CFD INVESTIGATION OF FILLING AND EMPTYING OF HYDROGEN TANKS

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ABSTRACT

During the filling of hydrogen tanks high temperatures can be generated inside the vessel because of the gas compression while during the emptying low temperatures can be reached because of the gas expansion. Excessively high or excessively low temperatures could affect the mechanical properties of the tank materials. CFD analyses of the filling and emptying processes have been performed in the HyTransfer project. To assess the accuracy of the CFD model the simulation results have been compared with new experimental data for different filling and emptying strategies. A satisfactory agreement between experiments and simulations is shown for the temperatures of the gas inside the tank, for the temperatures at the interface between the liner and the composite material, and for the temperatures on the external surface of the vessel.

1.0 INTRODUCTION

Currently compressed hydrogen is the technology selected by the automotive industry for the on-board storage in hydrogen powered vehicles like the fuel cell cars, which are already available on the market. Due to the large pressure increase during re-fuelling, the gas temperatures inside the tank increase and because of heat transfer also the temperatures of the vessel materials increase. In the emptying of a tank, both the gas and material temperatures decrease due to the gas expansion. In both situations, the temperatures can go beyond the design temperature range that is between -40 °C and +85 °C [1] and excessively high temperatures or excessively low temperatures can potentially affect the mechanical behaviour of the tank materials. Gas pre-cooling is used during filling to keep the temperature of the whole storage system below the threshold of +85 °C. However gas precooling causes an increase in the capital and operating costs of refuelling stations.

The main aim of the on-going HyTransfer project [2] is to develop and experimentally validate a practical approach for optimizing temperature control during fast transfers of compressed hydrogen to meet the specified temperature limit (gas or material), taking into account the system's thermal behaviour. The HyTransfer project is co- funded by the Fuel Cells and Hydrogen Joint Undertaking. Partners includes LBST, Air Liquide, CCS Global Group, Raufoss Fuel System, Honda R&D Europe, the European Commission Joint Research Centre, Centre National de la Recherche Scientifique (CNRS), and TesTneT Engineering.

An extensive campaign of experiments and numerical simulations (both Computational Fluid Dynamics methods and analytical models) has been carried out to support the main aim of the project. A crucial step for the application of numerical modelling is the validation of the model against the experimental measurements. The main objective of this paper is to describe the CFD benchmark exercises that have been performed in the project to assess the accuracy of the CFD model in describing filling and emptying of a 40 litre tank (type 3).

In previous CFD analysis by the same groups of researchers [3] – [6], only the filling stage was investigated and the main focus was on the gas temperature history in type 4 tanks. In this work, both filling and emptying are considered for a type 3 tank and the comparison between experiments and simulations is carried out for the gas temperatures, the temperatures at the interface between the liner and the composite layer, and for the temperature on the external surface of the tank, providing a more complete picture of the capabilities of the CFD model.

CFD numerical modelling of fast filling of hydrogen tanks has been performed by several research groups [7]-[15].

2.0 EXPERIMENTS

The experiments have been carried out at the JRC Institute for Energy and Transport (IET) in the compressed hydrogen Gas tanks Testing Facility (GasTeF), reference laboratory for safety and performance assessment of high-pressure hydrogen storage tanks [16]. The facility is able to reproduce cycling tests providing information on long-term mechanical and thermal behaviour of high-pressure tanks and their safety performance. The tests consist of a fast filling (with or without pre-cooled inlet gas), simulating the refuelling of the tank at the service station, followed by an emptying phase, representing the gas consumption during driving. During a test the tank is located inside a sleeve that can be heated up from room temperature to 100°C; the pressure in the tank can be increased up to ca. 85 MPa. Several parameters are monitored in order to evaluate the tank performance, such as tank wall temperature, temperature inside the material, internal gas temperature at different positions and deformation of the tank walls as well as the possible leakage or permeation of hydrogen; more details can be found in [1]

In the framework of the HyTranfer Project [2] several tests reproducing the filling and the emptying processes have been conducted at the GasTeF facility. In particular two filling and two emptying tests have been also simulated with a CFD code; tests details are described in Table 1 and in Table 2.

Table 1: Filling tests.

#	Initial pressure [bar]	Initial cylinder and gas temperature	Inlet gas temperature	Average mass flow rate [g/s]	Filling time [s]
FF_EXP01	20	20° C	-20° C	8	191
FF_EXP02	20	20° C	0° C for 75 s, then -40° C	8	197

Table 2: Emptying tests.

