VALIDATION OF CFD MODELS FOR HYDROGEN FAST FILLING SIMULATIONS

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ABSTRACT

High injection pressures are used during the re-fueling process of vehicle tanks with compressed hydrogen, and consequently high temperatures are generated in the tank, potentially jeopardizing the system safety. Computational Fluid Dynamics (CFD) tools can help in predicting the temperature rise within vehicle tanks, providing complete and detailed 3D information on flow features and temperature distribution. In this framework, CFD simulations of hydrogen fast filling at different working conditions are performed and the accuracy of the numerical models is assessed against experimental data for a type 4 tank up to 70 MPa. Sensitivity analyses on the main modeling parameters are carried out in compliance with general CFD Best Practice Guidelines.

1.0 INTRODUCTION

Hydrogen is widely seen as an energy carrier that could help to overcome issues such as green house gas emission, air pollution and security of energy supply. Nevertheless, for a realistic implementation of the “Hydrogen Economy”, all safety aspects related to its practical use in commercial systems have to be assessed: besides production and use of hydrogen, also all other market stages, like packaging, storage, delivery and transport, should be carefully addressed. In particular, hydrogen storage is a key enabling technology for the extensive use of hydrogen as an energy carrier [1]. Among all available technologies, compressed gas is currently the leading choice for storing hydrogen on board vehicles: high pressure hydrogen (35-70 MPa) is stored in cylindrical tanks packaged within the vehicle. At present four different tank designs are available, but mainly two of them are used because of weight minimization: type 3 tanks, constituted by a composite carbon-fiber and laminate external wrap with internal Aluminum liner, and type 4, with the same external composite wrap and internal plastic liner.

In order to be commercially competitive with current technologies, hydrogen refueling requires that three main targets are met [2], [3]: short refueling time, high refueling rate and high safety and reliability. Firstly, for a widespread adoption of hydrogen-powered vehicles, refueling time should be comparable with that for conventional fueling, which implies to refuel a passenger car in less than four minutes. The driving range of hydrogen-fueled vehicle is a main concern as well, since due to the low hydrogen volumetric energy density, high storing pressures (70MPa) are needed to compete with gasoline vehicle autonomy. When combining high pressure and short filling time, high temperatures can be reached in the tank during refueling because of nearly-adiabatic compression of the gas. The temperature increase during the filling represents a significant safety concern, and for safety reasons a maximum allowed temperature of 85°C is specified by the international regulation ISO 15869 [4]. It is therefore necessary to reach a deep knowledge of the phenomena taking place during the fast-filling transient in order to comply with the established safety margins.

Recent international research programmes [5] gave a strong contribution in this sense, encouraging both experimental and numerical investigations on hydrogen fast filling (e.g. within StorHy project [1] and HySafe NoE [6]). Among the analysis methods recently adopted for addressing fast filling issues ([7]-[14]) Computational Fluid Dynamics (CFD) methods have been identified as a promising tool for predicting the temperature rise within vehicle tanks, providing detailed information on flow features and temperature distribution. Nevertheless, CFD codes contain models (e.g. for simulating turbulence and heat transfer) which should be validated before they can be used with sufficient confidence in hydrogen safety applications. The necessary validation is performed by comparing model results against suitable experimental data, as previously done by several authors ([15]-[21]) for different hydrogen fast filling scenarios.

The current work aims at giving a contribution to the overall validation process, presenting CFD simulations of hydrogen fast filling at different working conditions; the accuracy of the numerical models is assessed against experimental data for a type IV tank up to 70 MPa.

2.0 GASTEF EXPERIMENTS

Considered experiments were conducted at JRC Institute for Energy (IE) in the compressed hydrogen Gas tanks Testing Facility (GasTeF), which represents a EU reference laboratory on safety and performance assessment of high-pressure hydrogen storage tanks through cycling and permeation tests [22]. The facility is sited in a half-buried strongly reinforced concrete bunker with annexed gas storage area. The 225 m3 room (10 x 7.5 x 3 m3) where the vessels are located is inertised using gaseous N2.

