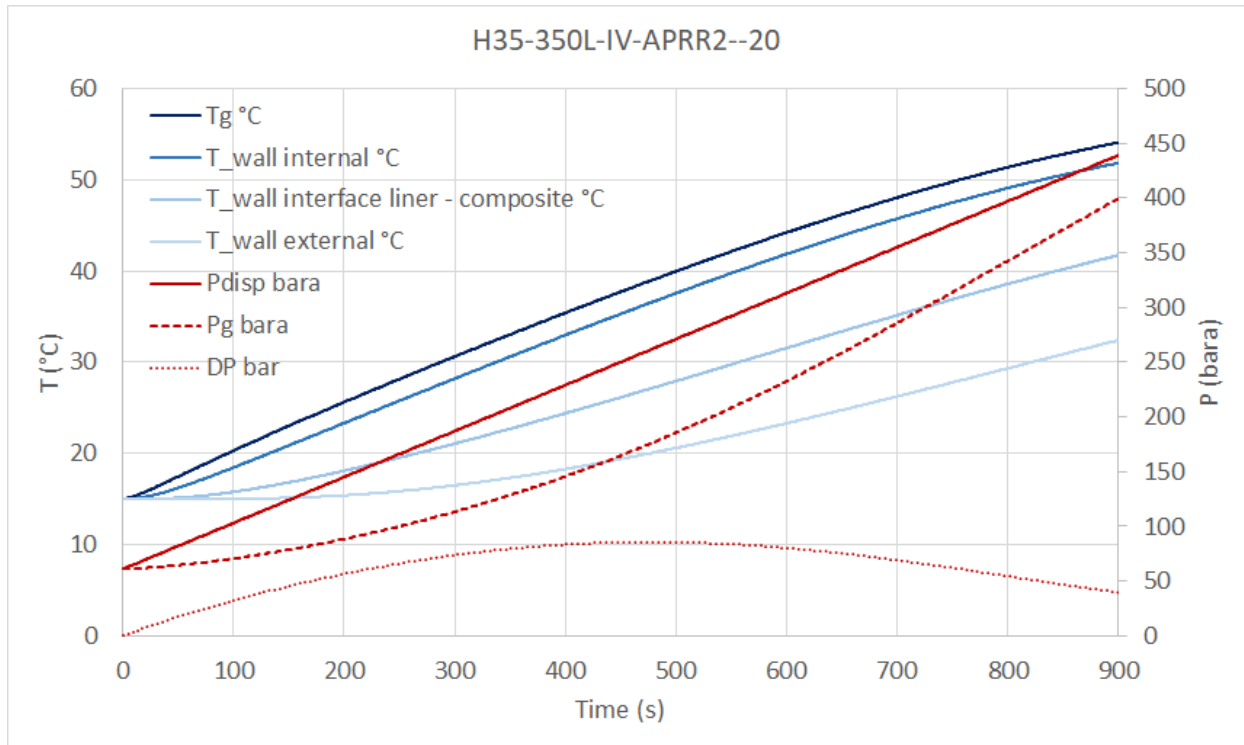


Figure C-16: Simulation of 15 minutes filling for NWP = 35 MPa, Type IV 350 L tank, inlet temperature = -20°C

D. H50 SIMULATIONS

Figures D.1-16 show the evolution of gas and wall temperatures, as well as pressure in the dispenser and the tank and their difference, for the sixteen H50 cases.

Note: seven simulations in Table 9 reached 100% SOC before the end of the filling. The graphs in Annex D show results until the end of simulation, even if the filling could have in practice been stopped earlier.

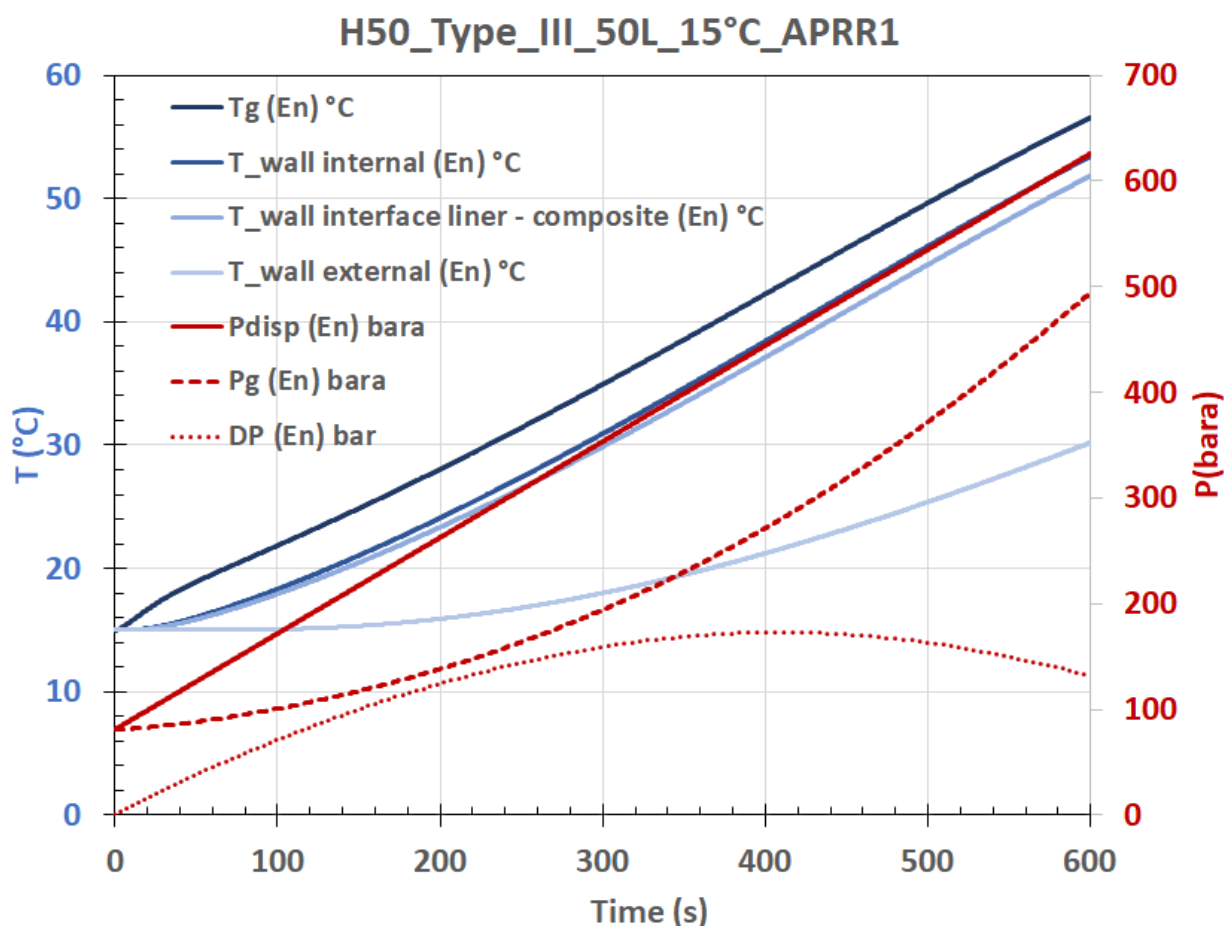


Figure D-1: Simulation of 10 minutes filling for NWP = 50 MPa, Type III 50 L tank, inlet temperature = 15°C

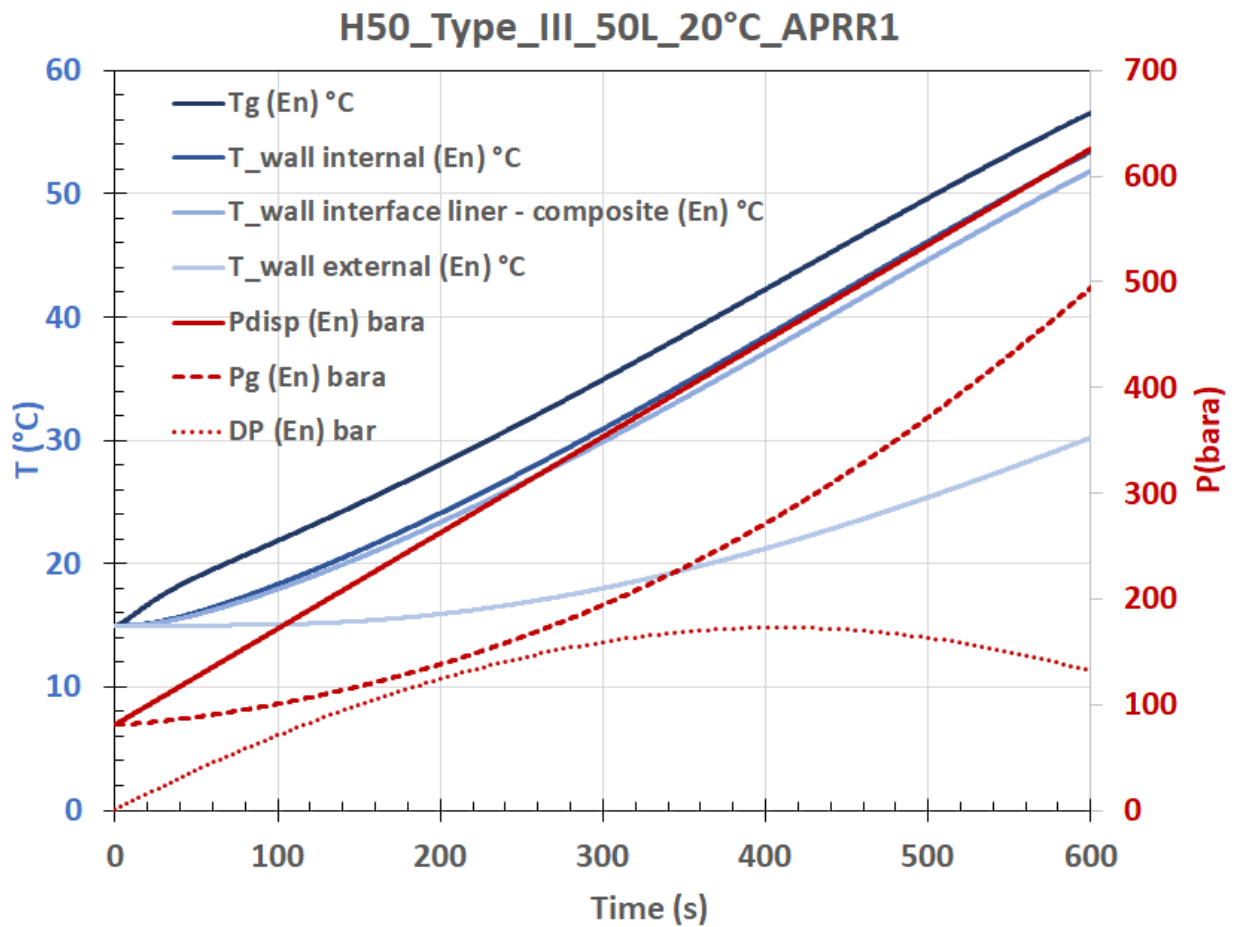


Figure D-2: Simulation of 10 minutes filling for NWP = 50 MPa, Type III 50 L tank, inlet temperature = -20°C

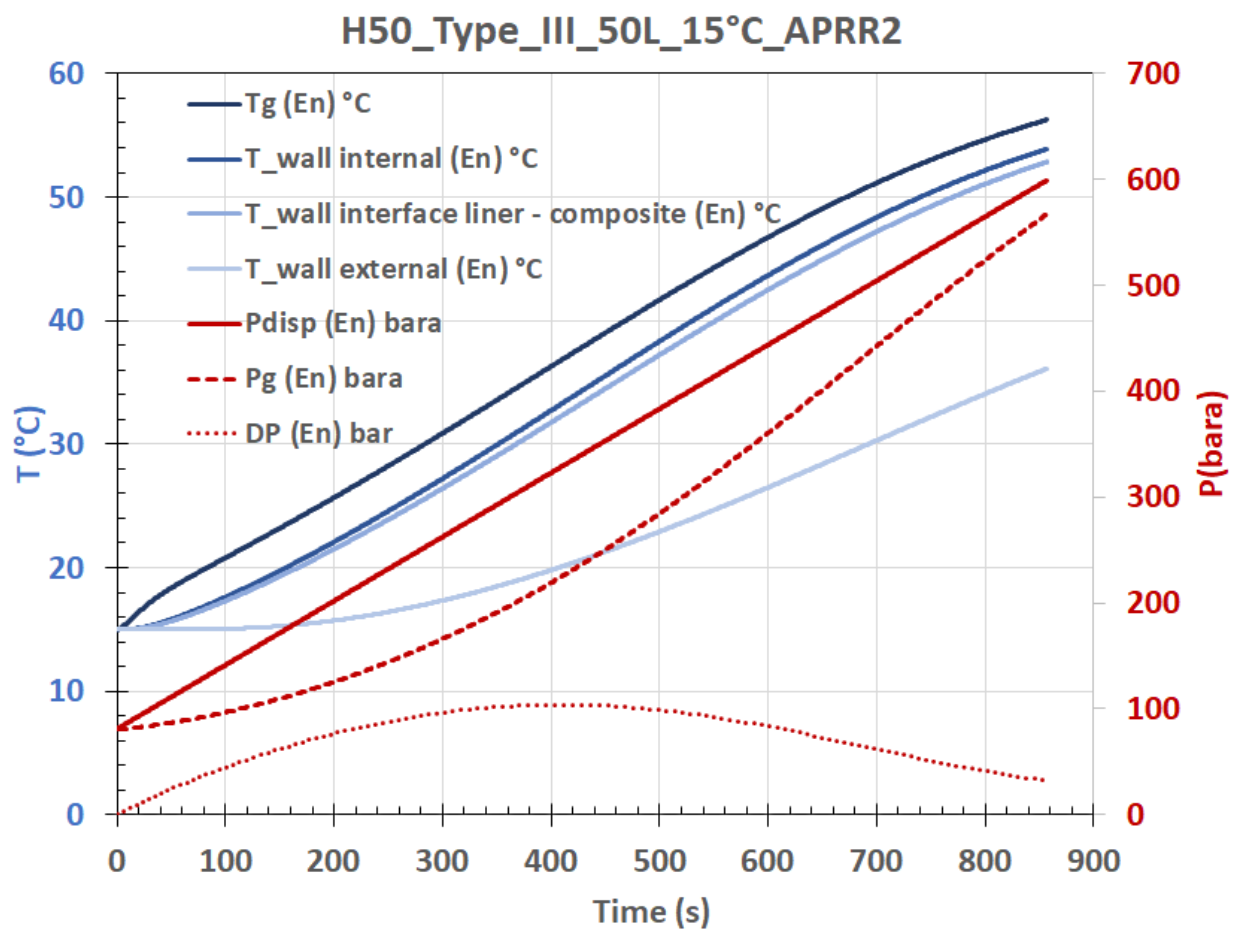


Figure D-3: Simulation of 15 minutes filling for NWP = 50 MPa, Type III 50 L tank, inlet temperature = 15°C