#	Initial S.O.C.	Initial cylinder and gas temperature	Average mass flow rate	Emptying time [s]
EM_EXP01	100 %	20° C	0.376 g/s	~ 3400
EM_EXP03	100 %	20° C	1.5 g/s for 500 s, then 0.2 g/s	~ 4000

The tank tested is a 40 litre type 3 which has two metallic bosses, a metallic liner (i.e. aluminium alloy) and an external wrapping of carbon fiber re-enforced composite (CFRC). A sketch of the tank with the location of the thermocouples is represented in Figure 1: there are thermocouples inside the tank (TTs in blue), between the liner and the CFRC (TCs in green) and at the external tank wall (EWTs in red).

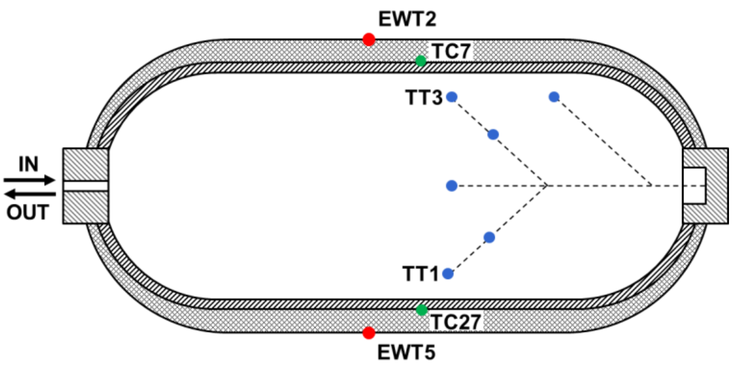

Figure 1: Approximate position of the selected tank thermocouples

In Figure 2 pressure, temperature measured at the tank inlet during the filling experiments are reported; in the figure the nominal inlet gas temperatures are represented with dashed lines. The red lines represent the test FF_EXP01, while the blue ones represent the test FF_EXP02.

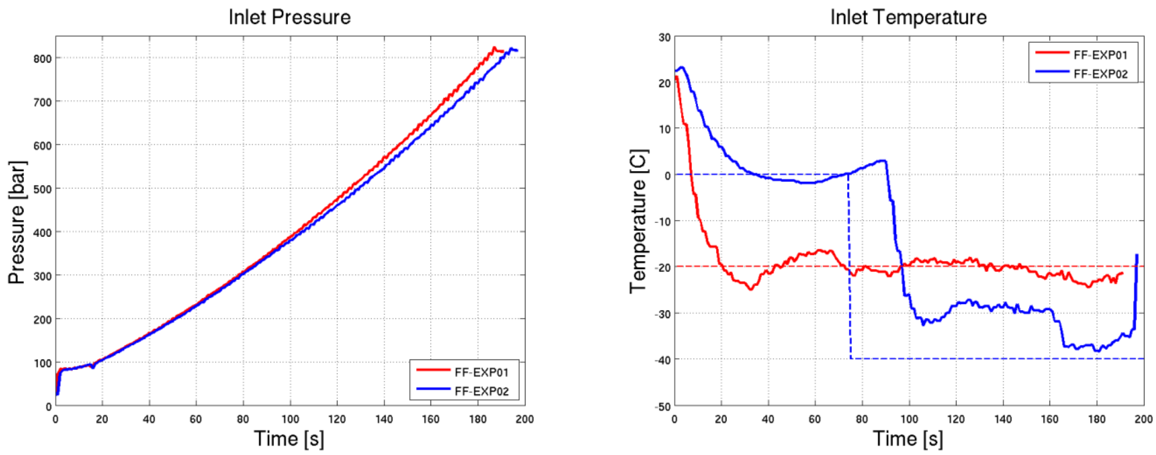

Figure 2: Pressure and temperature profile at the tank inlet for the two filling tests

In Figure 3 pressure and temperature measured at the tank outlet during the emptying experiments are reported. The yellow lines represent the test EM_EXP01, while the green ones represent the test EM_EXP03.