In the test room, a pressure vessel contains the component to be tested; the fuel tank is placed into a sleeve which, filled with inert gas, serves as safety chamber but also for measuring hydrogen permeation through the tank walls. The sleeve temperature can be varied from ambient to100°C, while the pressure in the tank can be increased up to ca. 80 MPa. Cycling tests aim at providing information on long-term mechanical and thermal behavior of high-pressure tanks and their safety performance. The tests consist of a fast filling (few minutes), simulating the refueling at the service station, followed by a slow emptying phase, representing the gas consumption. This transients' combination is repeated up to 1000 times to simulate the typical life of tanks. During the tests, several parameters are monitored in order to evaluate tank performance: external temperature, temperature and deformation of the tank walls as well as the possible leakage or permeation of hydrogen and internal gas temperature at different positions. More details on available data can be found in [23].

The tests considered in this work concern only the fast filling process of a Type IV tank up to 70MPa. Numerical simulations of the emptying phase are planned for future investigations. Measured temperatures at specific points in the tank (thermocouples arrangement Pos1 and Pos2 shown in Figure 1) are compared with predicted values during the filling transient, in order to validate CFD modelling. Originally a thermocouple was also positioned near the jet inlet but due to the high velocities reached in the filling transient and to the jet oscillations it was not working correctly and eventually broke. Working conditions of selected tests are summarized in Table 1; the corresponding transient (residual) pressure profiles measured at the tank inlet are shown in Figure 2.

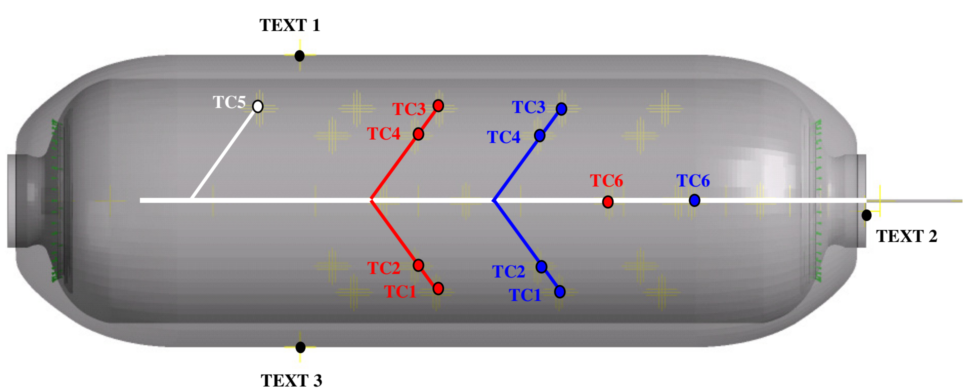

Figure 1. Thermocouples (TCs) position inside and outside the tank: Pos1 (blue), Pos2 (red), fixed internal (white) and external (black) ones.

Table 1 Tests Selected for CFD validation.

	H_2 P_{in} [MPa]	H_2 P_{fin} [MPa]	$t_{filling}$ [s]	T_{sleeve} [°C]	H_2 T_{ini} [°C]	TCs position
Test H2 10122010	0.02	71.7	330	16	21	Pos 2
Test H2 25022011	0.02	71.8	245	18	21	Pos1, Pos2

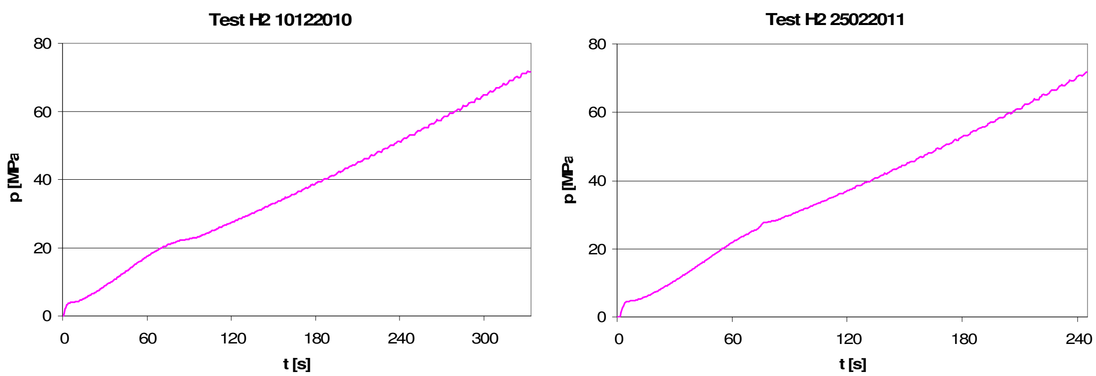

Figure 2. Hydrogen pressure profiles at tank inlet.