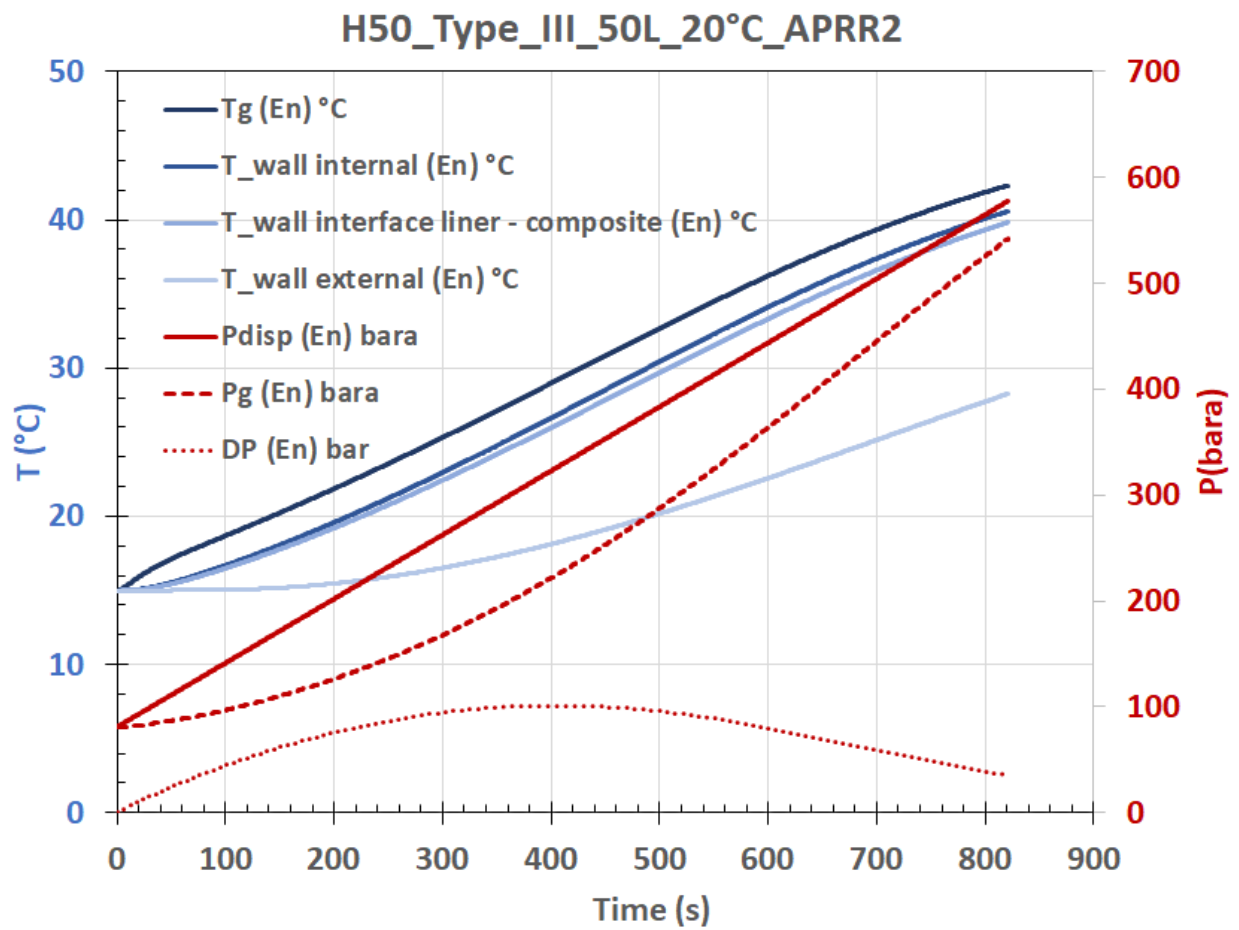


Figure D-4: Simulation of 15 minutes filling for NWP = 50 MPa, Type III 50 L tank, inlet temperature = -20°C

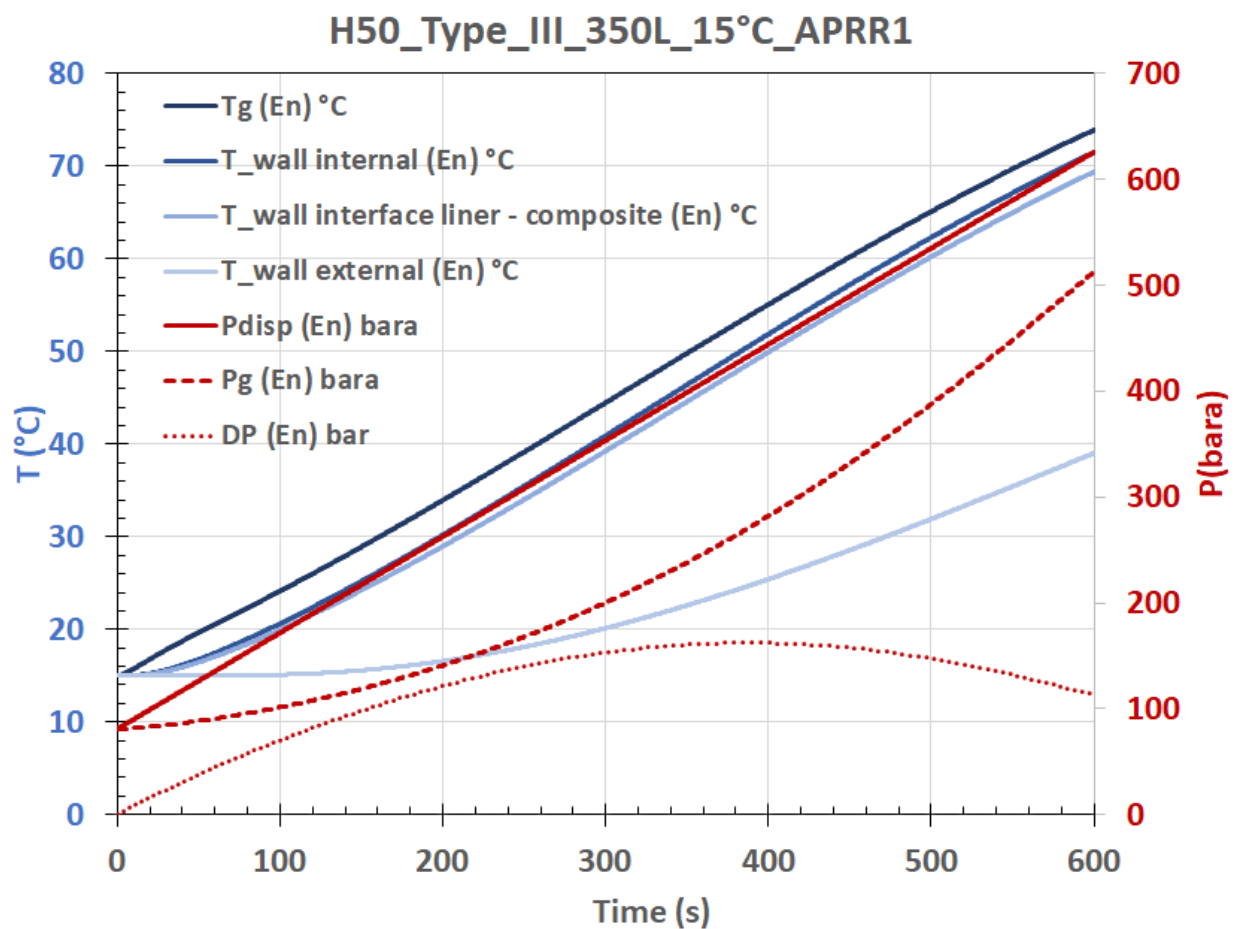


Figure D-5: Simulation of 10 minutes filling for NWP = 50 MPa, Type III 350 L tank, inlet temperature = 15°C

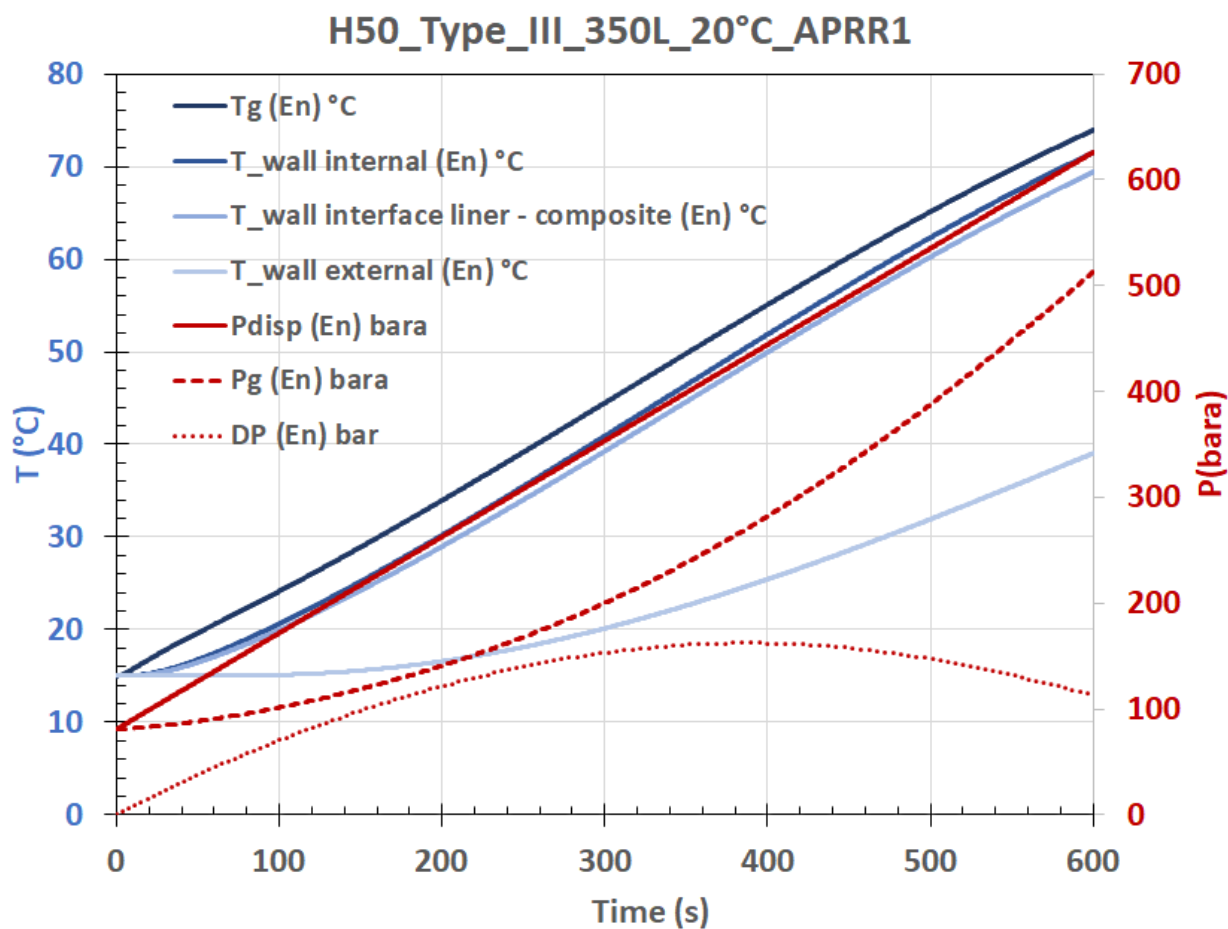


Figure D-6: Simulation of 10 minutes filling for NWP = 50 MPa, Type III 350 L tank, inlet temperature = -20°C

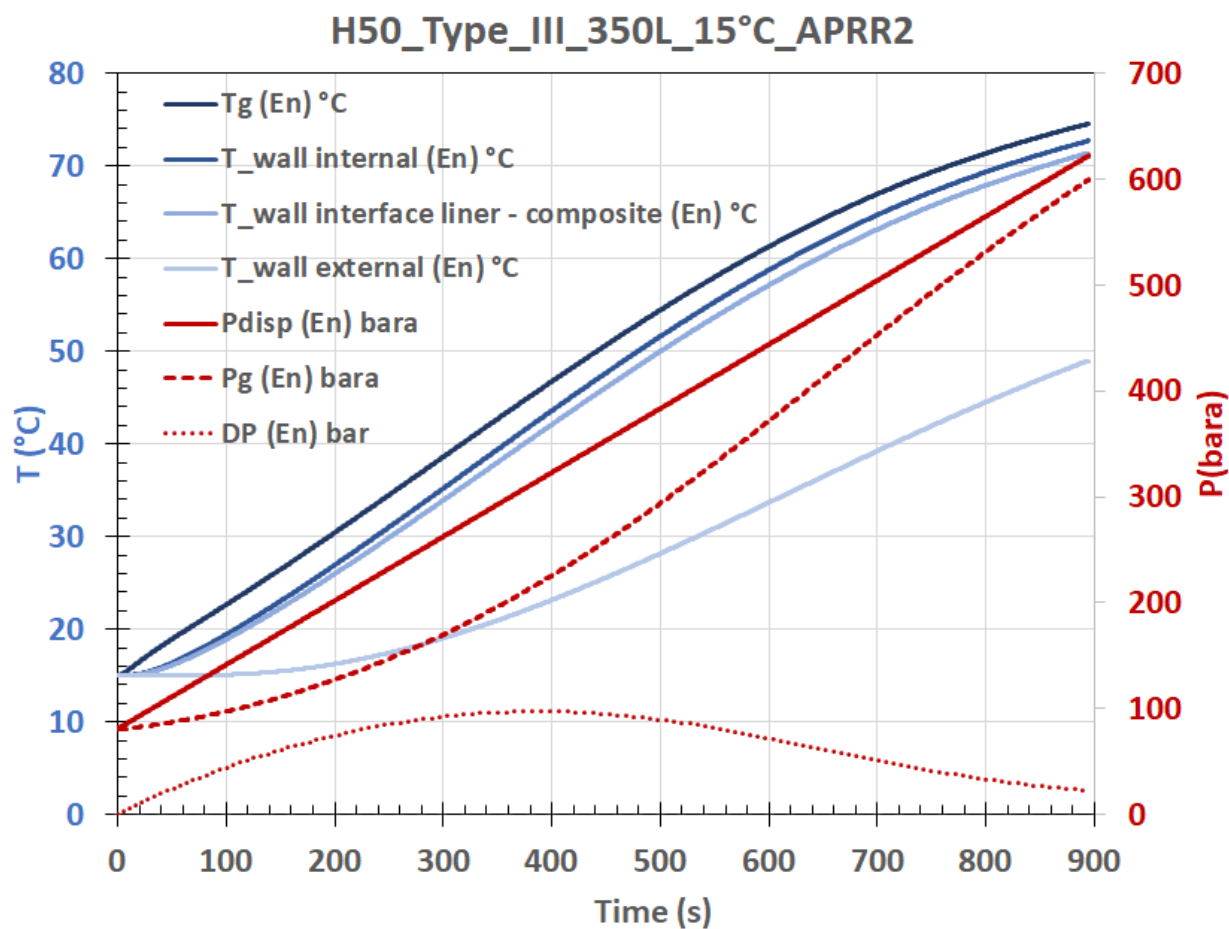


Figure D-7: Simulation of 15 minutes filling for NWP = 50 MPa, Type III 350 L tank, inlet temperature = 15°C

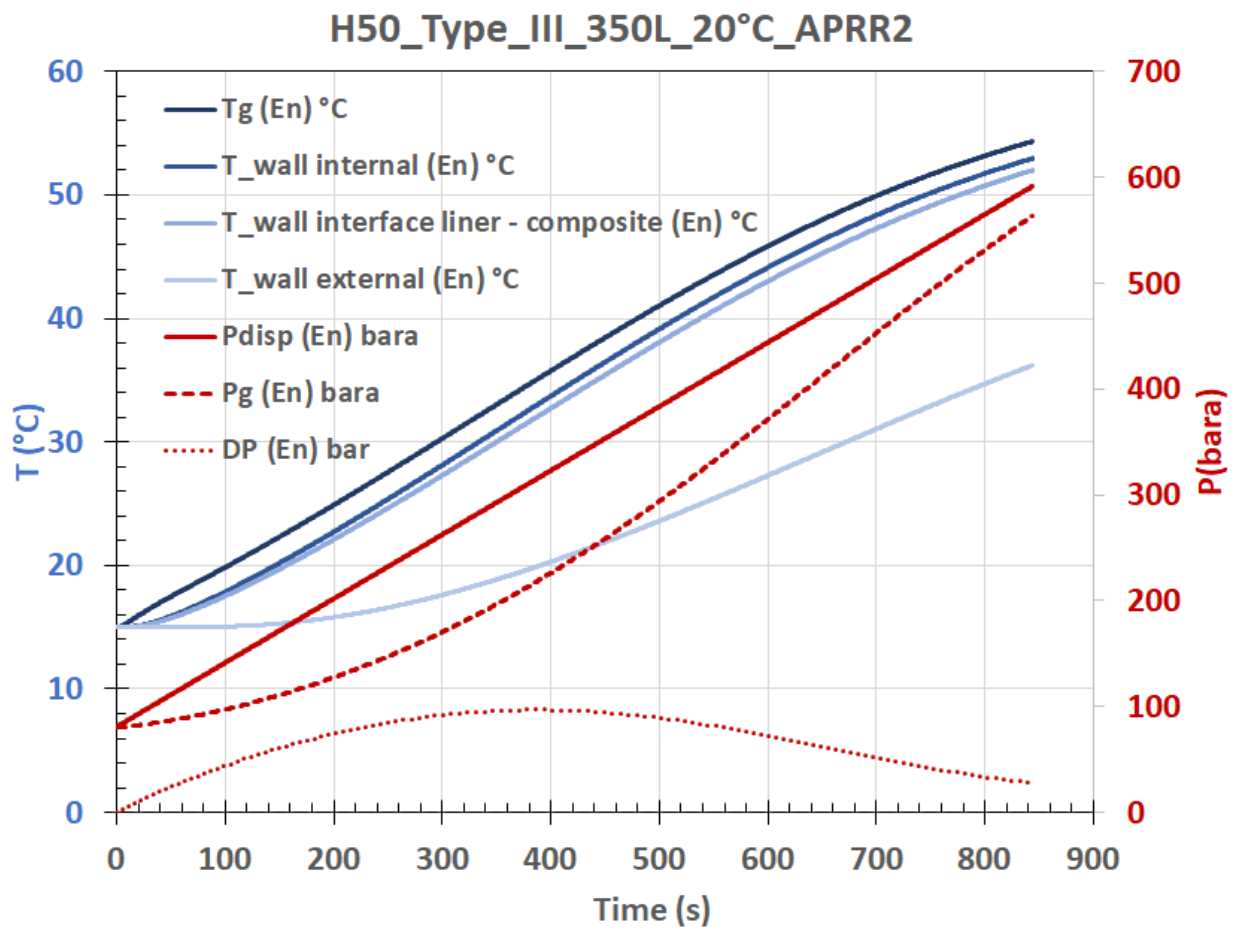


Figure D-8: Simulation of 15 minutes filling for NWP = 50 MPa, Type III 350 L tank, inlet temperature = -20°C