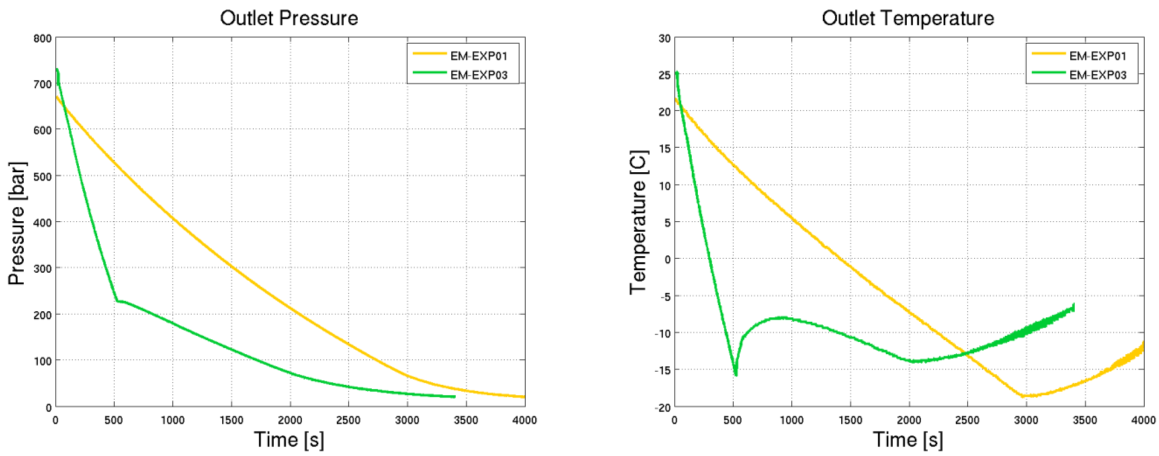

Figure 3: Pressure and temperature profile at the tank inlet for the two emptying tests

3.0 SIMULATION RESULTS

The CFD modelling strategy is based on the experience that was accumulated in the previous validation processes [3] – [5]. The numerical simulations have been performed with the commercial CFD software ANSYS CFX V14.0 [18]. The conjugate heat transfer model (CHT), available in CFX, has been used in order to evaluate the thermal conduction through solid materials coupled with the changing temperature in the fluid.

The numerical time scheme is based on a Second Order Backward Euler scheme. The high resolution scheme of CFX has been selected for the advection terms. Further details on the numerical scheme can be found in the ANSYS CFX manual [18]. A residual convergence criterion for RMS (root mean square) mass-momentum equations of 10^{-4} has been applied, ensuring the attainment of convergence of results. At the end of the fillings and at the beginning of the defueling the gas pressure inside the tank could reach values close to 750 bar; at those pressure values the ideal gas law is not able to describe properly the pressure and the temperature behaviour. For that reason a real gas equation of state for the evaluation of hydrogen properties has been used (Redlich, Kwong [19]). In addition a modified k-ε approach [20] was applied as turbulence model in order to reduce the jets spreading rate over-prediction of the standard model [20] - [22]. The initial conditions for each case have been assumed to be uniform and defined according to the experiment initial tank temperature and pressure; In addition the ambient temperature has been considered constant for the whole simulations.

The computational model adopted for the filling and empting simulations is constituted of five subdomains: one fluid part (i.e. the tank interior filled by hydrogen), the internal metallic liner, the external composite carbon fibre wrap (CFRC) and the two bosses at the tank ends. The material properties have been selected according to Monde [23]. The computational model represents half of the tank using the vertical symmetry plane passing through the inlet jet axis. Previous analyses using a domain representing the whole 3D geometry show slight differences, in terms of temperatures, compared with the half domain.

3.1. Filling simulations

The comparison between CFD results and experimental data is illustrated for both the fillings in Figure 4; the red and the blue colours refer to the FF_EXP01 and to the FF_EXP02 cases respectively, while the continuous lines represent the simulation results and the crosses represent the measurements. Temperature histories in the TT3 location (representing the gas temperature) are depicted on the left hand-side of Figure 4, in the TC7 position (representing the liner – CFRC temperature) in the middle and in EWT2 (representing the external wall temperature) in the right hand-side of the figure.

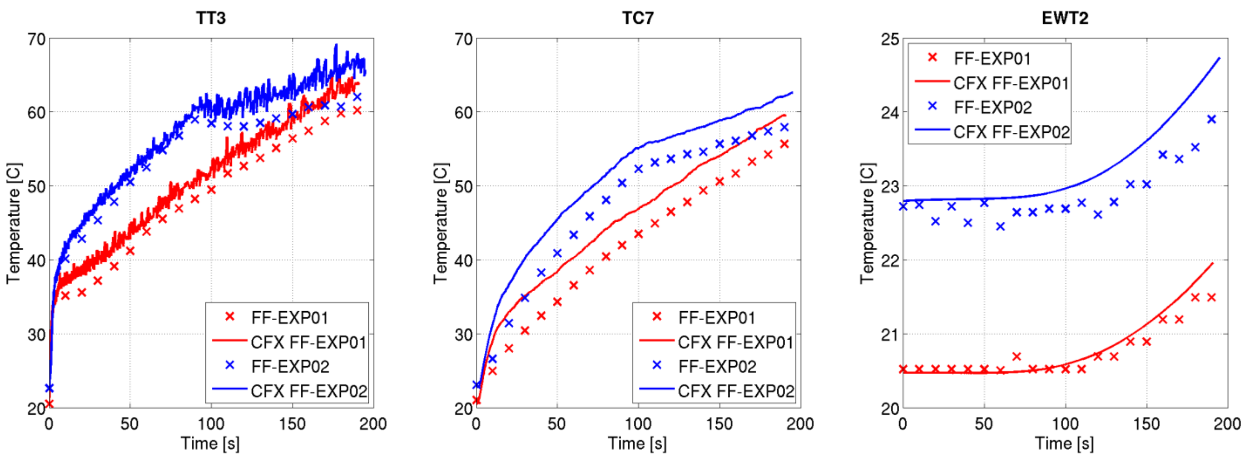

Figure 4: Comparison of simulation results and experimental data for the two types of filling.