3.0 CFD SIMULATIONS

The computational domain representing the studied type IV tank was generated with the meshing software GRIDGEN V15 [24]; then numerical simulations of GasTeF fast filling tests were performed by means of the commercial CFD code ANSYS CFX 12.1 [25]. ANSYS CFX solves the unsteady Navier-Stokes equations in their conservation form; it is an element-based finite-volume method with second-order discretization schemes in space and time. CFX includes also a conjugate heat transfer (CHT) capability which was applied in the present study, allowing calculation of pure thermal conduction through solid materials coupled with the calculation of temperature in the working fluid.

In the current analysis, numerical simulations were performed according to general Best Practice Guidelines (BPG) for the use of CFD codes [25] [26], in order to minimize numerical errors and to compare different modeling capabilities. A residual convergence criterion for RMS mass-momentum equations of 10^{-4} was used to ensure the attainment of negligible iteration errors.

3.1 Computational Model

The 3D computational domain consists of four different sub-domains, as shown in Figure 3:

1. Fluid domain, representing the interior of the tank filled by the hydrogen (blue);
2. Solid domain, representing the internal plastic liner (white);
3. Solid domain, representing the external composite carbon fiber wrap (black);
4. Solid domain, representing the two stainless steel bosses at the tank ends (grey).

Four different 3D computational grids were generated with slightly different geometry and various mesh refinement, as summarized in Table 2, to allow sensitivity analysis on grid refinement. Figure 3 shows some details of mesh size in the region near the inlet of the tank for the reference grid G4. For all the grid solutions, inlet pipe and solid domains are composed of hexahedral meshes, while the remaining fluid domain is made up by tetrahedral elements, as shown in the figure.

Table 2 Computational Grids (number of elements).

	TANK	LINER	BOSSES	INSULATION	TOT
G1	542780	95104	100352	140928	**879164**
G2	603489	95104	100352	140928	**938873**
G3	568540	95104	100352	140928	**904924**
G4	601867	95104	100352	140928	**938251**

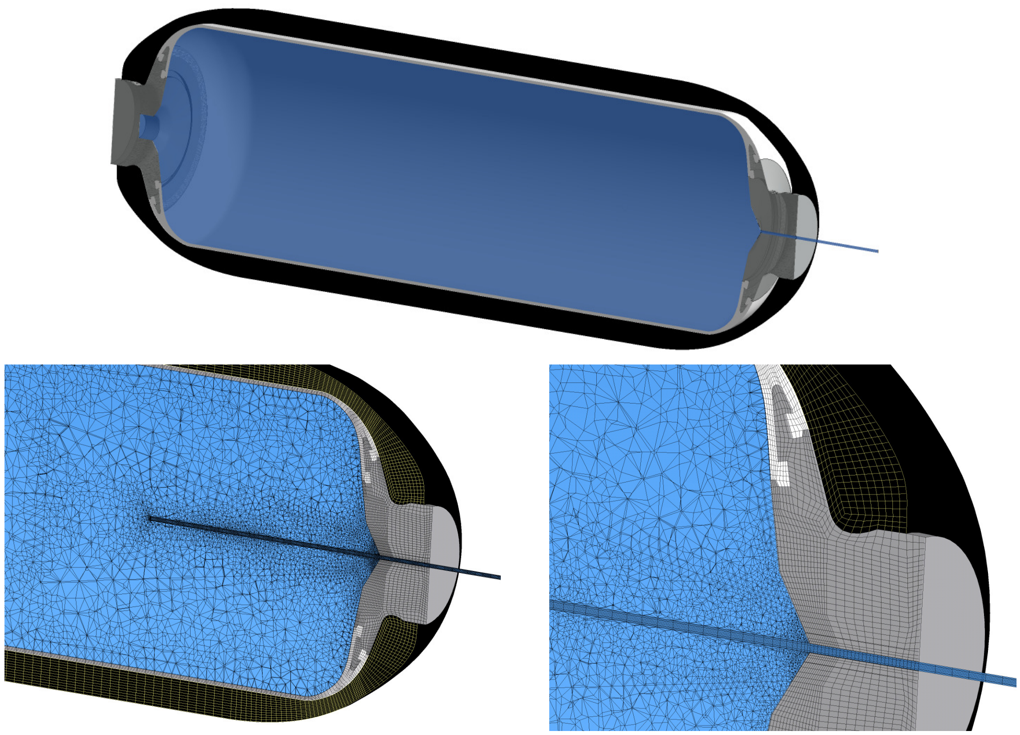

Figure 3. Computational domain.