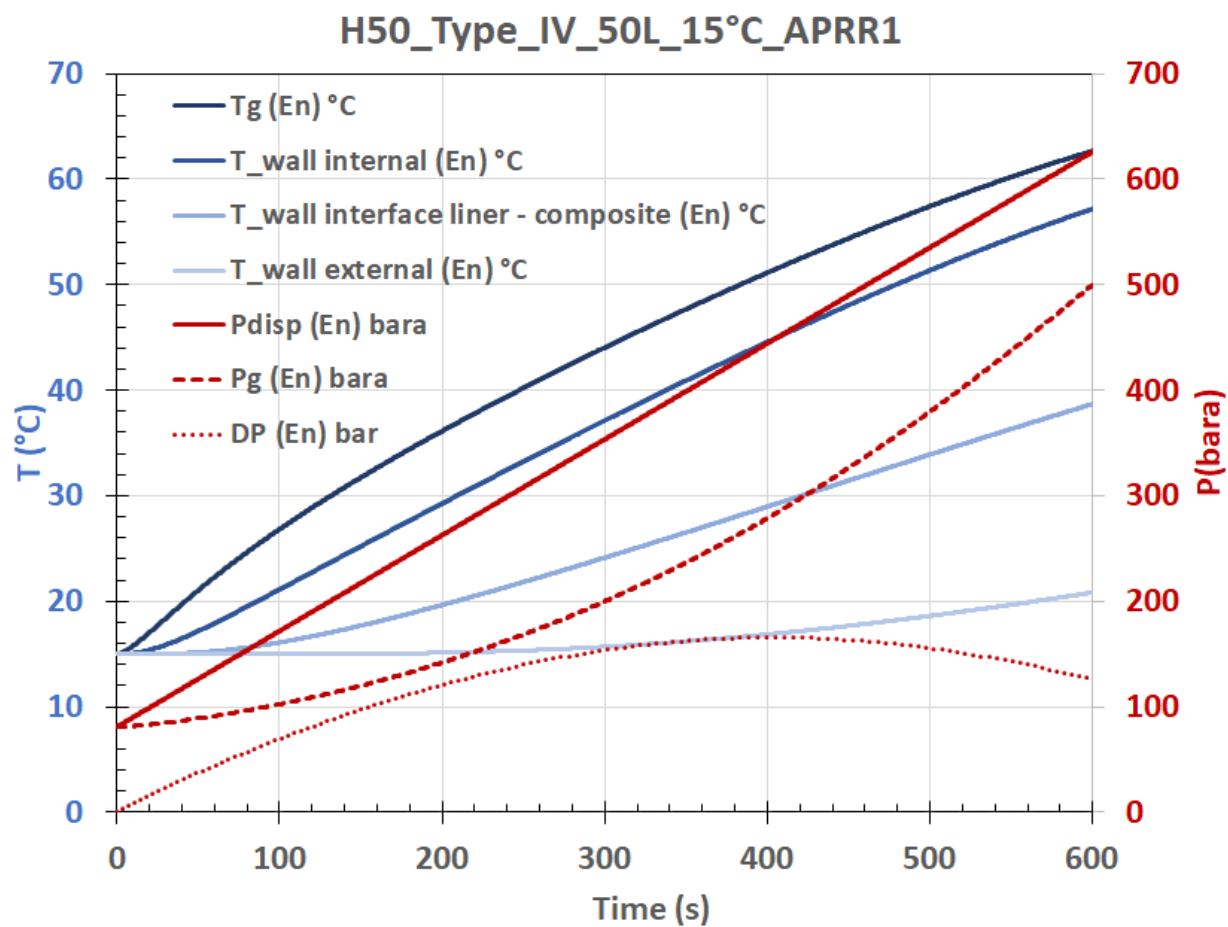


Figure D-9: Simulation of 10 minutes filling for NWP = 50 MPa, Type IV 50 L tank, inlet temperature = 15°C

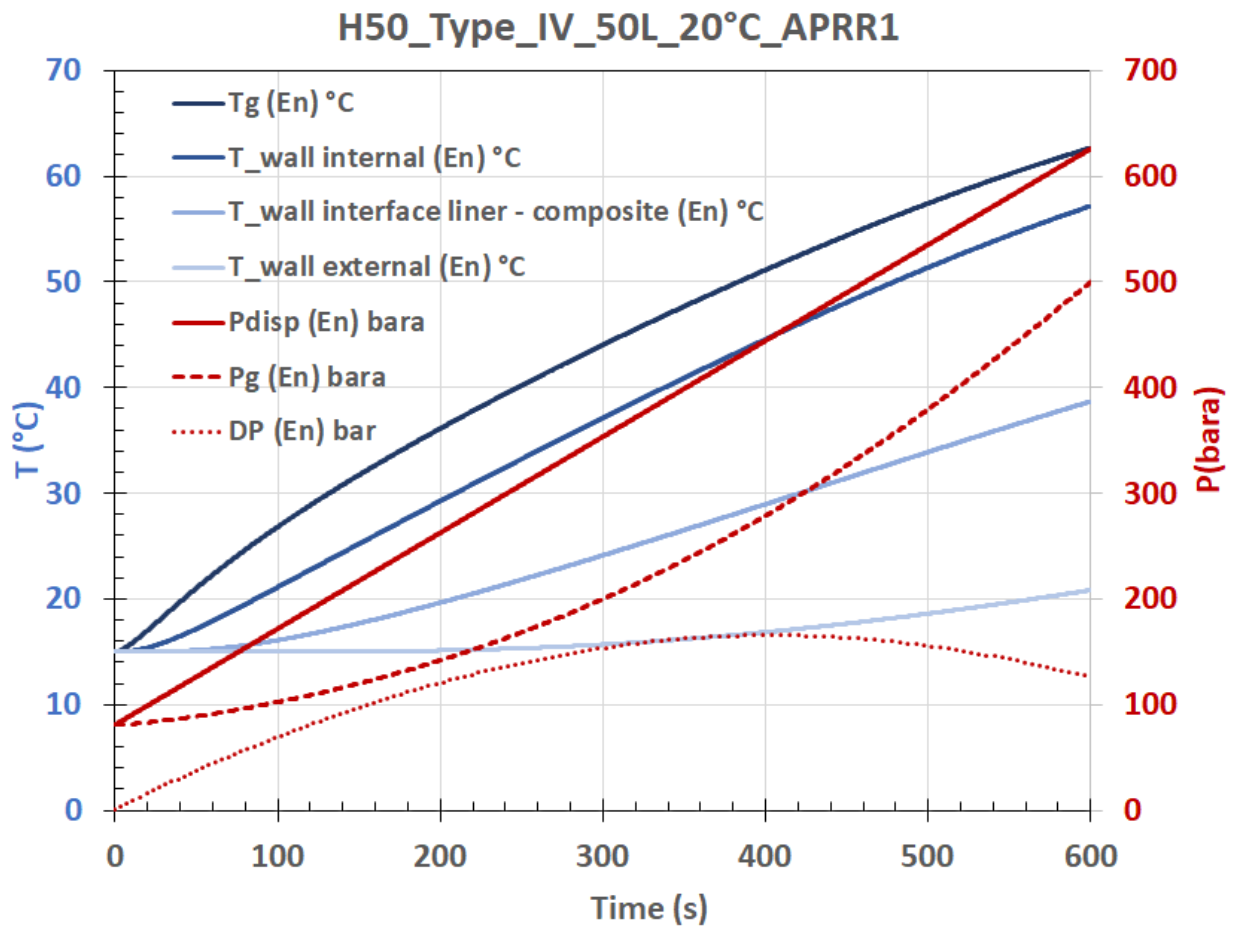


Figure D-10: Simulation of 10 minutes filling for NWP = 50 MPa, Type IV 50 L tank, inlet temperature = -20°C

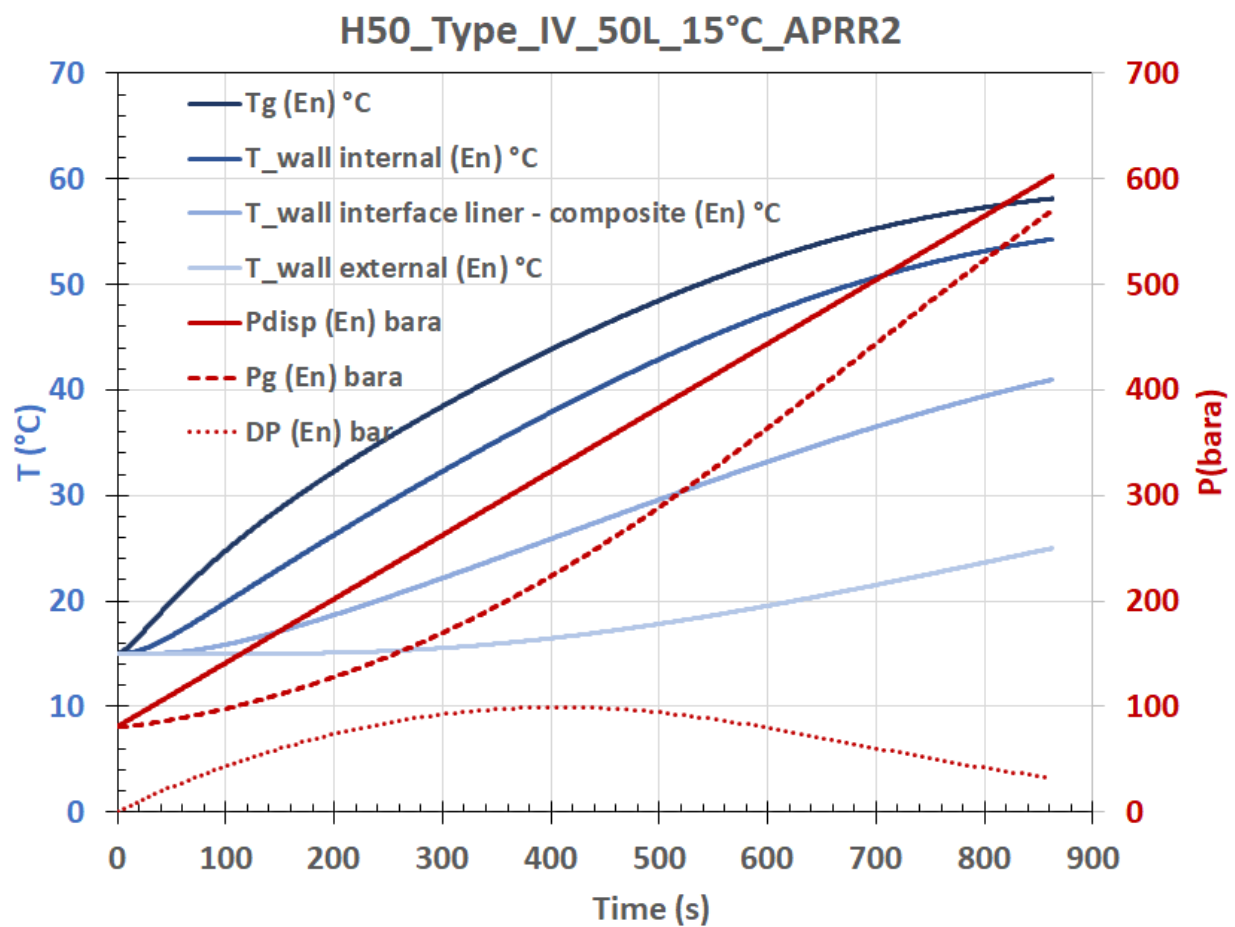


Figure D-11: Simulation of 15 minutes filling for NWP = 50 MPa, Type IV 50 L tank, inlet temperature = 15°C

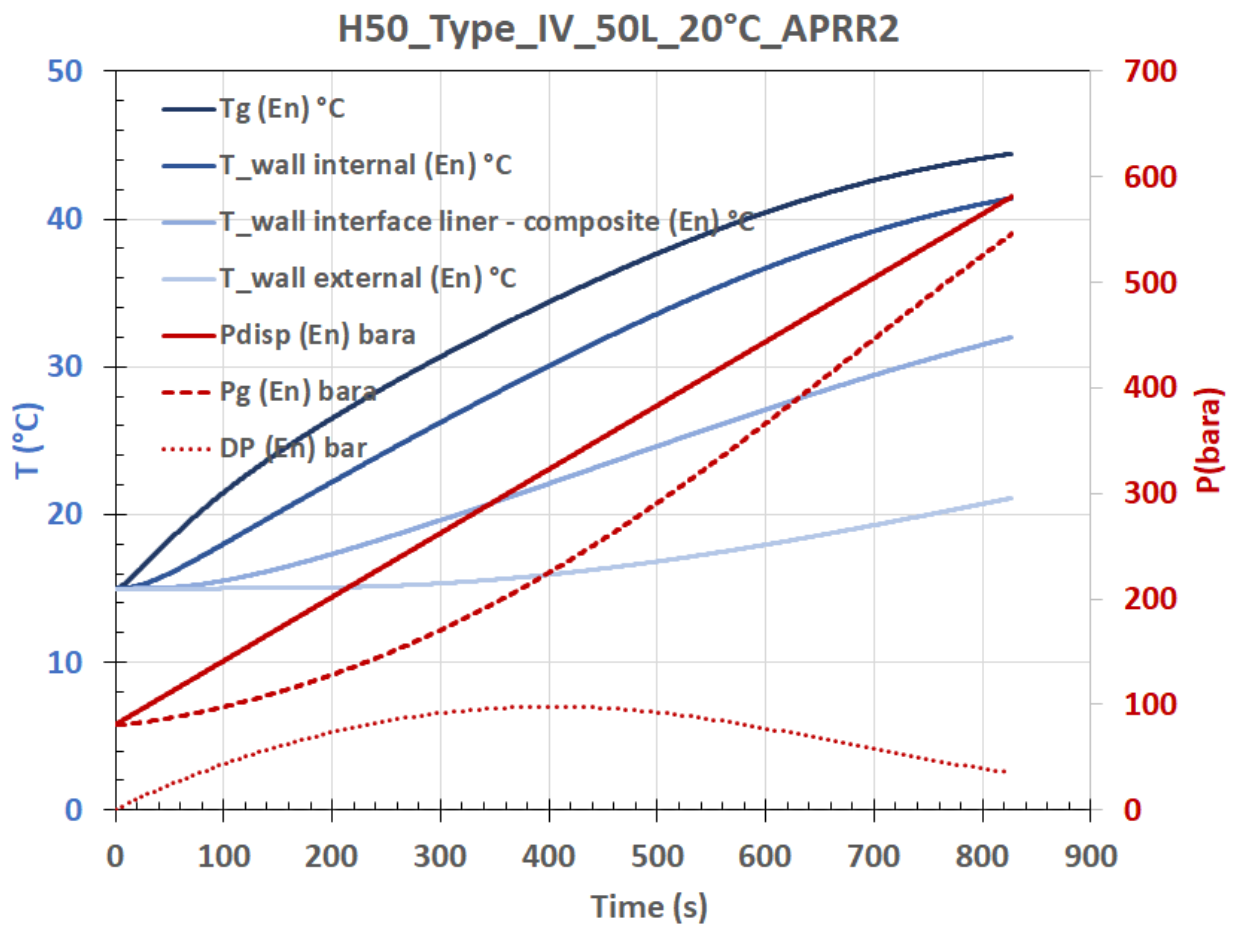


Figure D-12: Simulation of 15 minutes filling for NWP = 50 MPa, Type IV 50 L tank, inlet temperature = -20°C