The good agreement between experimental data and simulations is shown in Figure 4 and in Table 3, where the final temperatures and the difference ΔT between the simulated and measured temperatures at the end of the filling are reported at the three selected thermocouples.

Table 3: Filling test temperatures: CFD results vs. experimental data at the end of the simulations.

	TT3 Final	TT3 ΔT	TC7 Final	TC7 ΔT	EWT2 ΔT	EWT2 ΔT
FF-EXP01	60.38° C		55.42° C		21.49° C	
FF-EXP01 CFX	63.64° C	3.26	59.49° C	4.07	21.96° C	0.47
FF-EXP02	62.56° C	-	58.20° C	-	23.90° C	-
FF-EXP02 CFX	65.67° C	3.11	62.59° C	4.39	24.73° C	0.83

For both fillings, the difference between the simulations and the experiments are ~ 3° inside the tank (i.e. hydrogen temperature), ~ 4° between the liner and the CFRC and less than 1° at the external tank wall.

Comparing the two different types of filling, it is possible to note that the temperature histories are different, mainly due to the different inlet gas temperature history, but the final temperatures are comparable for the sensor inside the tank and the sensor at the liner – CFRC interface; on the other hand, the external wall temperature time histories are similar but shifted due to a slightly different initial wall temperature. For both cases the simulated temperatures slightly overestimate the experimental ones.

The temperature contours in the tank symmetry plane are reported for the two cases at the end of the filling in Figure 5. The homogeneity of the gas temperature is confirmed. If we do not consider the jet region which is colder due to the incoming cold gas, the tank temperature rang is between 68° C and 71° C for FF-EXP01 and it is between 70° C and 73° C for case FF-EXP02.

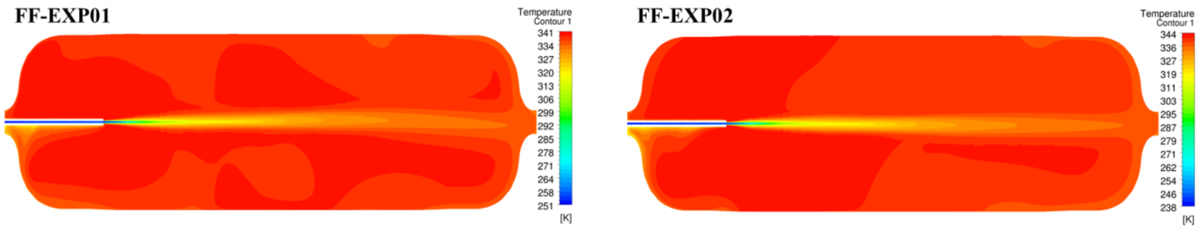

Figure 5: Simulation results. Gas temperature contours in the tank symmetry plane (end of the filling)

The temperature contours at the interface between the liner and the CFRC are shown in Figure 6 for the FF-EXP01 (left hand-side of the figure) and for the FF-EXP02 (right hand-side of the figure). A warmer zone is observed at the opposite zone with respect to the inlet injector as expected because the cold incoming gas has a cooling effect on the injector side.

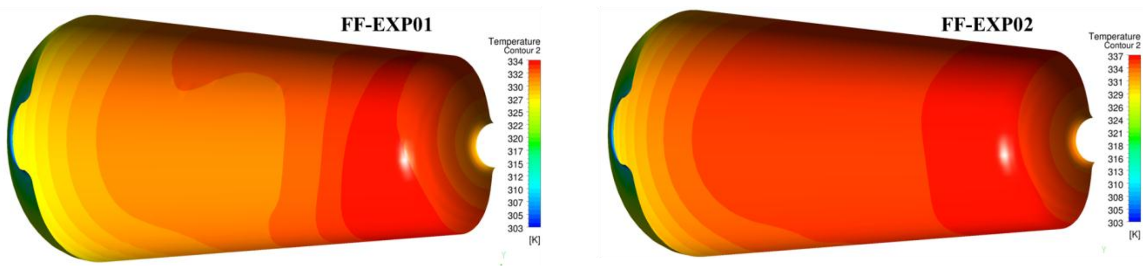

Figure 6: Simulation results. Temperature contours at the interface between liner and CFRC, inlet at the left-hand side.