Grid spacing was properly refined in the near-wall region in order to satisfy wall functions requirements for a suitable treatment of the near-wall turbulence. Grids G1, G3 and G4 are characterized by different lengths of the inlet pipe, while for grid G2 a prism layer was built adjacent to the wall in the fluid region as to increase mesh refinement in the near-wall region. G4 was selected as reference grid for simulations since it was reproducing more accurately the inlet pipe geometry.

Transient simulations were performed, solving all governing equations in their unsteady form. Due to gas high velocities at the inlet (especially at the beginning of the filling) and density variations along the transient, the following modeling choices were implemented:

- Compressibility effects were taken into account considering a real gas equation of state for the evaluation of hydrogen properties (Redliche-Kwong [25]);
- The gravitational source term was included into the momentum equation and within the turbulent kinetic energy and dissipation equations, in order to consider buoyancy effects;
- Turbulence produced by the hydrogen jet was predicted through a modified k-ε model [28] which corrects jets spreading rate over-prediction typical of the standard model [28]-[30].

Transient pressure and temperature experimental profiles were imposed at the tank inlet to reproduce fast filling conditions (as from Figure 2). A non-slip boundary condition was applied at inner tank and inlet pipe walls. At the outer tank and bosses walls, a constant heat transfer coefficient was imposed to determine the heat transfer to the environment, while pipe wall was considered adiabatic. Ambient temperature was assumed to be constant throughout the filling. Initial conditions were defined by H_2 initial temperature and pressure within the tank, which were assumed to be uniform. Tank walls were considered to be at the same temperature as the gas. In order to assess model capabilities, sensitivity analyses were performed on grid refinement, turbulence modeling, boundary conditions on inlet pressure, inlet pipe geometry, external wall heat transfer coefficient and material properties.

3.2 Main Results

Results for the reference simulation of **Test H2 10122010** are shown in the following figures, compared with corresponding experimental data. Figure 4 shows the evolution of temperature distribution inside the tank during the transient, as well as the final temperature distribution on the outer surface of the tank wrap.