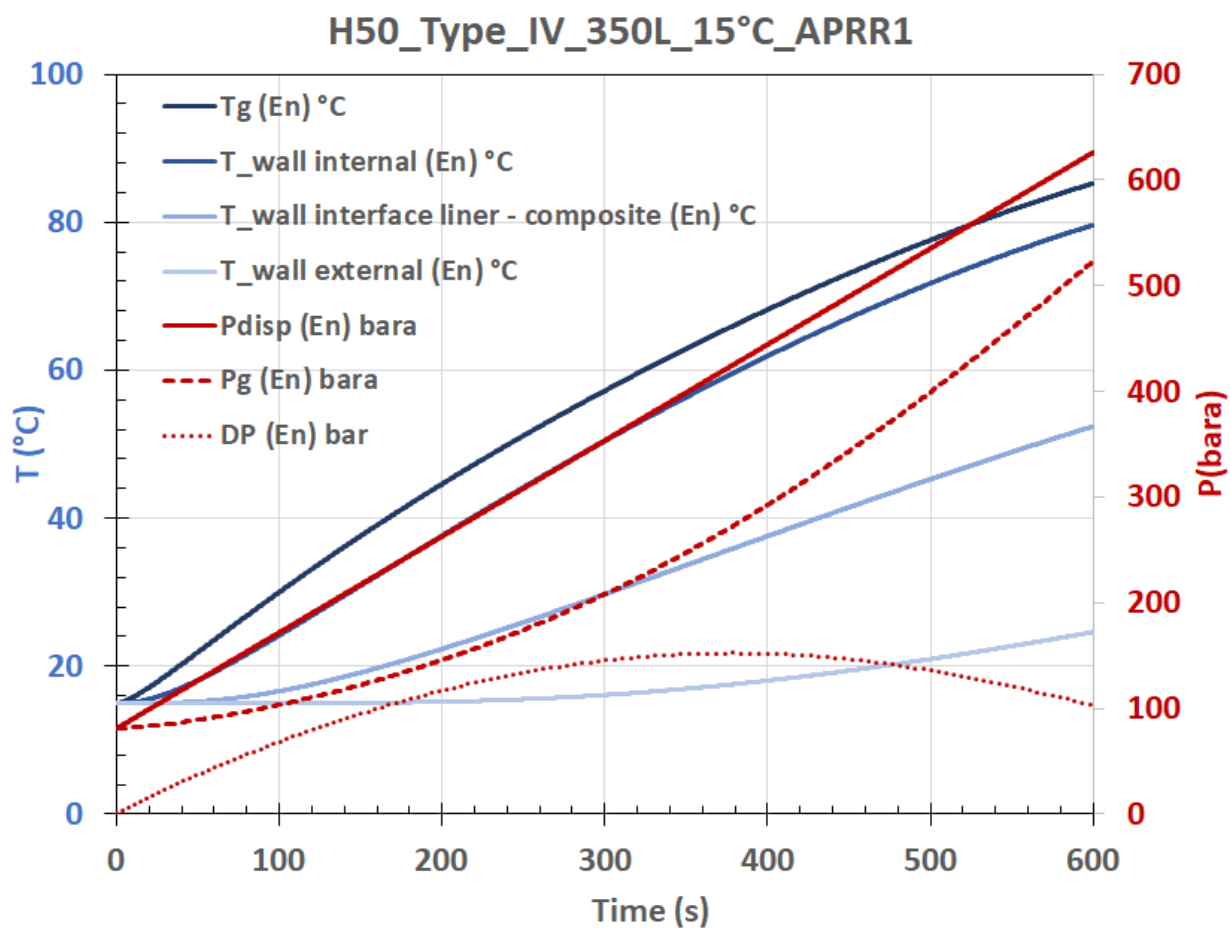


Figure D-13: Simulation of 10 minutes filling for NWP = 50 MPa, Type IV 350 L tank, inlet temperature = 15°C

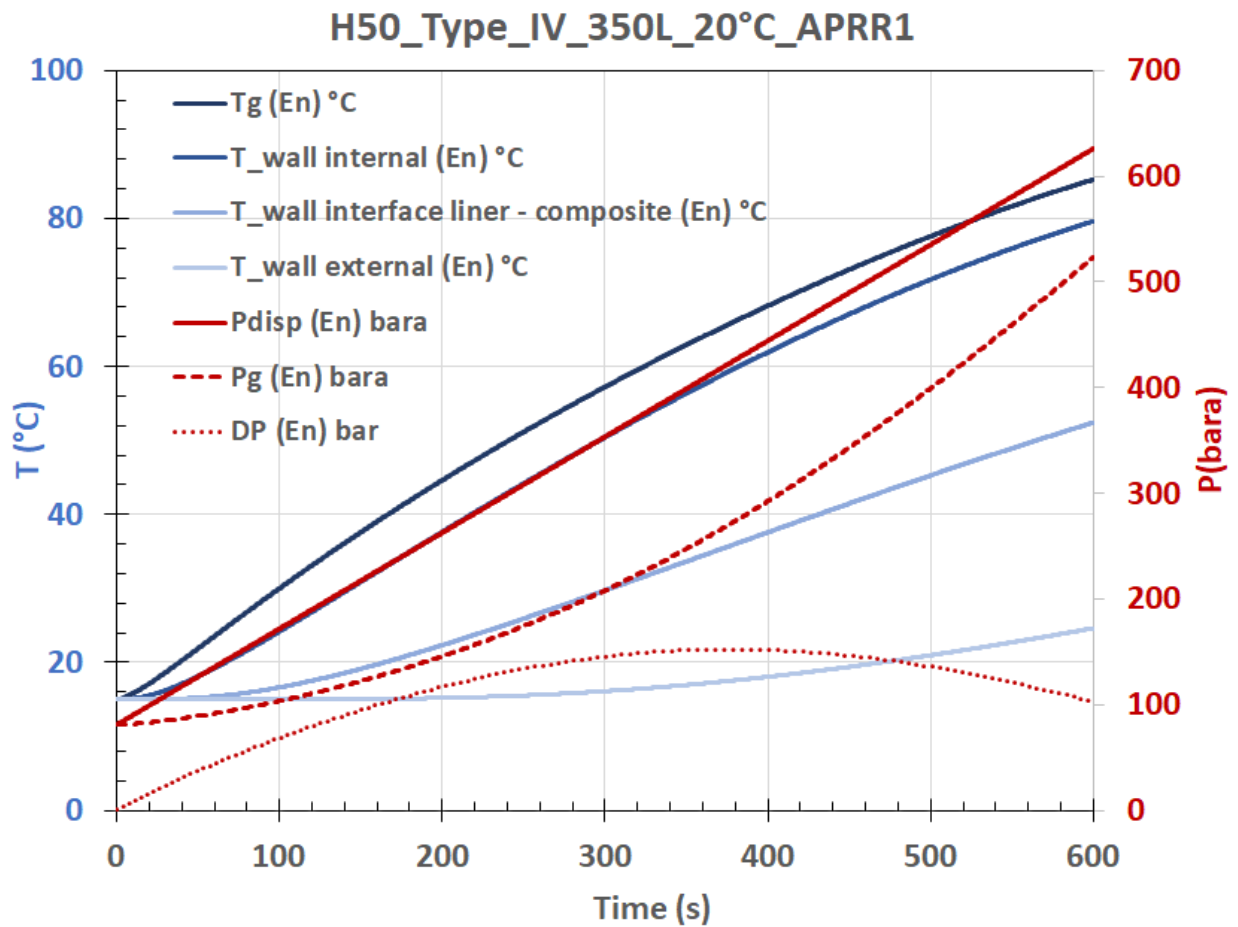


Figure D-14: Simulation of 10 minutes filling for NWP = 50 MPa, Type IV 350 L tank, inlet temperature = -20°C

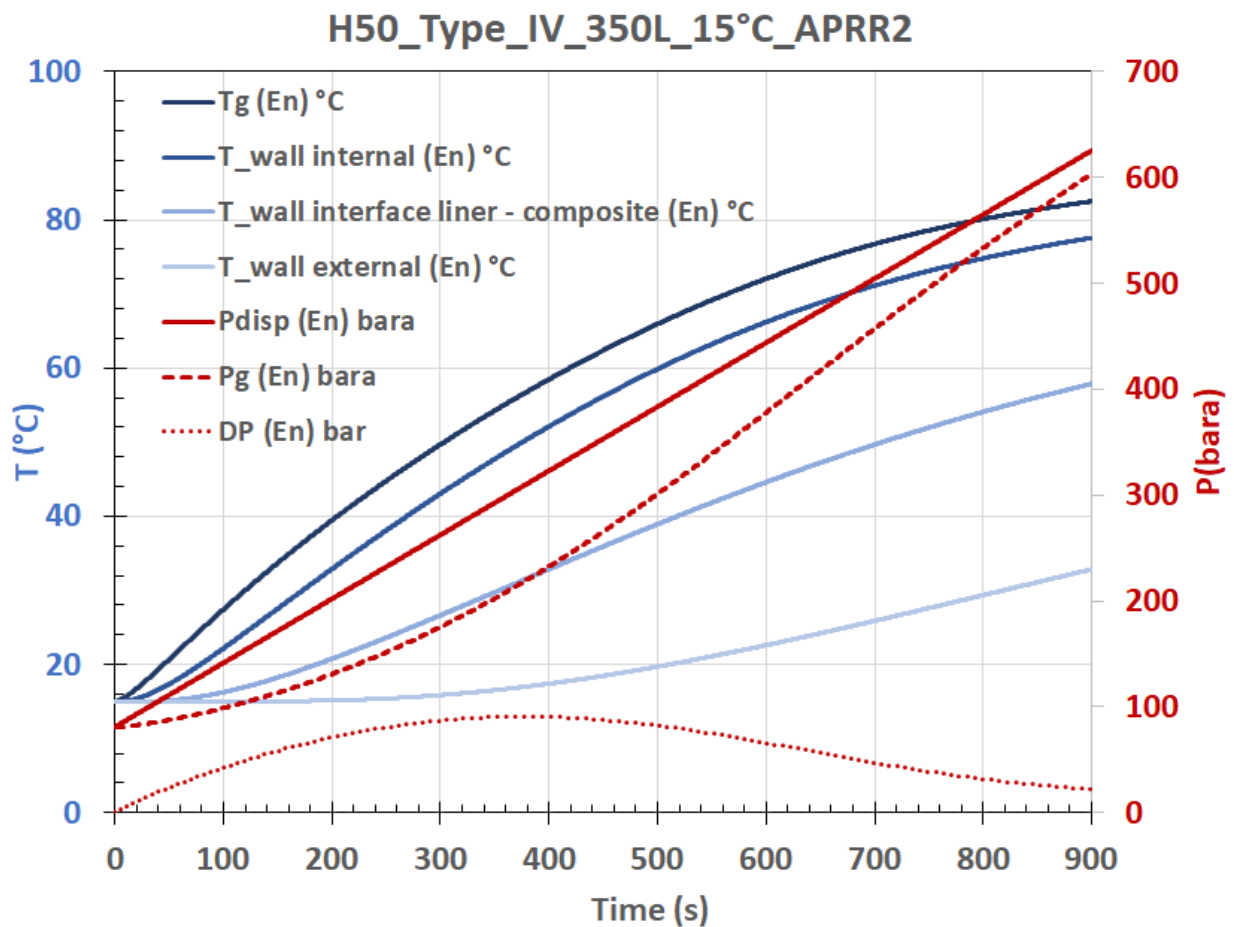


Figure D-15: Simulation of 15 minutes filling for NWP = 50 MPa, Type IV 350 L tank, inlet temperature = -20°C

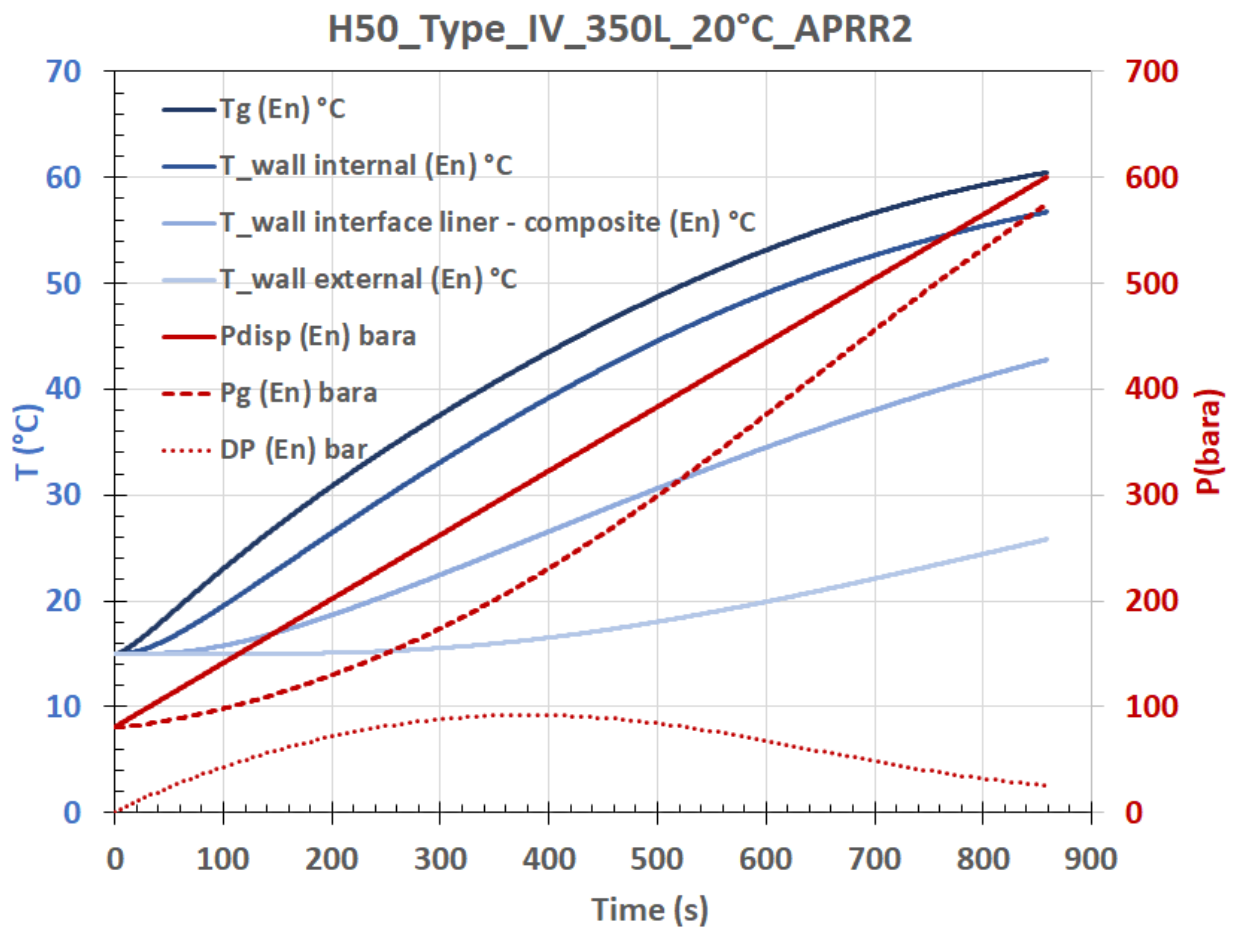


Figure D-16: Simulation of 15 minutes filling for NWP = 50 MPa, Type IV 350 L tank, inlet temperature = -20°C

E. H70 SIMULATIONS

Figures E.1-16 show the evolution of gas and wall temperatures, as well as pressure in the dispenser and the tank and their difference, for the sixteen H70 cases.

Note: seven simulations in Table 10 reached 100% SOC before the end of the filling. The graphs in Annex E show results until the end of simulation, even if the filling could have in practice been stopped earlier.