The minimum, the average and the maximum temperatures at the interface between liner and CFCR during the filling are reported in Figure 7: on the left hand side the temperatures related to the case FF-EXP01 and on the right side the ones related to the case FF-EXP02 are shown respectively. The trend of the average (the blue curve in the figure) and the maximum (the red curve in the figure) temperatures are similar for both the cases and, obviously, the maximum curves are shifted above the averaged ones: at the end of the filling the difference of the maximum and the averaged temperatures is 3° for case FF-EXP01 and it is 2° for case FF-EXP02. The minimum temperatures for both the simulation are located in the regions that are affected by the inlet cold gas.

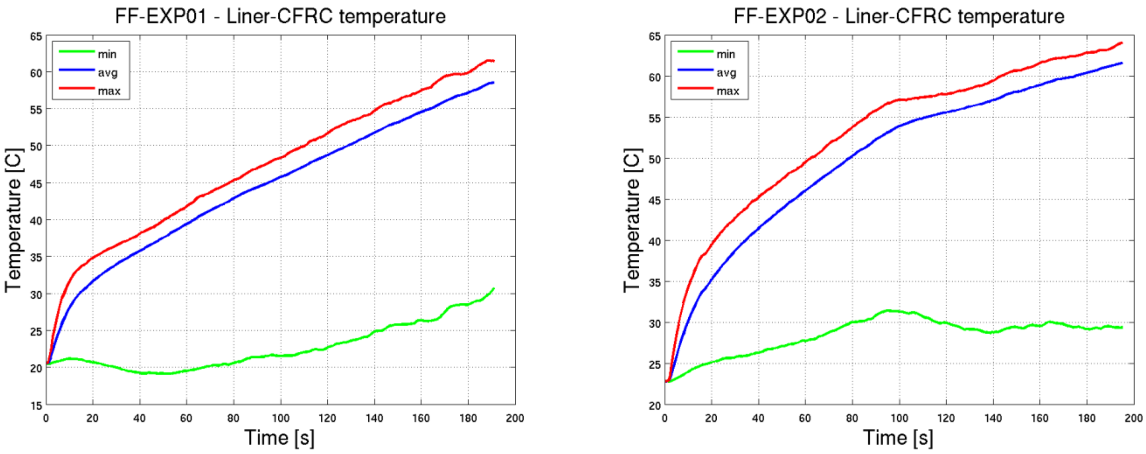

Figure 7: Simulation results. Minimum, averaged and maximum and average temperatures at the interface between liner and CFRC for the two type of filling

The liner and the CFRC of the tank, as explained in Paragraph 2.0, are made of different material (i.e. aluminium and composite carbon fiber respectively). The material properties of the two materials are different, in particular the liner has a higher thermal diffusivity than the CFRC; in addition the CFRC is much thicker than the liner one. For those reasons, the thermal behaviour inside the two types of material is different, as reported at the end of the filling in Figure 8 (the blue curve is related to the case FF-EXP01 and the red curve is related to the case FF-EXP02). For both cases, at the end of the filling the liner temperatures are almost constant through the material thickness and they are similar to the temperature of the gas region close to the wall.

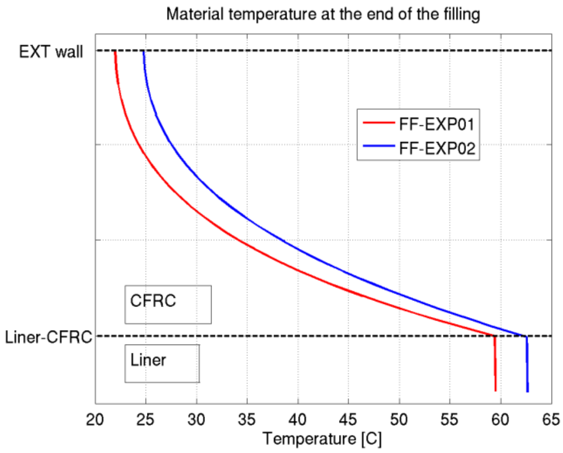

Figure 8: Simulation results. Temperature inside the material at the end of the filling for the two fillings

The temperatures of the CFRC decrease from 59.85° C for case FF-EXP01 and from 62.56° C for case FF-EXP02 in the gas, to 21.85° C for case FF-EXP01 and from 24.76° C for case FF-EXP02 at the external wall, as reported in Table 4. It means that the CFRC ΔT at the end of the filling is almost 38° for both fillings.

Table 4: Simulation results. CFRC wall temperatures: comparison between the two fillings.