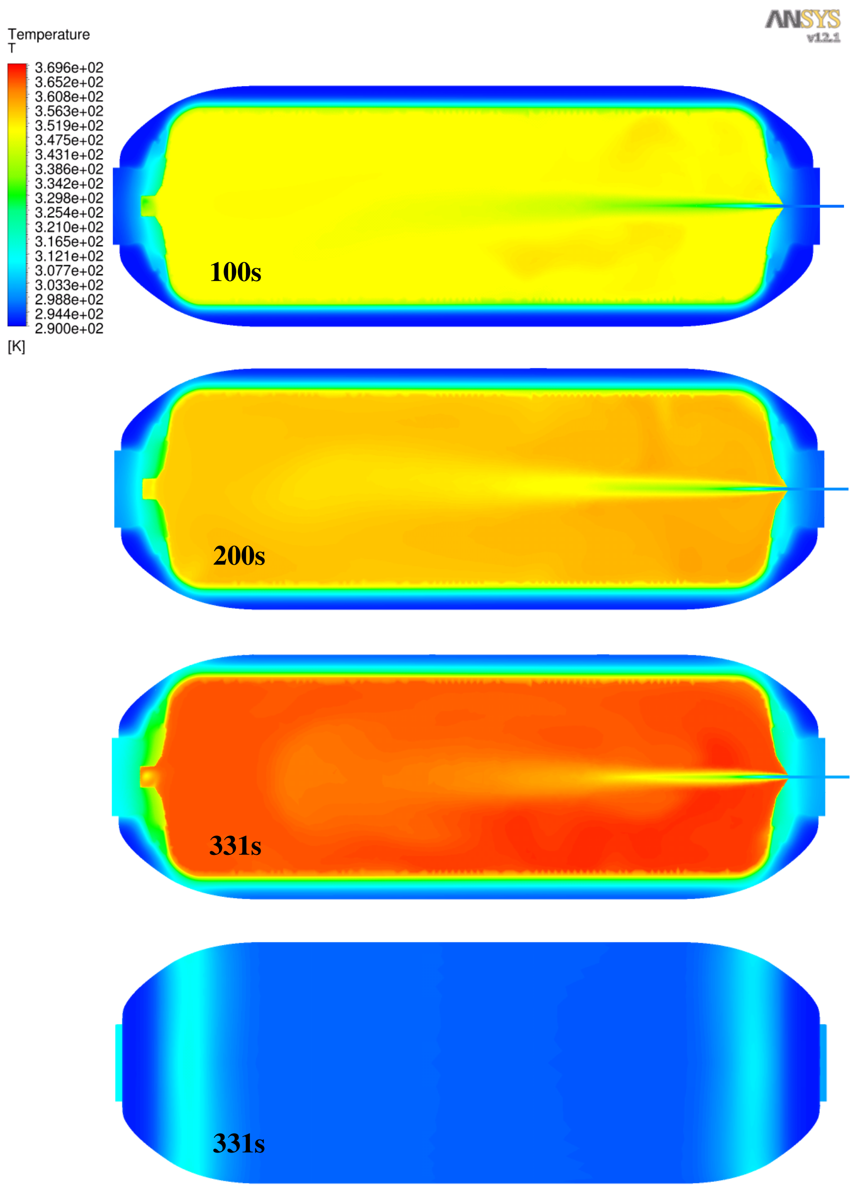

Figure 4. Temperature contours plot at different time interval from the start of the filling, inside and outside the tank (figure at the bottom) (Test H2 10122010).

It is worth mentioning that, as it happens in many filling scenarios from high pressure vessels, a standing shock wave is generated at the entrance of the tank in front of the inlet. Due to high pressure ratio between the pressure in the tank and the pressure of compressor at the beginning of the transient, M=1 is reached at the end of the inlet pipe, generating a Mach disk in front of the inlet. The CFX code is capable of simulating supersonic flows and caught the physics of that phenomenon, even if a finer mesh would be required to sharply capture the shock wave structure. Nevertheless, within 4 seconds from the beginning of the filling the pressure ratio between the pressure in the tank and the pressure of compressor decreases below 1.9, the flow becomes subsonic at the end of the inlet and the Mach disk disappears from the flow field. Therefore the local effect of the Mach disk on the temperature distribution is limited to the first 4 seconds. Temperature profiles predicted at internal and external thermocouples location are compared with experimental data in Figure 5 and Figure 6. As can be observed from Figure 4, up to 100s from the start of the filling the heat transferred from the hydrogen mainly affects the liner, while in the following part of the transient also the composite material is involved. Due to the short duration of the filling transient, no temperature stratification is produced within the tank but two warmer regions of fluid are created at the ends of the cylinder. Accordingly, higher temperatures are developed in the composite wrap at the rounded edges, were the tank wall is thinner (see Figure 4 bottom); moreover, the rear end of the tank and the rear boss resulted to be slightly warmer than the corresponding regions near the inlet. A similar behavior was recently observed in experiments by other authors through thermal imaging camera [31]. Temperature histories inside the tank are generally in good agreement with experimental data, as shown in Figure 5, with minor under-predictions (below 4%) for high pressures (>35 MPa).

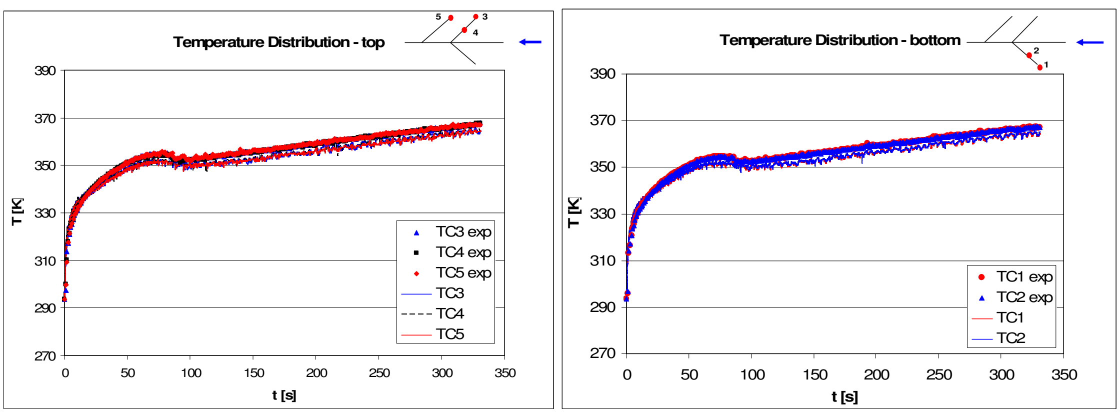

Figure 5. Predicted temperature inside the tank at thermocouples position, compared with experimental data (Test H2 10122010).