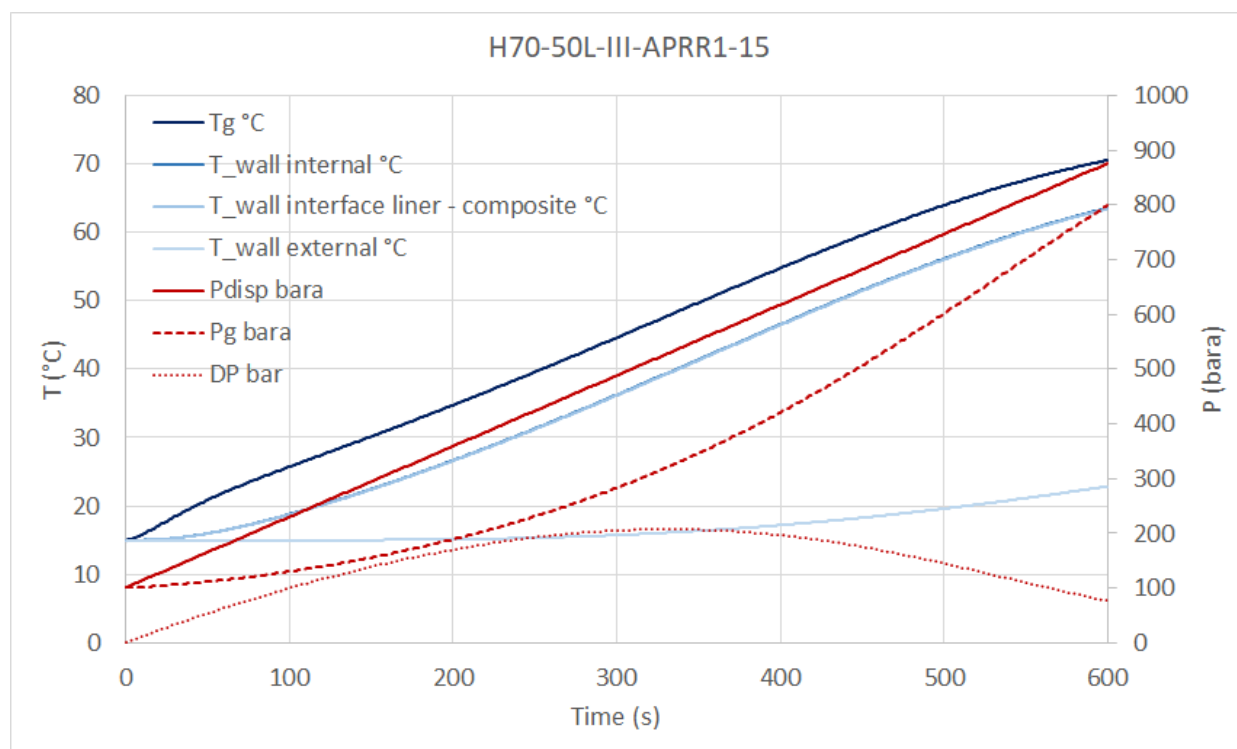


Figure E-1: Simulation of 10 minutes filling for NWP = 70 MPa, Type III 50 L tank, inlet temperature = 15°C

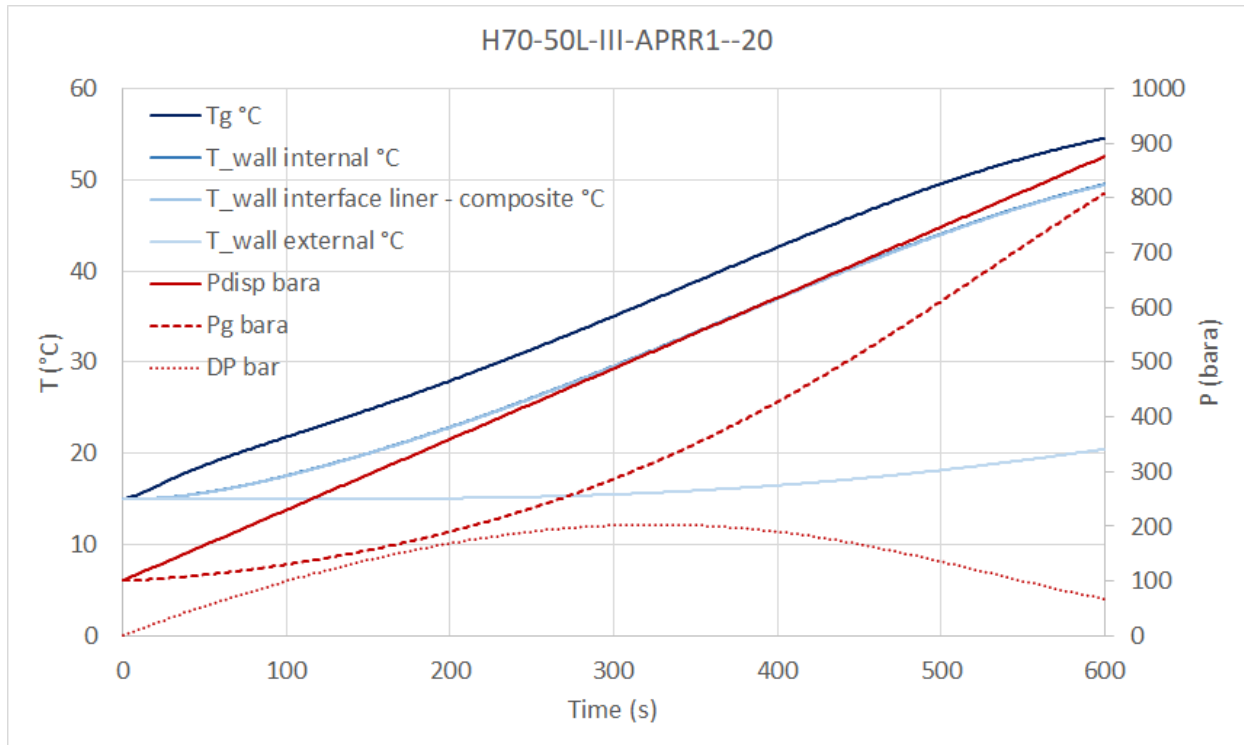


Figure E-2: Simulation of 10 minutes filling for NWP = 70 MPa, Type III 50 L tank, inlet temperature = -20 $^{\circ}\text{C}$

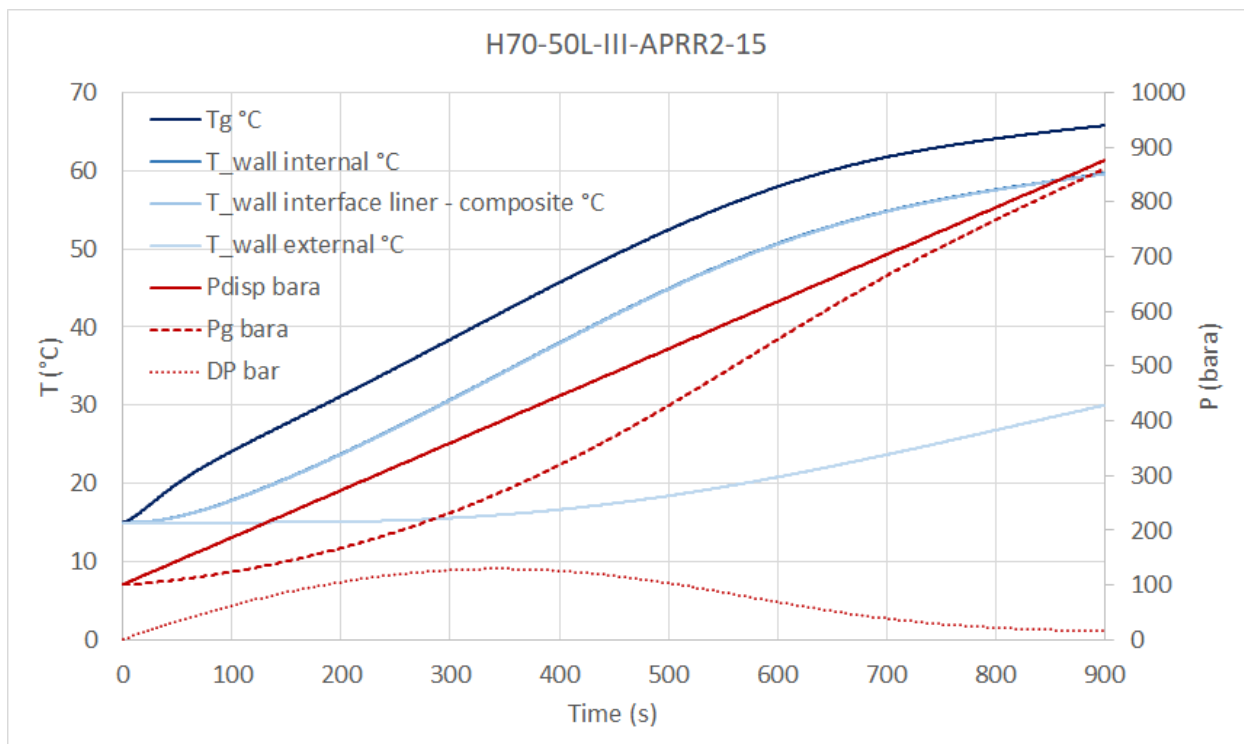


Figure E-3: Simulation of 15 minutes filling for NWP = 70 MPa, Type III 50 L tank, inlet temperature = 15 $^{\circ}\text{C}$

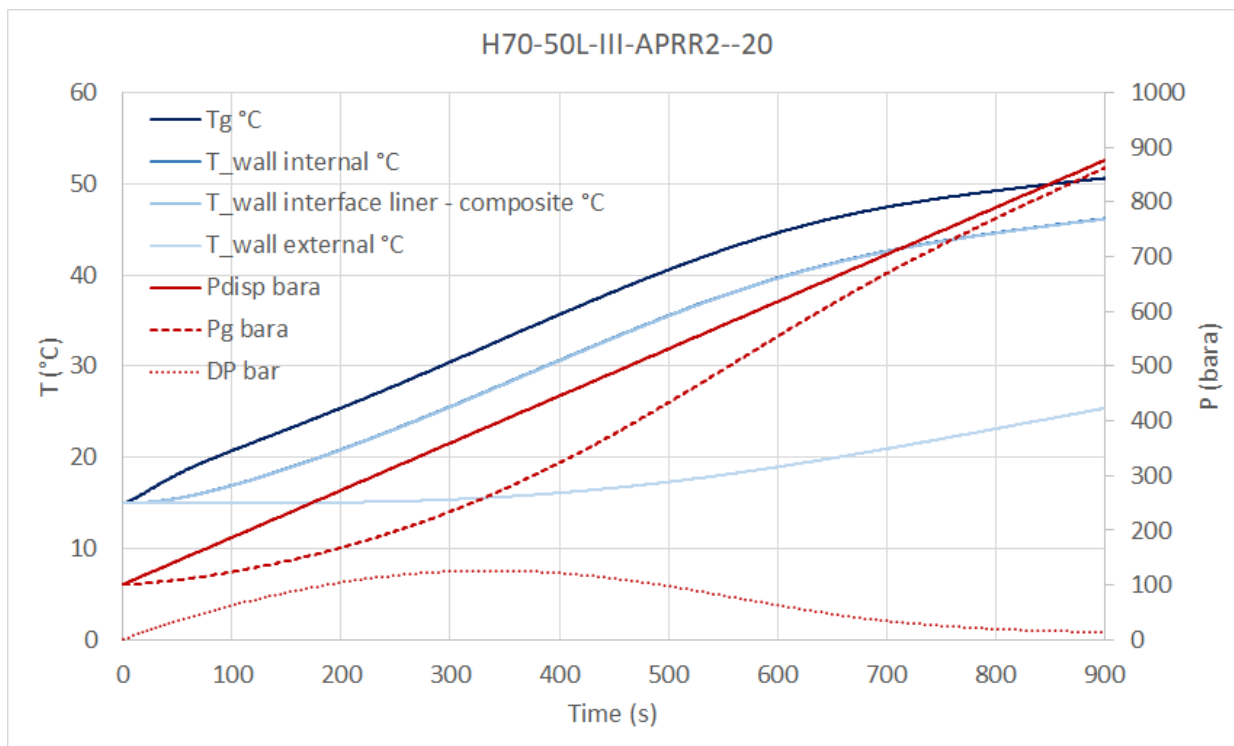


Figure E-4: Simulation of 15 minutes filling for NWP = 70 MPa, Type III 50 L tank, inlet temperature = -20°C

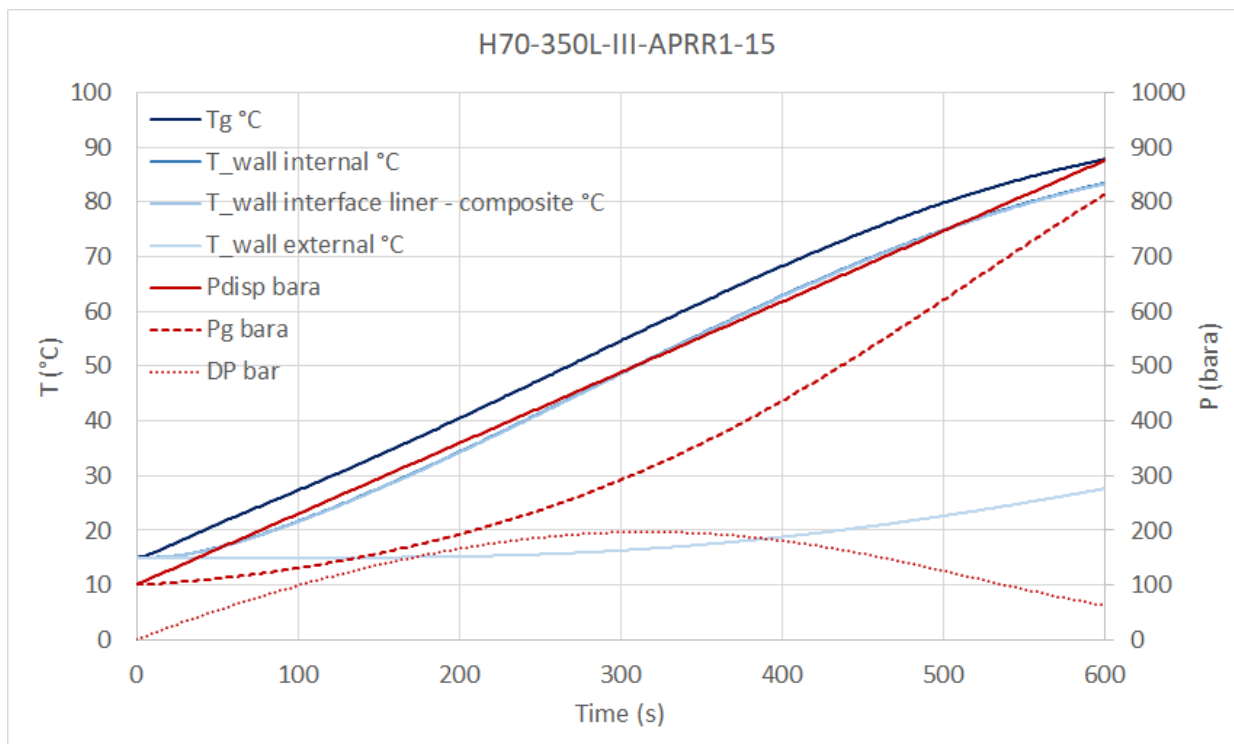


Figure E-5: Simulation of 10 minutes filling for NWP = 70 MPa, Type III 350 L tank, inlet temperature = 15°C

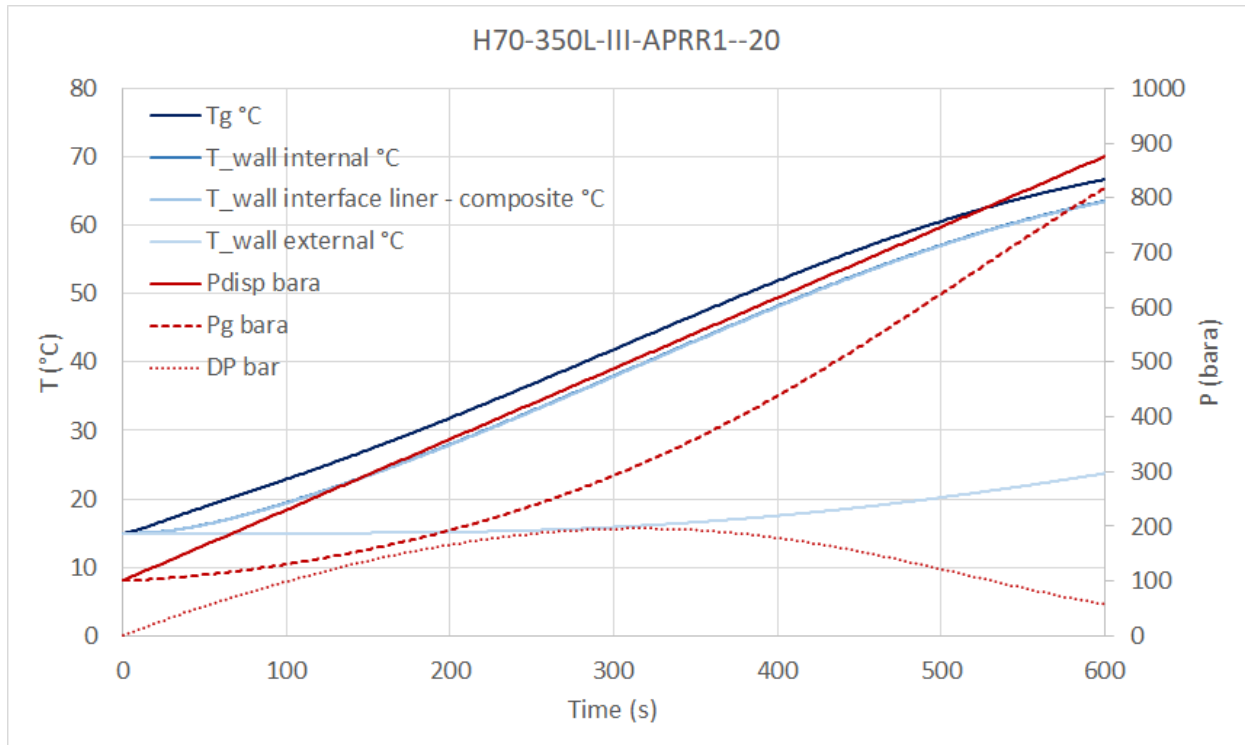


Figure E-6: Simulation of 10 minutes filling for NWP = 70 MPa, Type III 350 L tank, inlet temperature = -20°C