	FF-EXP01	FF-EXP02
Liner-CFRC T [C]	59.85	62.56
External wall T [C]	21.85	24.76
ΔT	38.00	37.80

3.2. Emptying simulations

The comparison between the CFD results and the experimental data are reported in Figure 9; the yellow and the green colours refer to the EM_EXP01 and to the EM_EXP03 cases respectively, while the continuous lines represent the simulations and the crosses represent the experiments. Temperature histories in the TT1 location (representing the gas temperature) are depicted on the left hand-side of Figure 9, in the TC27 position (representing the liner – CFRC temperature) in the middle and in EWT5 (representing the external wall temperature) in the right hand-side of the figure.

A faster depressurization generates a larger drop in the gas temperature as depicted in Figure 9 for the first 500 s in the EM-EXP03 case. During the emptying the pressure decrease inside the vessel causes a decrease of the gas temperature while the heat transfer from the environment to the tank tends to produce the opposite effect. The two effects are competing against each other for the whole duration of the process and the de-pressurization effect is dominant for most of the emptying. Towards the end of the emptying the rate of the pressure decrease becomes very slow as illustrated in Figure 3 and the heat transfer effect prevails on the de-pressurization effect, producing an increase of the gas temperature. The temperatures of the gas and of the surface between the liner and the CFRC start to increase after 3000 s for the case EM-EXP01 and after 2000 s for case EM-EXP03.

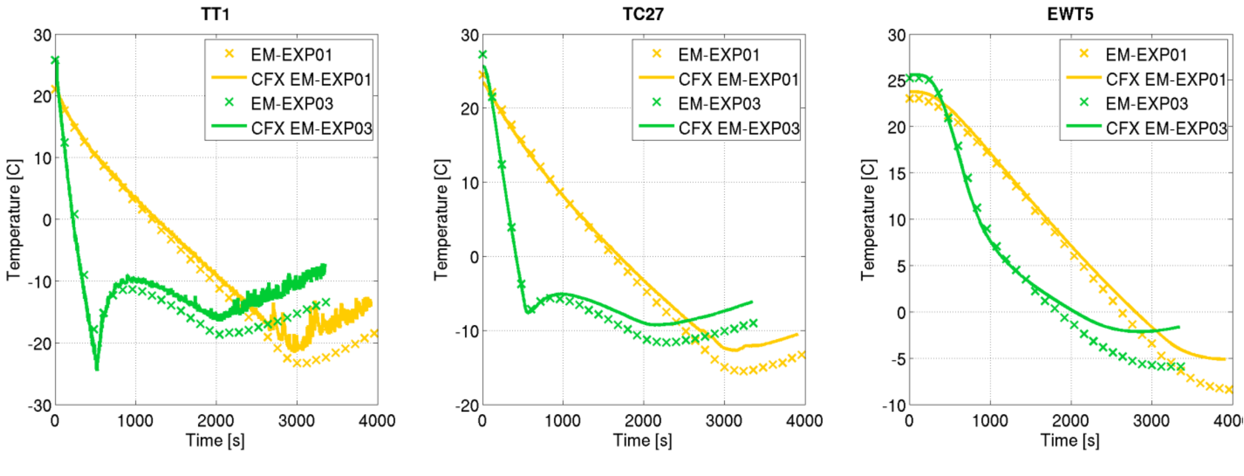

Figure 9: Comparison of simulation results and experimental data for the two types of emptying

The good agreement between experimental data and simulations is shown in Figure 9 and in Table 5, where the final temperatures at the end of the filling are reported for the fillings at the three selected thermocouples. The difference between the simulated and the measured temperatures is between 2.9° and 5.9° for both the cases.

Table 5: Emptying test temperatures: CFD results vs. experimental data at the end of the simulations.

	TT1 Final	TT1 ΔT	TC27 ΔT	TC27 ΔT	EWT5 ΔT	EWT5 ΔT
EM-EXP01	-18.82		-13.50		-8.40	
EM-EXP01 CFX	-14.13	4.69	-10.52	2.98	-5.11	3.29
EM-EXP03	-13.51		-9.04		-5.91	
EM-EXP03 CFX	-7.58	5.93	-6.14	2.90	-1.64	4.24

The temperature contours in the tank symmetry plan are reported at the time when the gas temperature reaches its minimum value (i.e. 3000 s and 2000 s for EM-EXP01 and EM-EXP03 respectively) in Figure 10. In both cases, stratification occurs with higher temperatures at the top regions of the tank and lower temperatures at the bottom. For the selected experiments, emptying is a much slower phenomenon than filling. Due to the low gas velocity inside the vessel during the emptying, the buoyancy becomes more relevant than during the filling. The heat transfer from the environment to the tank warms up the gas in contact with the tank inner walls and the heated gas tends to move upwards because of buoyancy, producing a stratified temperature field. For both simulations the difference between the upper and the lower part of the tank is around 12°. The liner and CFRC temperatures are higher than the gas temperature. In Figure 10 on the bottom surface of the cylinder the gas that is heated by the heat transfer from the liner is moving upwards, forming elongated and in some cases convoluted shapes in the lower regions of the tank.