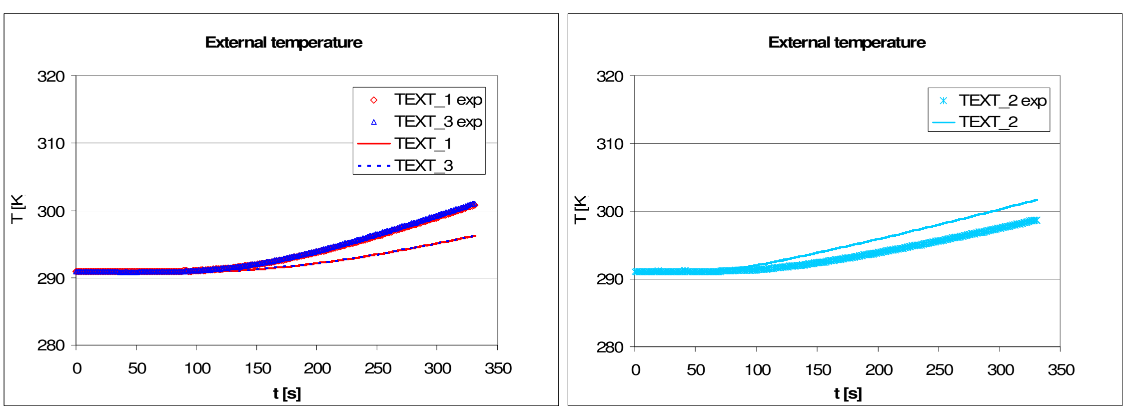

Figure 6. Predicted temperature outside the tank (left) and on the inlet boss (right) at TCs position, in comparison with experimental data (Test H2 10122010).

Some differences were also observed for calculated temperatures outside the tank (see Figure 6): the central part of the tank resulted in slight under-prediction (maximum error of 4.5 ºC) while for the inlet boss temperature was slightly over-predicted (maximum error of 3 ºC). Estimated errors for calculated values of maximum temperature at thermocouples position are drawn in Figure 7. It is worth noting that, even if measured and predicted maximum temperatures exceeded the allowed limit of 85°C specified by the regulation, this issue is not addressed within the present paper, as performed experiments aimed at testing tank capabilities in extreme situations and numerical simulations focused on CFD models validation prior to application. Sensitivity analyses were performed to evaluate the influence of main problem parameters on results accuracy. A refined grid (G2) was considered for performing simulations with the SST turbulence model; some differences (~10%) were observed in calculated temperature profiles, so that further investigation is needed in this direction. Sensitivity studies were also conducted varying pressure boundary condition at the inlet to account for pressure measurement errors (~0.4 MPa); as a result, only within the first 10s results were slightly affected, but the influence on the predicted maximum temperature was negligible. More relevant effects on calculated temperature profiles were due to variations in inlet pipe geometry and material properties. The first parameter (reduced length of the inlet pipe was considered) strongly influenced hydrogen temperature history at the beginning of the transient, causing up to 20 degrees of heating overestimation. Changes within material properties for the carbon fiber wrap strongly influenced predicted temperature outside the tank, as shown in Figure 8. On the contrary, modifying the internal plastic liner materials or setting adiabatic boundary condition on the wrap external surface (instead of constant heat transfer coefficient) produced negligible temperature variations (<0.5 degrees).

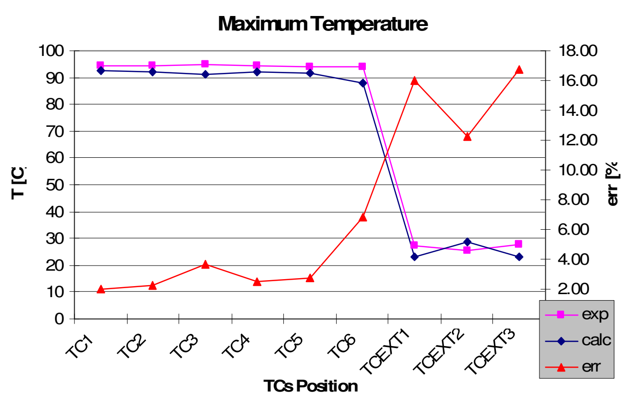

Figure 7. Accuracy of predicted maximum temperature at TCs position (Test H2 10122010).