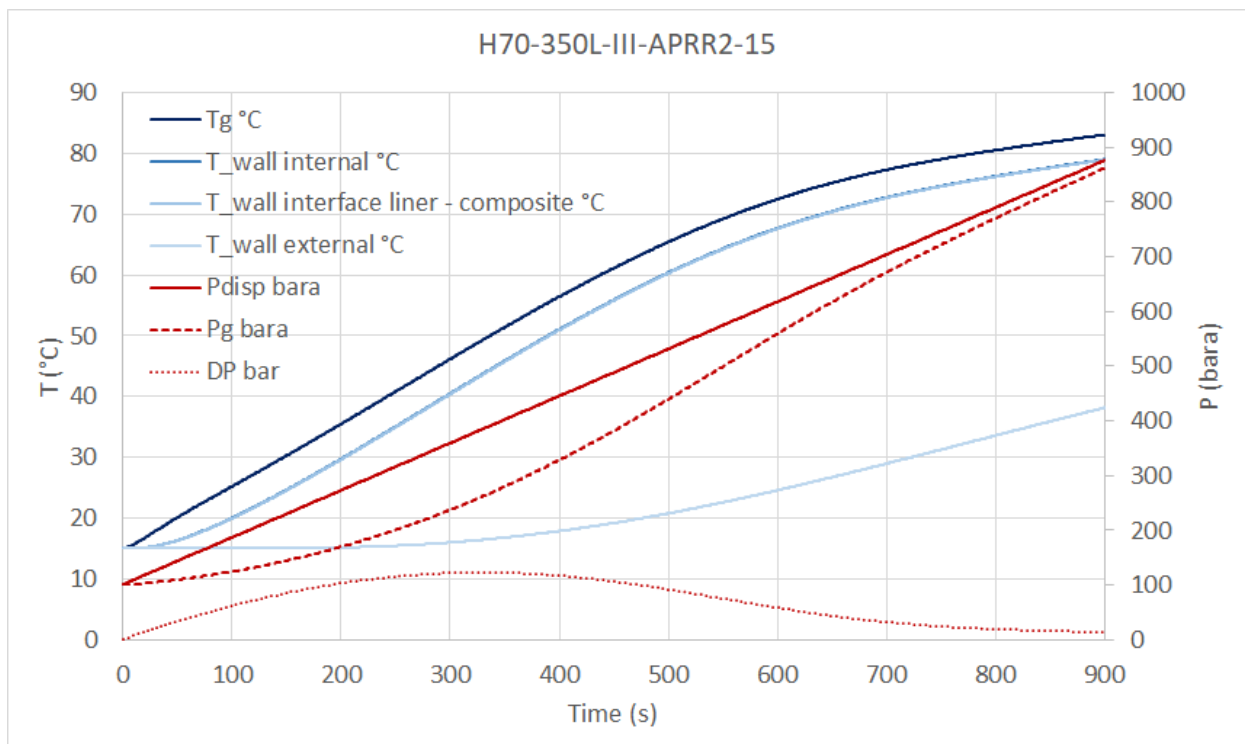


Figure E-7: Simulation of 15 minutes filling for NWP = 70 MPa, Type III 350 L tank, inlet temperature = 15°C

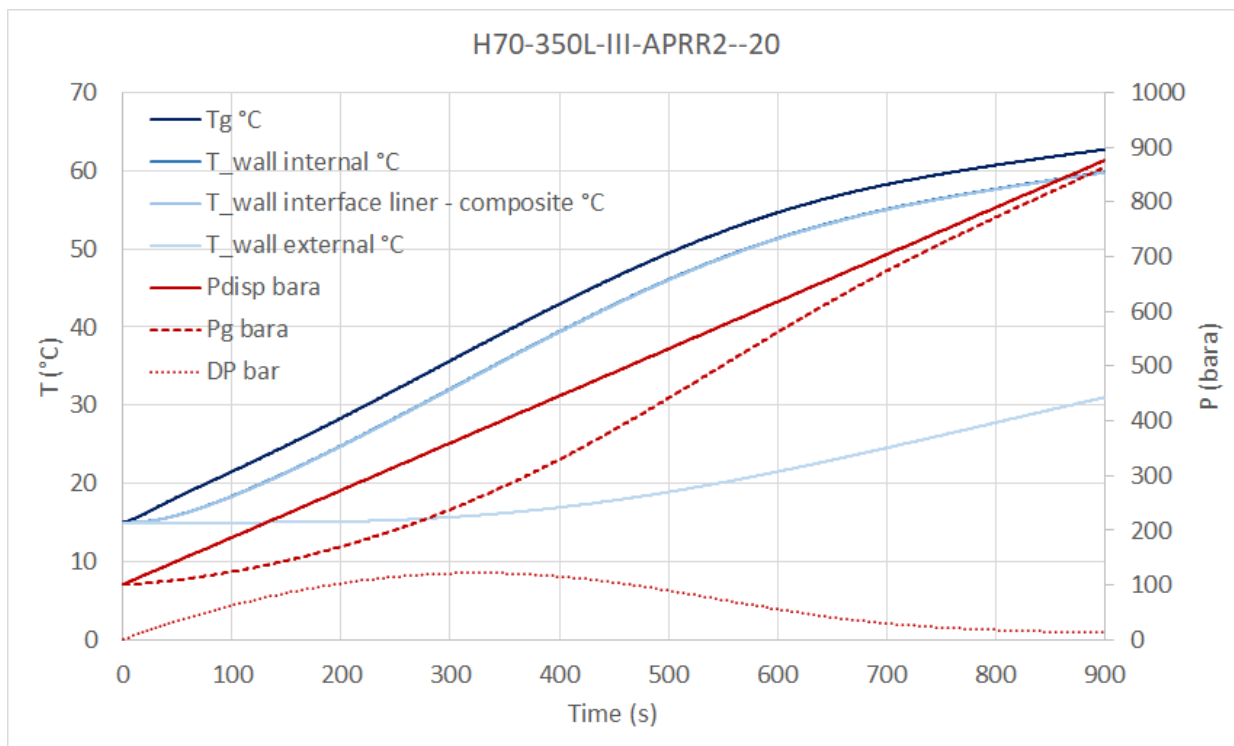


Figure E-8: Simulation of 15 minutes filling for NWP = 70 MPa, Type III 350 L tank, inlet temperature = -20°C

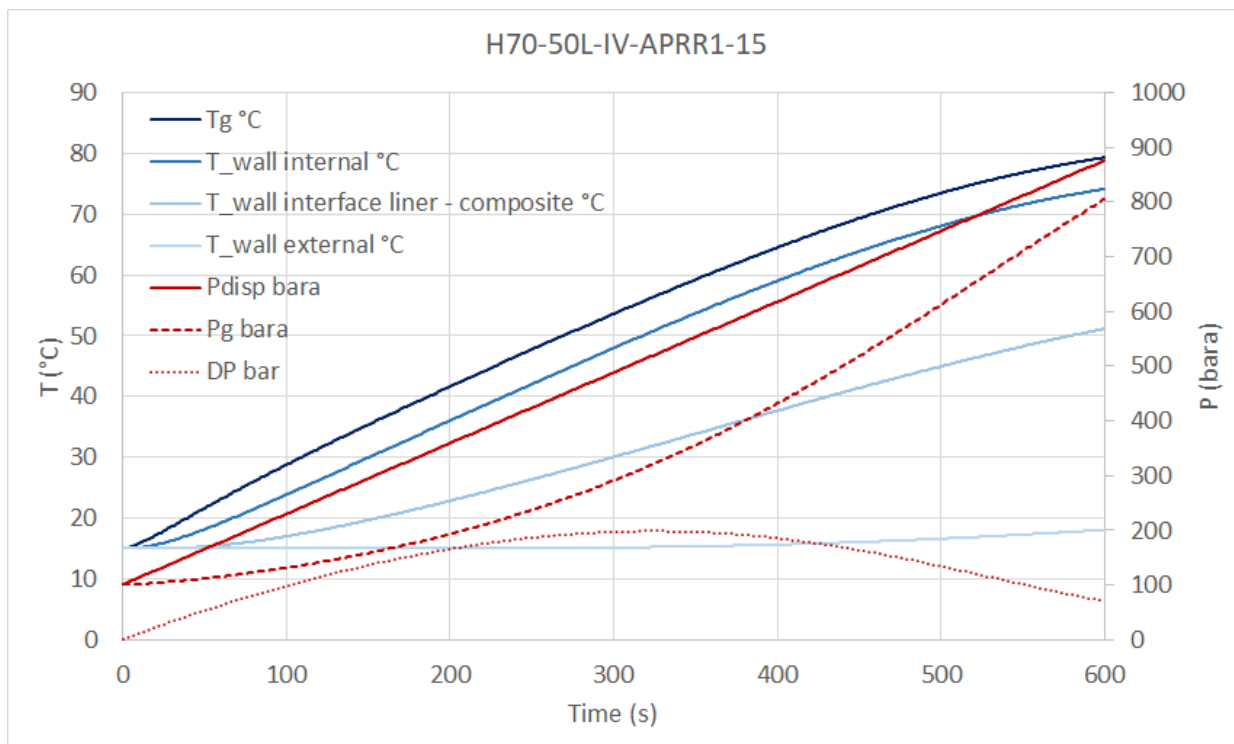


Figure E-9: Simulation of 10 minutes filling for NWP = 70 MPa, Type IV 50 L tank, inlet temperature = 15°C

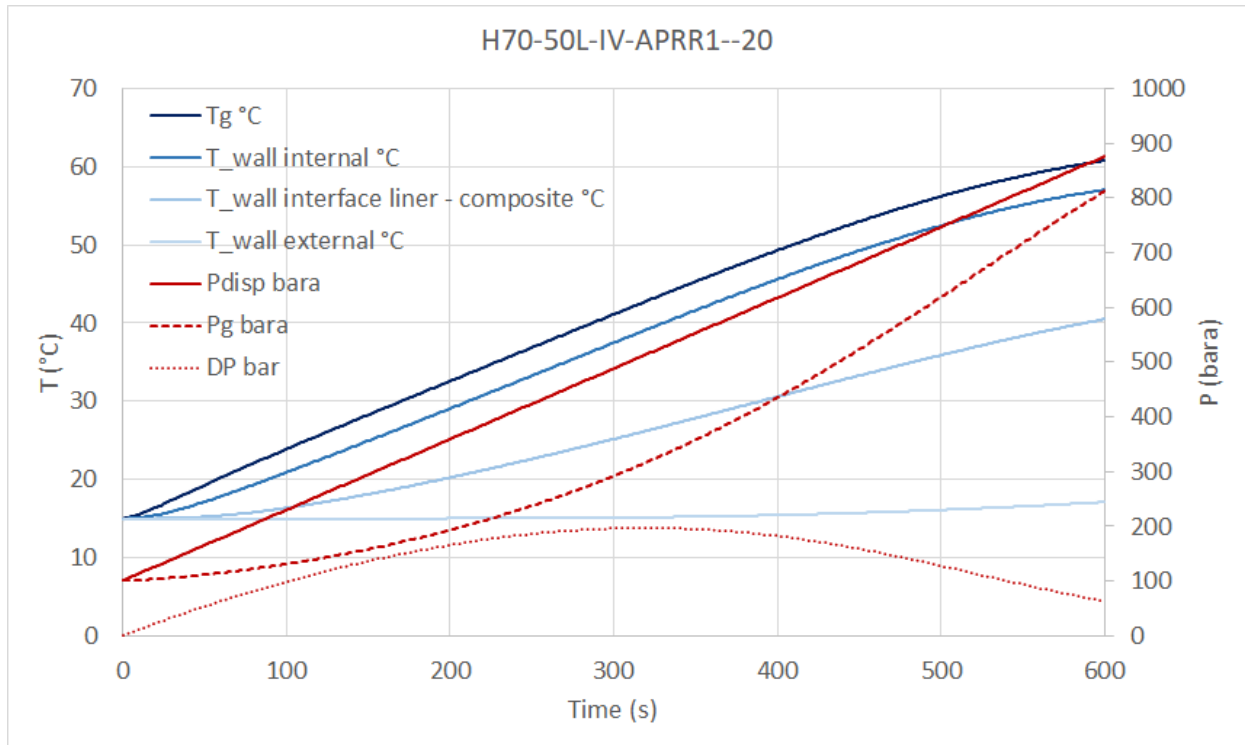


Figure E-10: Simulation of 10 minutes filling for NWP = 70 MPa, Type IV 50 L tank, inlet temperature = -20°C

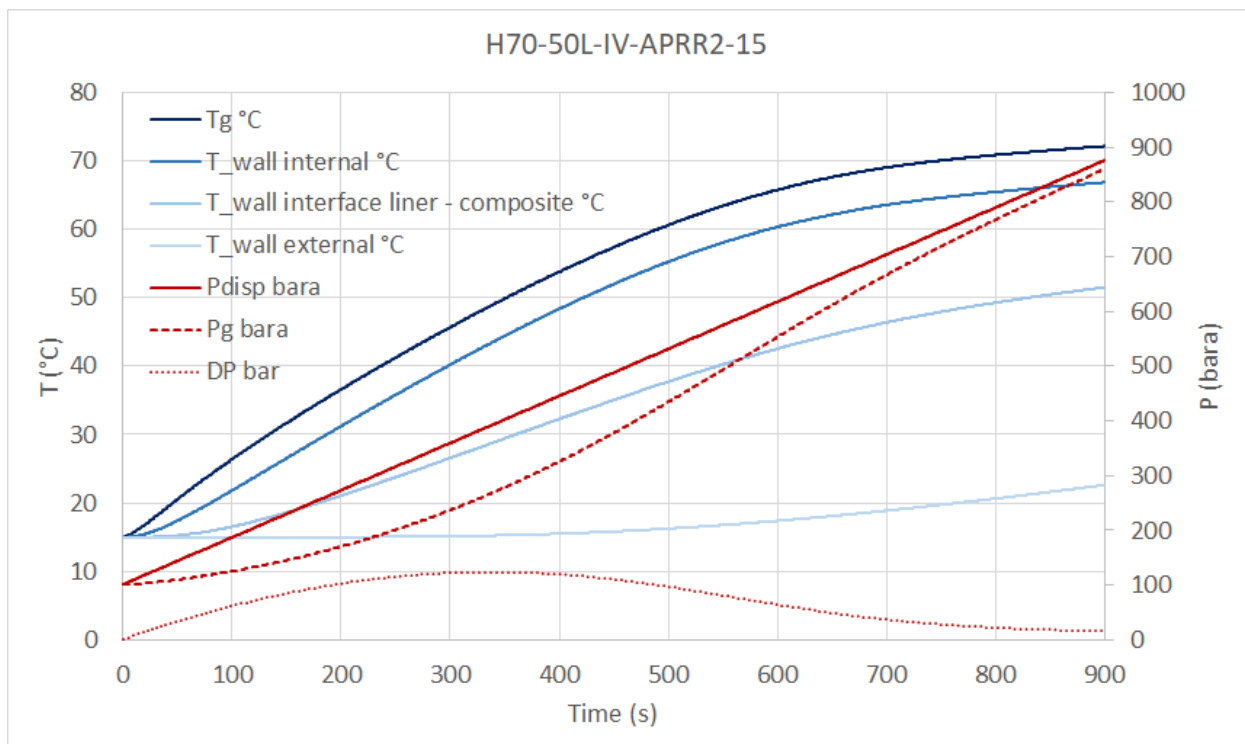


Figure E-11: Simulation of 15 minutes filling for NWP = 70 MPa, Type IV 50 L tank, inlet temperature = 15°C

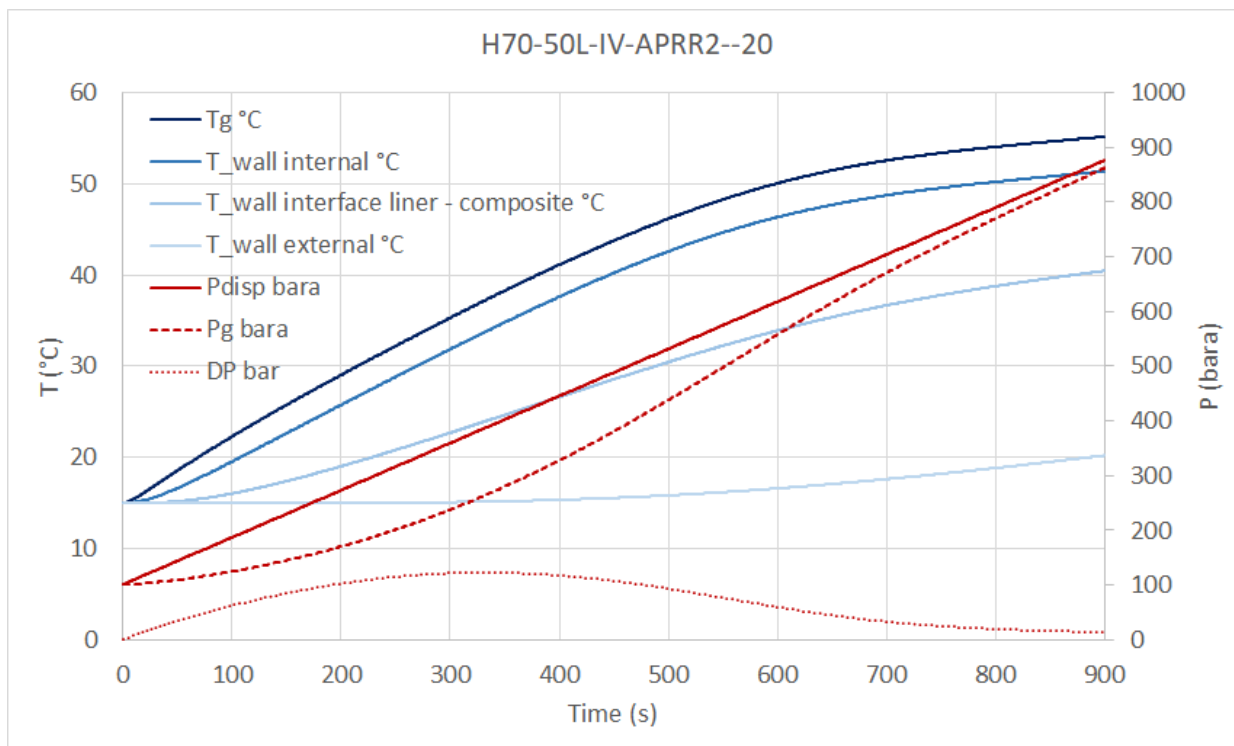


Figure E-12: Simulation of 15 minutes filling for NWP = 70 MPa, Type IV 50 L tank, inlet temperature = -20°C