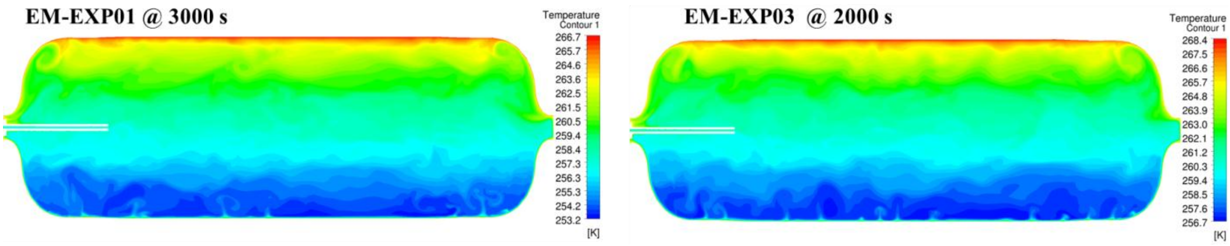

Figure 10: Simulation results. Temperature contours at the tank symmetry plane

The temperature contours at the interface between the liner and the CFRC are described in Figure 11 for the EM-EXP01 (left hand side of the figure) and for the EM-EXP02 (right hand side of the figure). Due to the stratification phenoma occuring in the gas, the upper part is hotter than the lower part.

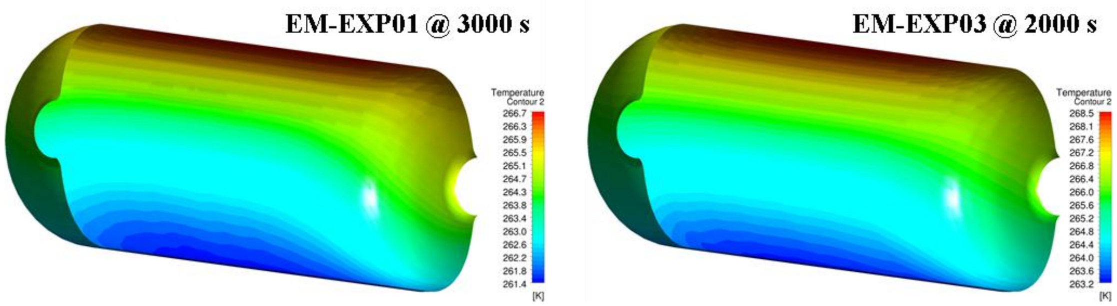

Figure 11: Simulation results. Temperature contours at the interface between liner and CFRC

The minimum, the average and the maximum temperature time history at the interface between liner and CFRC for case EM-EXP01 and for case EM-EXP03 are reported on the left and on the right side of Figure 12 respectively. For case EM-EXP03, the difference between the minimum and the maximum temperature is larger at 500 s, when the gas mass flow is 1.5 g/s (i.e. ~ 12°), while, at the end it is ~3°.

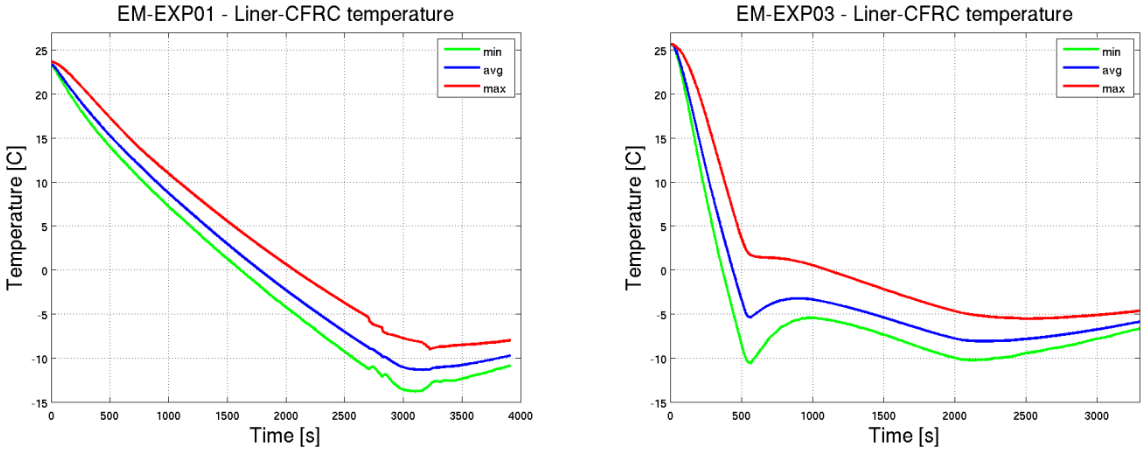

Figure 12: Simulation results. Minimum, average and maximum temperatures at the interface between liner and CFRC for the two emptying

The temperatures across the materials at the lower part of the tank are reported in Figure 13.

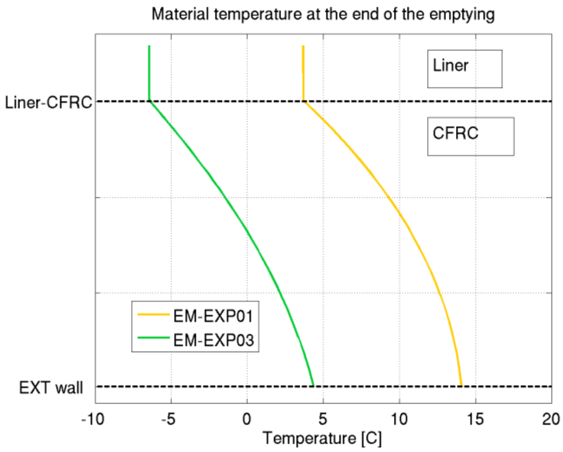

Figure 13: Simulation results. Temperature inside the materials at the end of the filling for the two emptying

For both the cases at the end of the emptying the temperature inside the liner is almost constant and it is influenced by the gas temperature; inside the CFRC the two temperatures have similar profiles (i.e. the ΔT is 8.28° for EM-EXP01 and 10.21° for case EM-EXP03) and the EM-EXP01 external wall CFRC temperature is larger than the EM-EXP03 one, as reported in Table 6.

Table 6: Simulation results. CFRC wall temperatures: comparison between the two emptying.

	EM-EXP01	EM-EXP03
External wall T [C]	14.07	4.34
Liner-CFRC T [C]	3.68	-6.45
ΔT	10.39	10.79

4.0 CONCLUSIONS

The main objective of this paper was to describe the CFD benchmark exercises that were performed in the HyTranfer Project to assess the accuracy of the CFD model in describing filling and emptying of a 40 litre tank, type 3.

Two filling experiments have been taken into account in the paper with a starting internal tank pressure of 20 bar and an initial gas and material temperature of 20° C; the inlet hydrogen mass flow rate is the same for both cases (i.e. 8 g/s), but the nominal inlet gas temperature is -20° C for one case and 0° C for 75 s of filling, and then -40° C for the other case. For both fillings, due to the short time of the filling itself (i.e. less than 200 s), the gas temperature inside the tank is quite homogeneous; even if the two fillings have a different precooling processes, the final gas temperature differs by only few degrees.

Two emptying experiments with a 100% initial state of charge (SOC) and with initial gas and material temperature of 20° C were considered; the difference between the two emptying experiments is the nominal mass flow rate of the gas coming out from the tank: for one case it is constant and equal to 0.376 g/s, for the other case it is 1.5 g/s for 500 s, and then 0.2 g/s until the end of the emptying. In both cases, temperature stratification occurs with higher temperatures at the top regions of the tank and lower temperatures at the bottom.

The comparison between the simulation and the experimental data for the temperature histories shows good agreement. For the filling cases, the difference between the measurements and the simulation results at the end of the process is about 3°C for the gas temperature, it is just above 4°C for the temperature at the interface between the liner and the CFRC layer, it is less than 1°C for the temperature on the external surface of the cylindrical part on the tank walls. For the emptying cases, the difference between the experimental data and the calculated values at the end of the process is about 5° - 6° C for the gas temperature, it is less than 3° C for the temperature at the interface between the liner and the CFRC layer, it is about 3° - 4°C for the temperature on the external surface of the cylindrical part on the tank walls. Since the simulation results are in a satisfactory agreement with the measurements, the computed temperature distributions were analysed to investigate the hottest regions in the filling and the coldest regions in the emptying where the temperatures could potentially exceed the design temperature range.

In the filling simulations the gas temperature distribution is uniform. At the interface between the liner and the composite layer, during the filling the region closer to the jet injection is colder compared to the other regions, due to the cooling effect of the incoming jet. Because of that effect, the maximum temperature difference between the coldest region and the hottest region at the interface reaches about 30°C.

During the emptying the gas temperature stratification affects significantly the temperature distribution in the material. At the interface between the liner and the composite layer, the maximum temperature difference between the coldest region and the hottest region at the interface reaches about 5°C with a constant flow rate of 0.376 g/s while it reaches about 12°C with a flow rate of 1.5 g/s in the first 500 s and then 1.5 g/s for the remaining time.

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