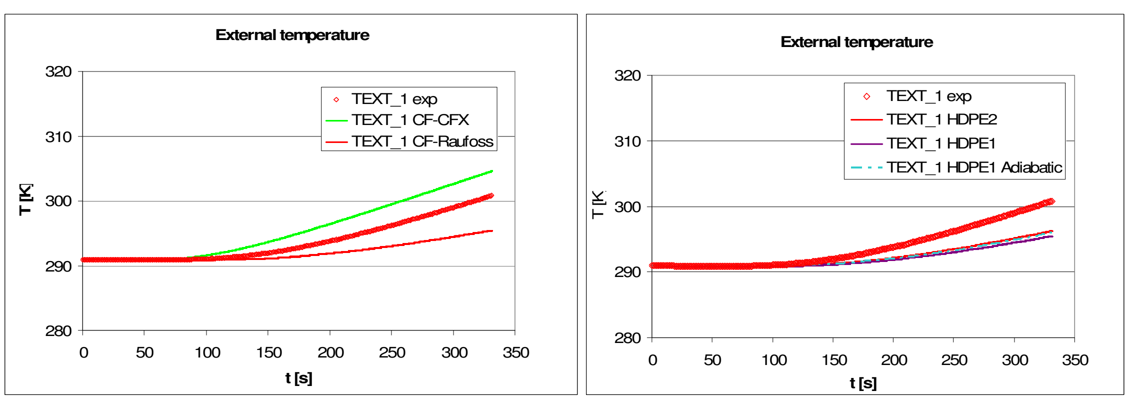

Figure 8. Sensitivity to material properties (left) and external heat transfer BC (right) (Test H2 10122010).

The same reference input was adopted for simulating the second test case, **Test H2 25022011**, characterized by a shorter filling time (245 s) at the same operating conditions. Temperature profiles predicted at two thermocouples (TC2, TC4) position are shown in Figure 9, for Pos1 (left) and Pos2 (right). As observed from Figure 10, results are in very good agreement with experimental data for both positions, and errors on maximum calculated temperatures are below 6%. Nevertheless, error in the evaluation of external temperature increased respect to the previous case, so that further investigation should focus on material properties and heat exchange between fluid, tank walls and environment.