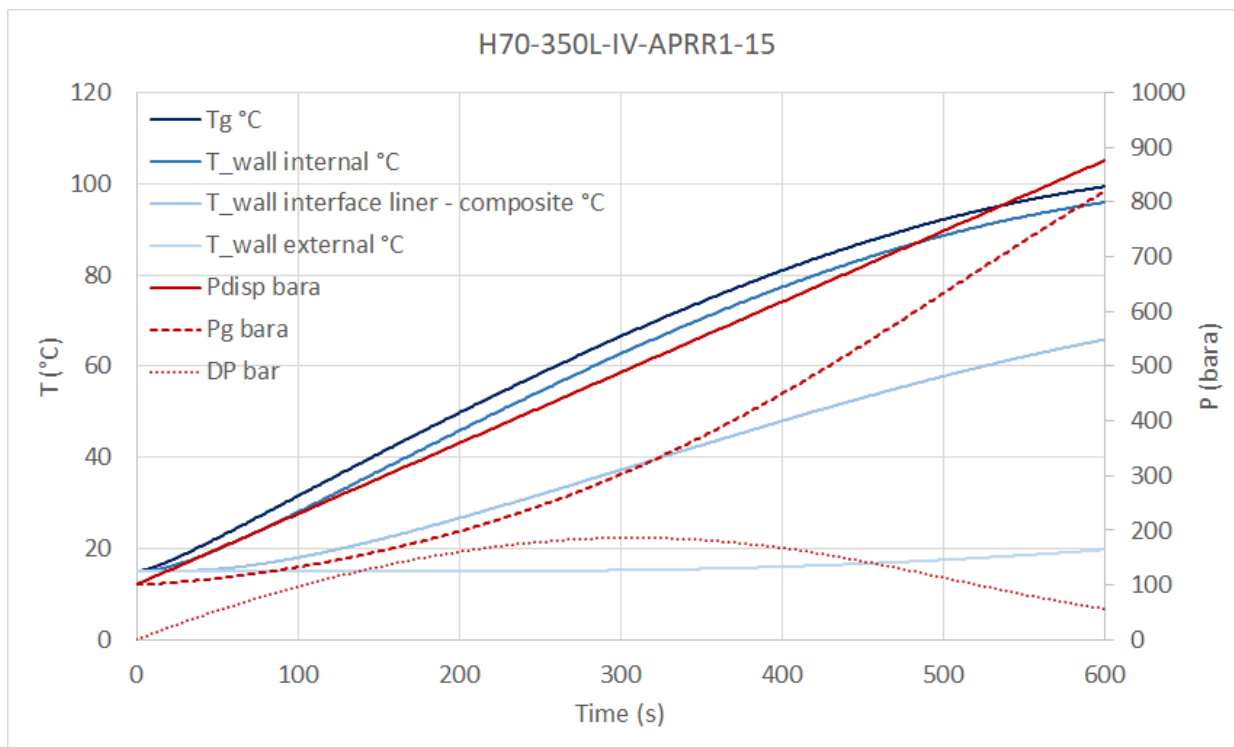


Figure E-13: Simulation of 10 minutes filling for NWP = 70 MPa, Type IV 350 L tank, inlet temperature = 15°C

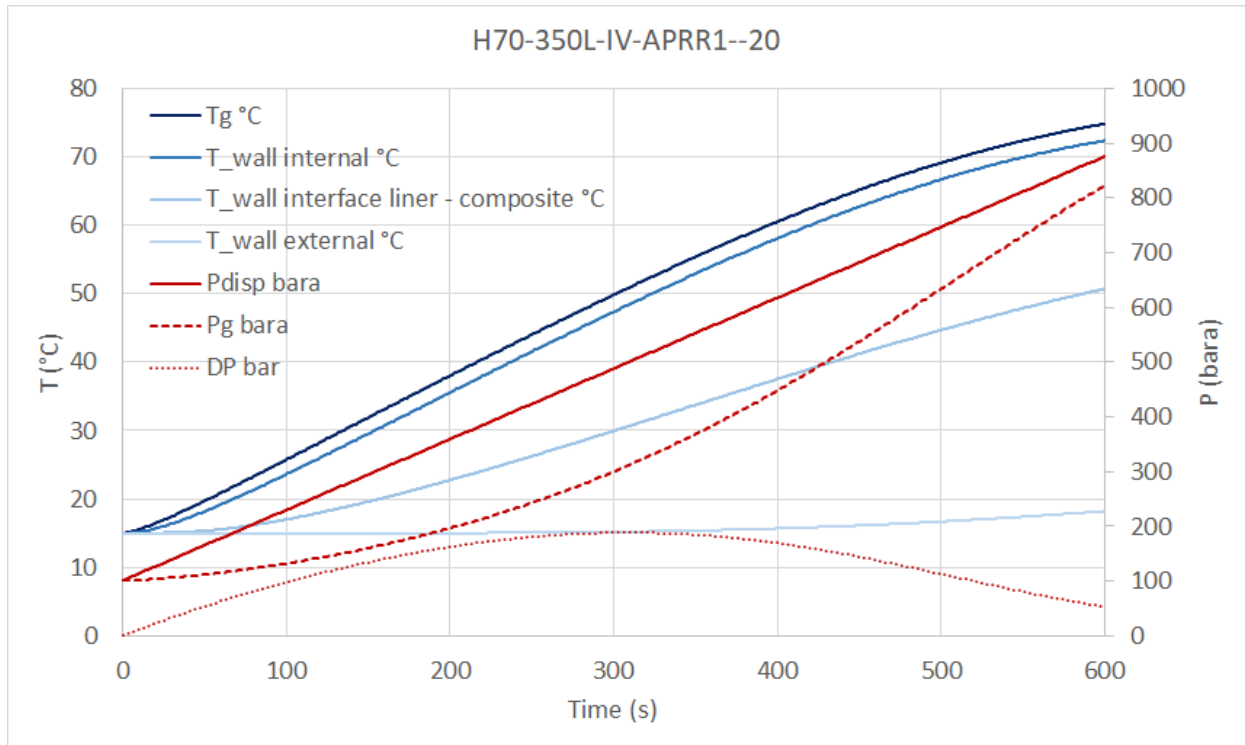


Figure E-14: Simulation of 10 minutes filling for NWP = 70 MPa, Type IV 350 L tank, inlet temperature = -20°C

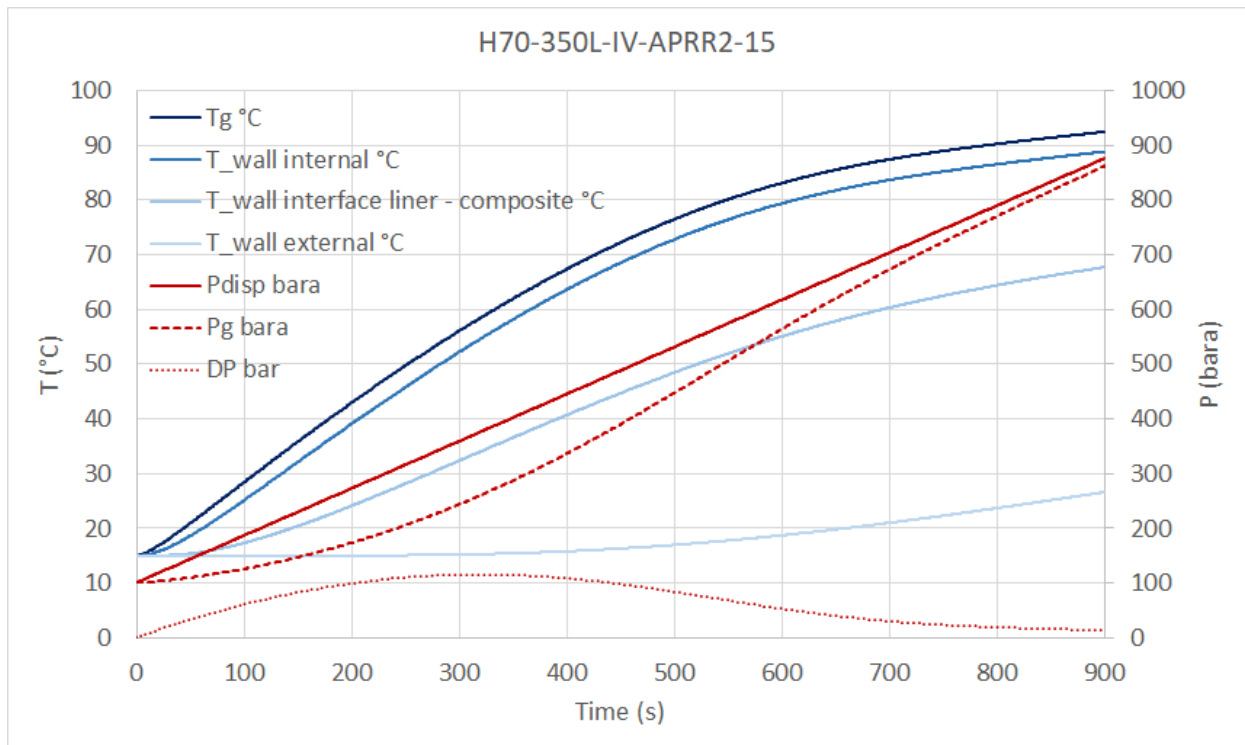


Figure E-15: Simulation of 15 minutes filling for NWP = 70 MPa, Type IV 350 L tank, inlet temperature = 15°C

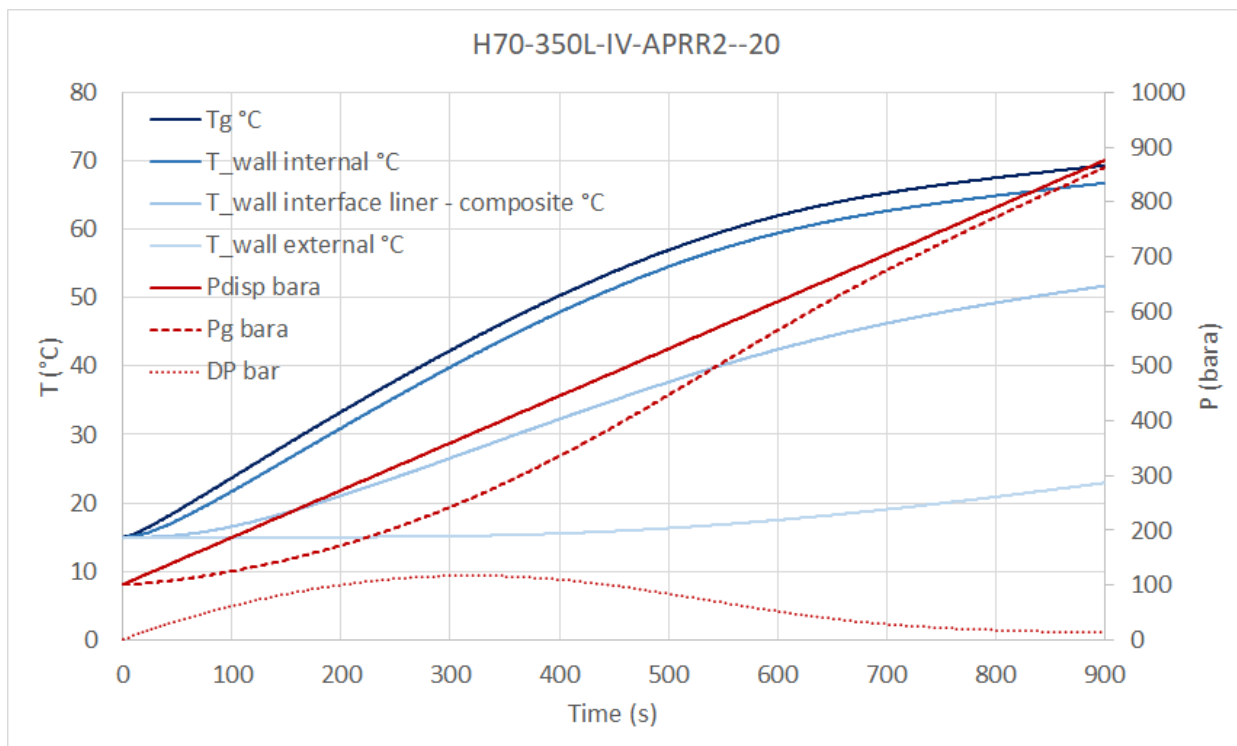


Figure E-16: Simulation of 15 minutes filling for NWP = 70 MPa, Type IV 350 L tank, inlet temperature = -20°C

F. H35 SIMULATIONS WITH AMBIENT TEMPERATURE OF 40°C

Figures F.1-6 show the evolution of gas and wall temperatures, as well as pressure in the dispenser and the tank and their difference, for the six H35 cases, with ambient temperature at 40°C.

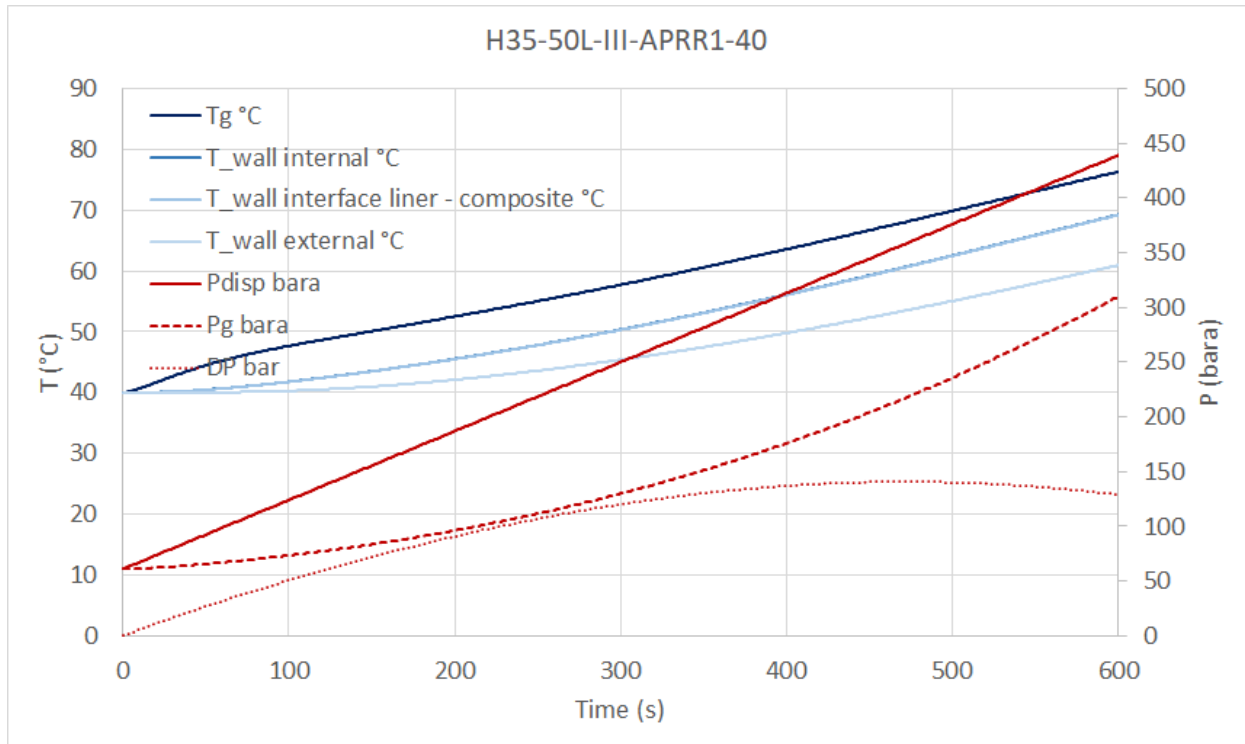


Figure F-1: Simulation of 10 minutes filling for NWP = 35 MPa, Type III 50 L tank, inlet temperature = 40°C, ambient temperature = 40°C