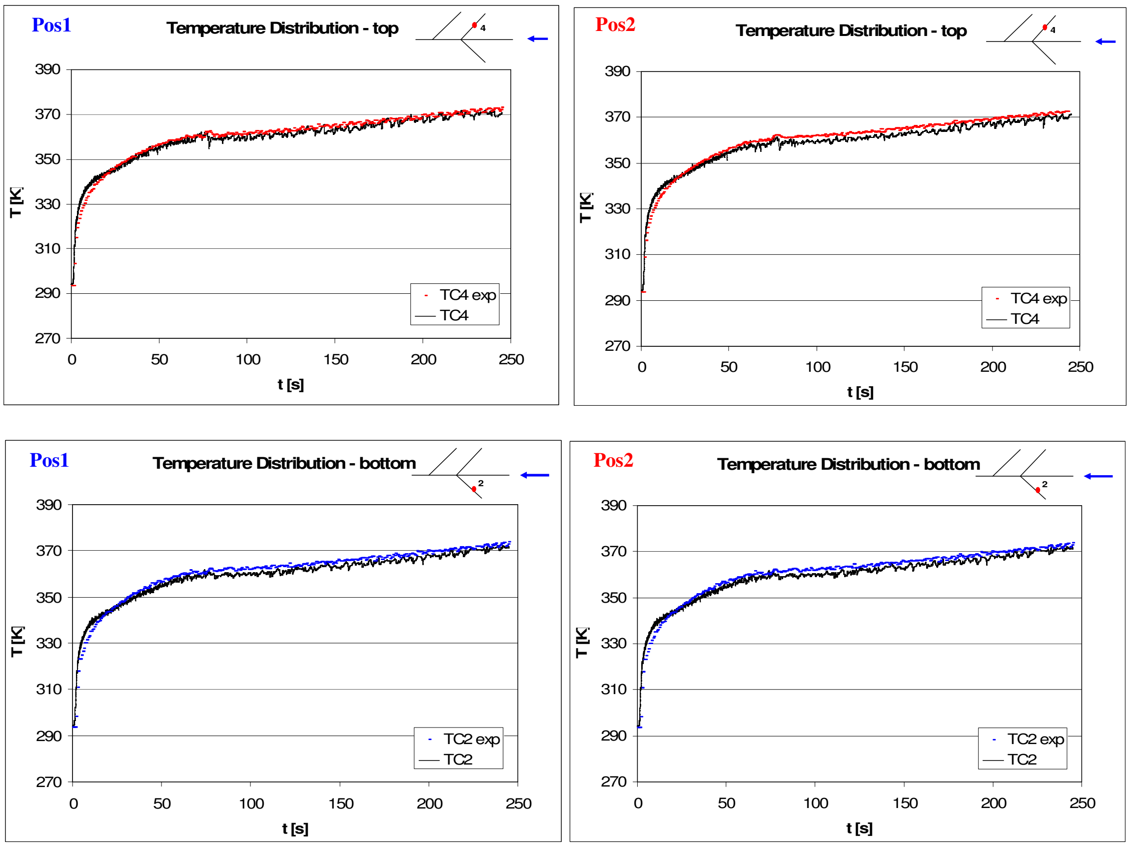

Figure 9. Predicted temperature inside the tank at thermocouples position, compared with experimental data (Test H2 25022011).

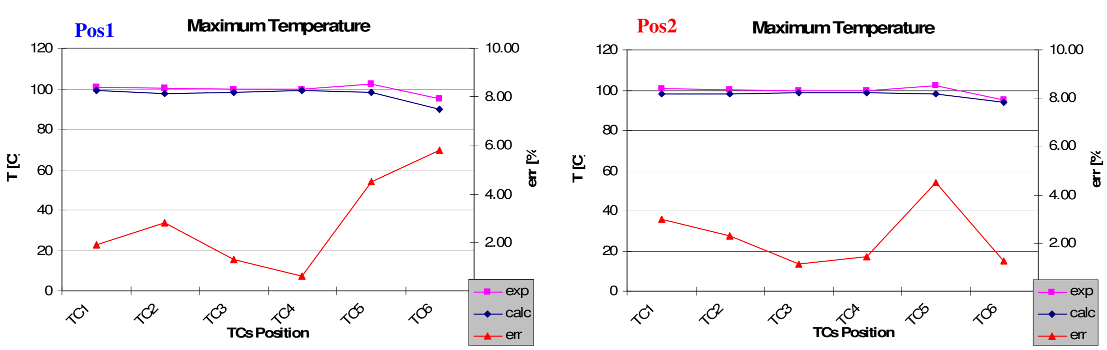

Figure 10. Accuracy of predicted maximum temperature at TCs position for Pos1 and Pos2 (Test H2 25022011).

4.0 CONCLUSIONS

CFD modeling validation against experimental data for hydrogen fast filling prediction up to 72 MPs has been presented. Two different experimental tests were considered, characterized by analogous working conditions but different filling time (245 s and 330 s).

The developed CFD model was first tested against the longer refueling scenario, which was expected to be less demanding from the computational point of view. Sensitivity analyses were performed in compliance with general Best Practice Guidelines for the use of CFD codes, in order to assess model response respect to variations in the main problem parameters (e.g. grid refinement, turbulence modeling and boundary conditions). Predicted temperature inside the tank was found to be in very good agreement with experimental data for both test cases, and errors on maximum calculated temperatures did not exceed 7%. Nevertheless, the evaluation of external tank and front boss temperatures resulted to be less accurate (errors above 10%) and strongly dependent on material properties. The developed model proved to accurately predict internal temperature distribution also for the shorter filling time case, while errors in the evaluation of external temperature increased. Further investigation is then required on material properties and heat exchange between fluid, tank walls and environment, as well as on grid refinement and turbulence modeling effects. This aspect is particularly important when considering that during a usual refilling the only temperatures accessible are those external to the tank. When fully validated the CFD model will allow reliable prediction of fast filling scenarios, and will then constitute a valuable complementary tool to experimental campaigns for optimizing the filling pressure ramp within the safety limits established by the international regulation.

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