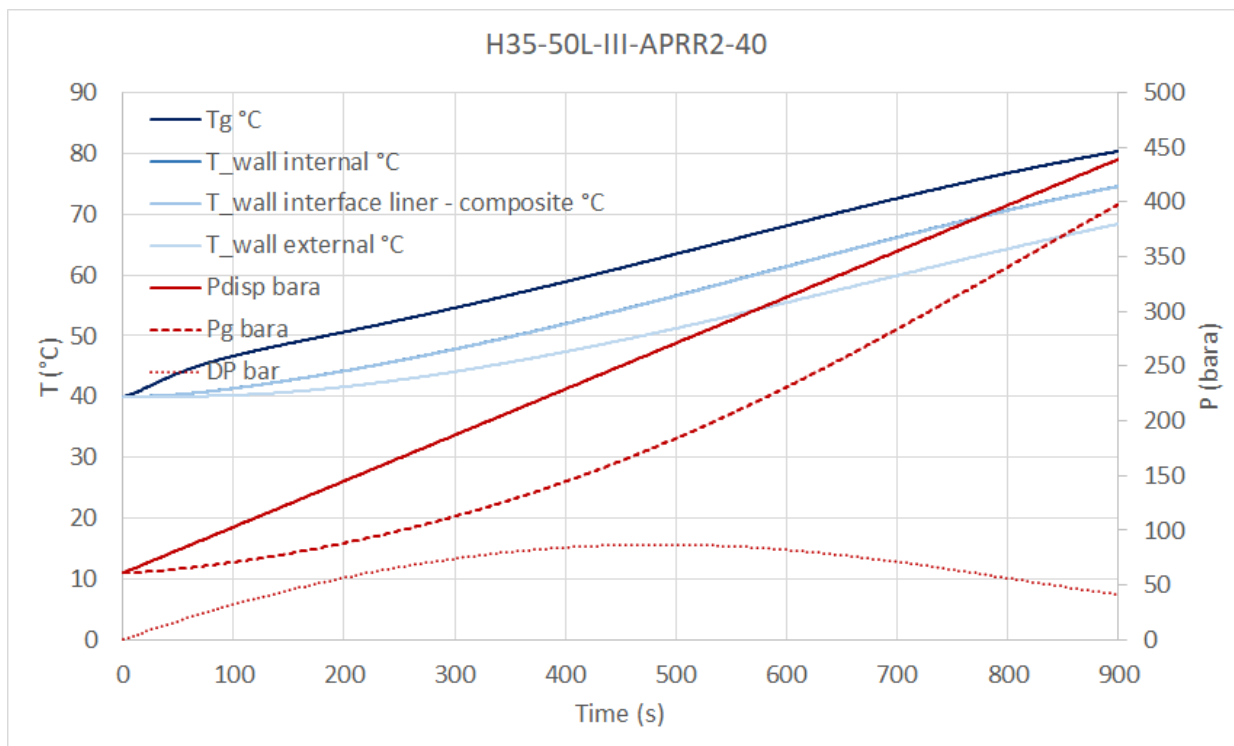


Figure F-2: Simulation of 15 minutes filling for NWP = 35 MPa, Type III 50 L tank, inlet temperature = 40°C, ambient temperature = 40°C

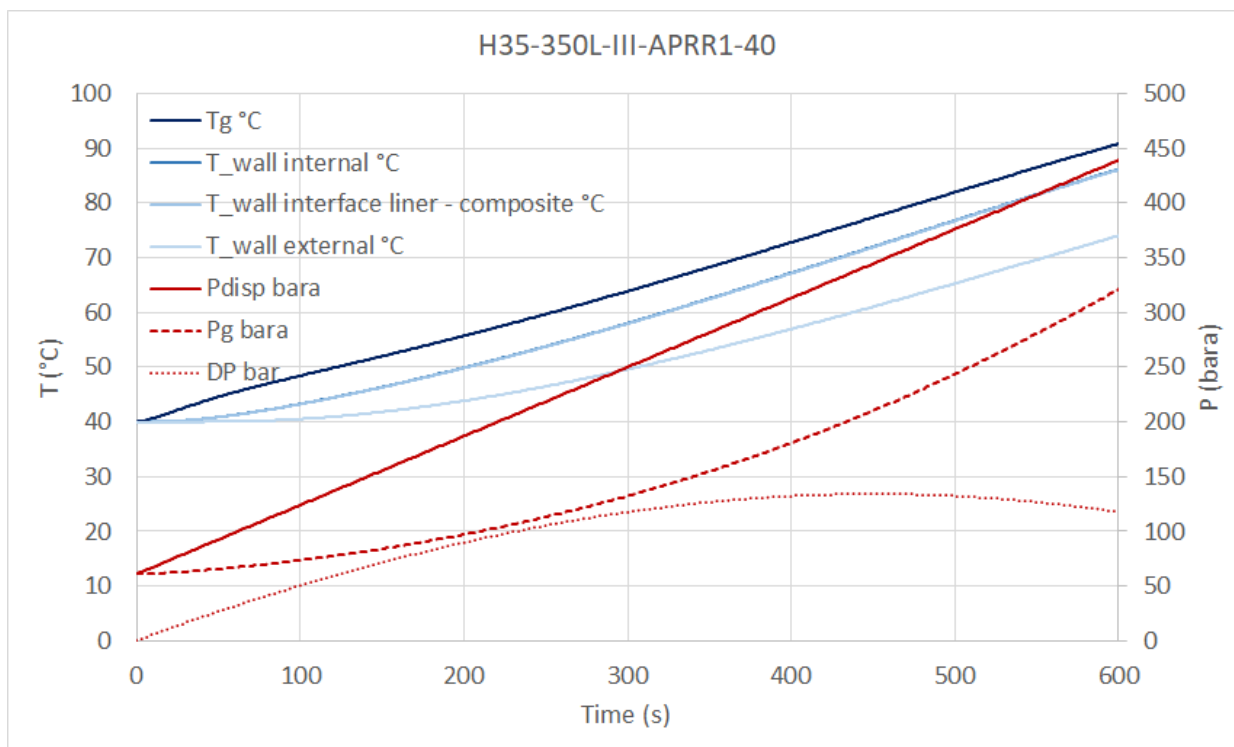


Figure F-3: Simulation of 10 minutes filling for NWP = 35 MPa, Type III 350 L tank, inlet temperature = 40°C, ambient temperature = 40°C

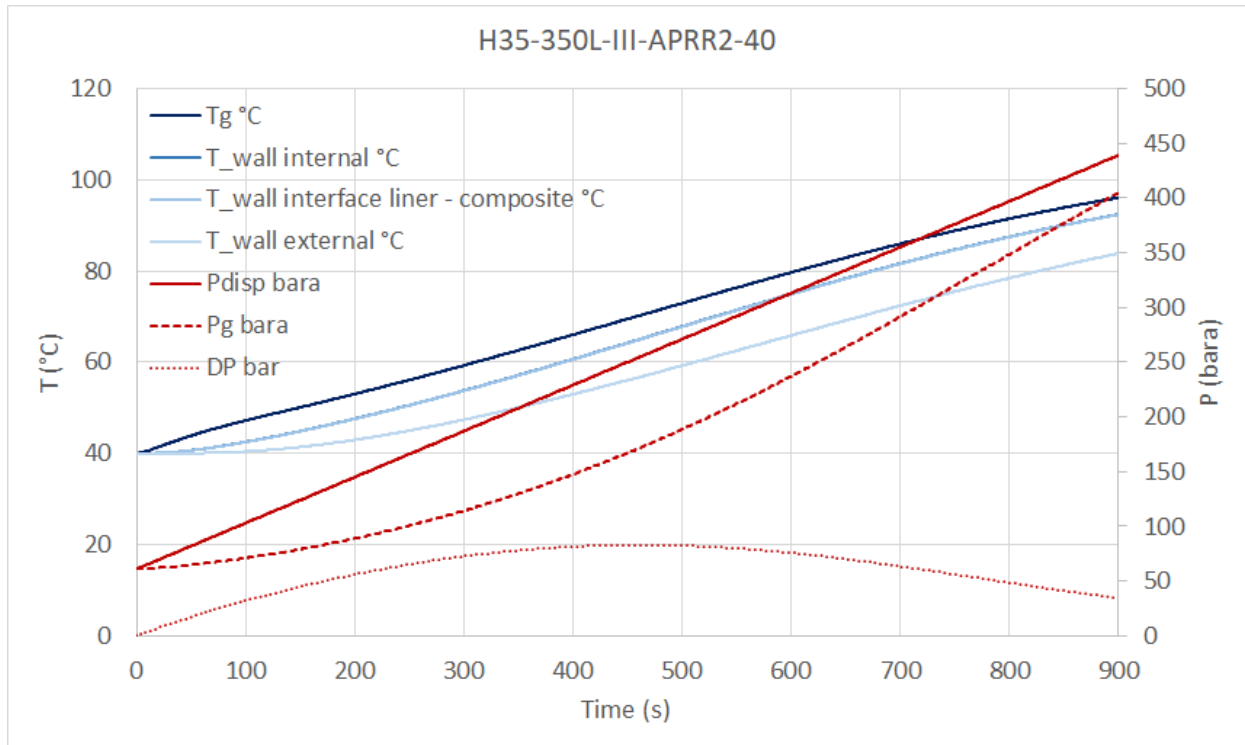


Figure F-4: Simulation of 15 minutes filling for NWP = 35 MPa, Type III 350 L tank, inlet temperature = 40°C, ambient temperature = 40°C

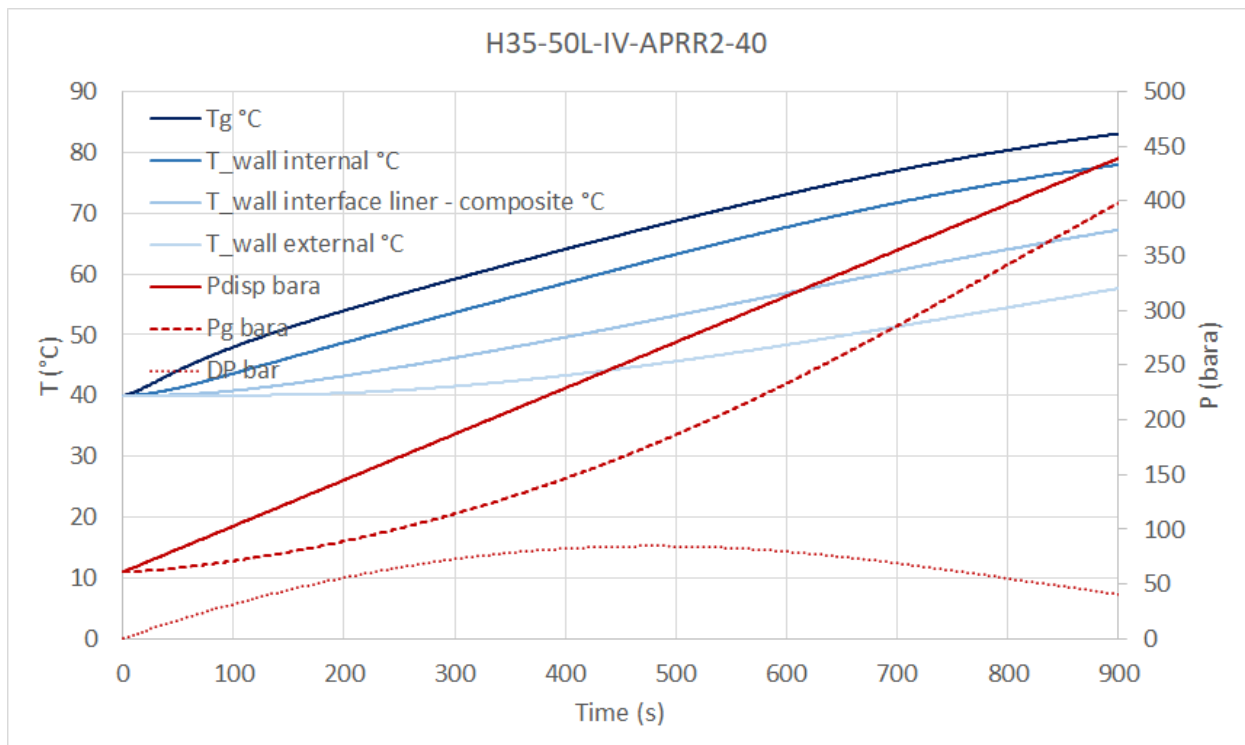


Figure F-5: Simulation of 15 minutes filling for NWP = 35 MPa, Type IV 50 L tank, inlet temperature = 40°C, ambient temperature = 40°C

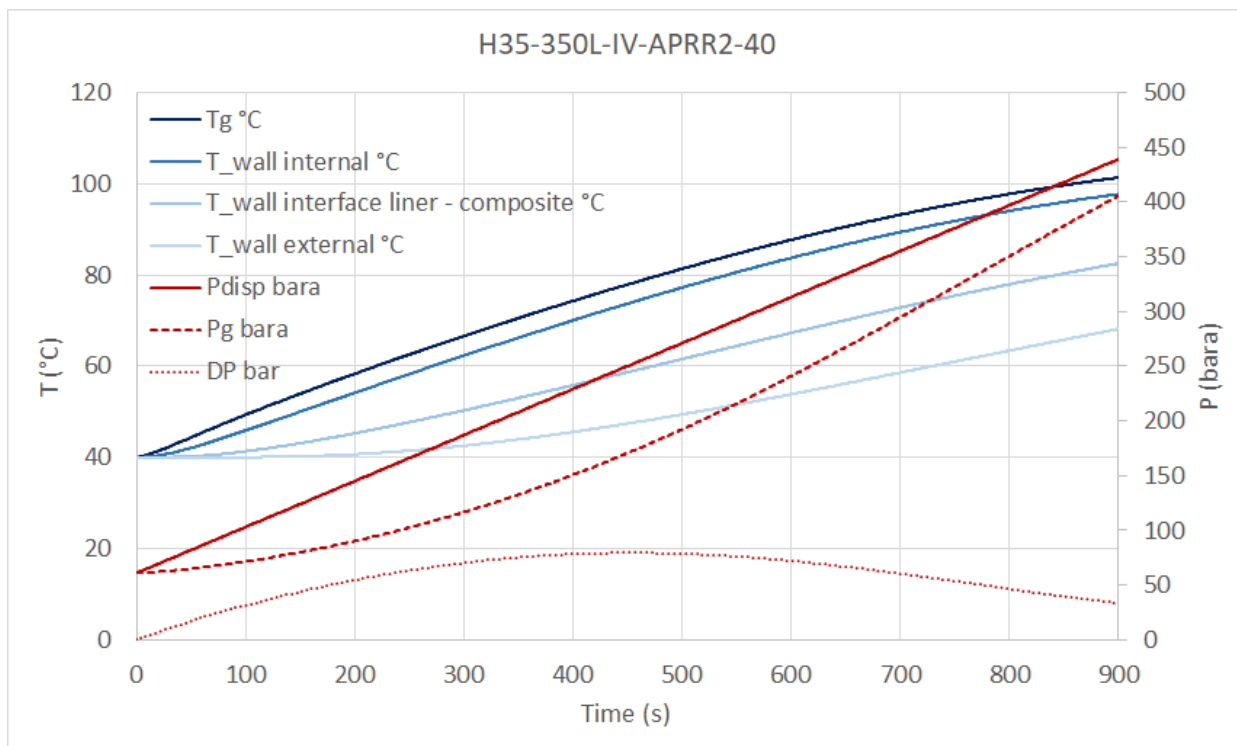


Figure F-6: Simulation of 15 minutes filling for NWP = 35 MPa, Type IV 350 L tank, inlet temperature = 40°C, ambient temperature = 40°C



FUEL CELLS AND HYDROGEN
JOINT UNDERTAKING

What is PRHYDE?

With funding from the Fuel Cells and Hydrogen 2 Joint Undertaking (FCH 2 JU), the PRHYDE project is aiming to develop recommendations for a non-proprietary heavy duty refuelling protocol used for future standardization activities for trucks and other heavy duty transport systems applying hydrogen technologies.

Based on existing fuelling protocols and current state of the art for compressed (gaseous) hydrogen fuelling, different hydrogen fuelling protocols are to be developed for large tank systems with 35, 50, and 70 MPa nominal working pressures using simulations as well as experimental verification. A broad industry perspective is captured via an intense stakeholder participation process throughout the project.

The work will enable the widespread deployment of hydrogen for heavy duty applications in road, train, and maritime transport. The results will be a valuable guidance for station design but also the prerequisite for the deployment of a standardized, cost-effective hydrogen infrastructure.

Further information can be found under <https://www.prhyde.eu>. For feedback on the PRHYDE project or the published deliverables, please contact info@prhyde.eu.

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Members of the PRHYDE Consortium:



With contributions by:

