CFD SIMULATIONS OF THE REFUELING OF LONG HORIZONTAL H2 TANKS

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ABSTRACT

The understanding of physical phenomena occurring during the refueling of H2 tanks used for hydrogen mobility applications is the key point towards the most optimal refueling protocol. A lot of experimental investigations on tank refueling were performed in the previous years, for different types and sizes of tank. Several operating conditions were tested through these experiments. For instance, the HyTransfer project gave one of the major outputs on the understanding of the physical phenomena occurring during a tank refueling. From a numerical perspective, the availability of accurate numerical tools is another key point. Such tools could be used instead of the experimental set-ups to test various operating conditions or new designs of tanks and injectors. The use of these tools can reduce the cost of the refueling protocol development in the future. However, they first need to be validated versus experimental data. This work is dedicated to CFD (Computational Fluid Dynamics) modeling of the hydrogen refueling of a long horizontal 530L type IV tank. As of now, the number of available CFD simulations for such a large tank is low as the computational cost is significant which is often considered as a bottleneck for this approach. The simulated operating conditions correspond to one of the experimental campaigns performed in the framework of the HyTransfer project. The 3D CFD model is presented. In a first validation step, the CFD results are compared with experimental data. Then, a deeper insight into the physics predicted by the CFD is provided. Finally, two other methodologies with the aim to reduce the computational cost have been tested. This work was co-financed by Air Liquide and the European funds from the Fuel Cells and Hydrogen 2 Joint Undertaking under grant agreement No 874997 – PRHYDE.

1.0 INTRODUCTION

Hydrogen is a new energy vector, which can help achieve the objectives defined by the COP21 to reach the 1.5°C target. Hydrogen will comprise 20% of the energy demand by 2050. This leads to an increase by a factor 10 of the hydrogen market, namely from 70 Mtpy to 700 Mtpy.

Hydrogen is one of the most promising technologies dedicated to mobility applications. The fast and aggressive development of the heavy duty mobility applications imposes more constraints on the Hydrogen Refueling Stations: for example the vehicle tanks should be refueled fast enough to be compatible with gasoline and diesel fuels. The safety of the refueling should be guaranteed by the refueling protocol to avoid tank overheating, i.e composite temperature not higher than 85°C, and overfilling which means that gas density should remain less than 24 kg/m3 and 40.2 kg/m3 for 350bar and 700bar tanks respectively. Economical consideration also must be taken into account to reduce the final price per kg of the dispensed hydrogen via for instance the reduction of the pre-cooling. Nowadays, complementary approaches including experiments and numerical simulations are used for protocol developments.

A lot of experimental investigations on tank refueling were performed in the last past years, for tanks of different types, namely types III and IV, of different size, from 29L up to 531L, and of different shapes with different aspect ratio, i.e the ratio between the diameter and the length of the tank. Operating conditions such as the pressure ramp rate, pre-cooling temperature or type of injectors were varied in these experiments. For instance the HyTransfer project [1] gave one of the first and major outputs on the understanding of the physical phenomena occurring during a tank refueling which in turn is of great value for refueling process optimization.

From a numerical perspective, the availability of accurate numerical tools is another key point. Such tools could be used instead of the experimental set-ups to test various operating conditions as well as new designs of tanks and injectors. The use of these numerical tools could significantly reduce the cost of the refueling protocol development in the future. However, these numerical tools first need to be validated versus experimental data.

Two main modeling strategies have been developed in the past decade. The first strategy consists in developing thermodynamic models [2-6]. These are transient 0D or 1D models in which energy and mass balance equations are solved. Depending on their level of sophistication, they allow for the prediction of the averaged temperature and pressure in the gas volume during the refueling process, as well as the averaged temperature at the different solid interfaces for the most complete models. They can provide a reliable estimation of the thermal behaviour of the tank during the refueling. They are commonly used to design refueling protocols. The limits of these useful and quick-to-run models is that they cannot provide local information or be used to get a comprehensive understanding of all the phenomena occurring during the refueling. For this reason, a second strategy of modeling is based on CFD [7-15]. CFD enables a 2D or 3D description of the turbulent flow and heat transfer involved in the tank as well as in its solid components. The main variables of interest such as temperature and gas velocity can be assessed at each cell of the mesh in the entire geometry. As a consequence these CFD models provide critical information such as the location and value of maximum temperature. Unfortunately, this approach is far more computationally intensive than its 0D and 1D counterparts.

Due to the significant computational cost of CFD models, this strategy has mainly been limited to small tanks, i.e a few tens of liters, and fast refueling processes. Indeed, the review by Bourgeois et al. [16] reported that CFD simulations had been restricted to tank volumes in the range [15L-150L] up to now, which is typical of car tank fueling. For some other mobility applications such as bus or heavy duty, the order of magnitude is rather hundreds of liters. The number of CFD works for this range of large tanks remains limited.

In the framework of the HyTransfer project, a large tank of 531 liters has been used to perform experimental refueling tests. During this project, CFD simulations of this tank were performed for several of the experimentally tested operating conditions. To go further, the study presented in this article aims at simulating another refueling case for the large 531 liters tank. The availability of experimental data allows for a reliable validation of the model. In parallel, several CFD strategies aiming at reducing the simulation time have been tested.

2.0 DESCRIPTION OF THE PROBLEM

The problem studied is the refueling of a H_2 tank. The target protocol for these experiments consists of refueling a tank with a constant mass flow rate. More details are provided below.

2.1 Materials and operating conditions

The tank considered in this study is the HEX531 produced by Hexagon Lincoln. The volume of the tank is V = 0.531m3, its internal diameter is D = 0.50m and its internal length is L = 2.70m. The aspect ratio is 5.4, which falls into the long tank range. It is a type IV tank, i.e it is made of a plastic liner and a composite wrapping. The gas is injected through a horizontal axial injector.

The theoretical operating conditions of the experimental test are described hereafter. The H_2 is pre-cooled before being injected into the tank with the aim to limit the maximal temperature inside the tank during the refueling. The target value of the injected gas temperature is -20°C. The gas is injected at an average mass flow rate of 2g/s through an injector of an internal diameter of 0.003m. Note that the mass flow rate is automatically controlled during the entire refueling in order to reach this target value which generates some fluctuations.

The initial pressure and gas temperature in the tank were respectively 29.24bar(a) and 30.35°C. The experimental test took place outside at an ambient temperature around 28°C. A strong wind was reported during this experimental campaign. The refueling lasted about 6200s to reach a final pressure of 463bar(a). It corresponds to a pressure ramp with a rate of 0.07bar/s.

Numerous sensors were installed within the tank, making it possible to finely monitor pressure and temperature at various locations every 0.5s. Pressure was measured inside the tank and also about 0.1m upstream the injection. Temperature was measured 0.1m upstream the injection, in 5 locations in the gas volume at different heights and different distances from symmetrical axis in the rear part of the tank thanks to a thermocouple tree, in 30 regularly spaced locations around the tank in the vertical symmetrical plane at the liner-wrapping interface and at 6 locations around the tank in the vertical symmetrical plane at the external wall of the tank. The position of the different thermocouples is shown in Figure 1.

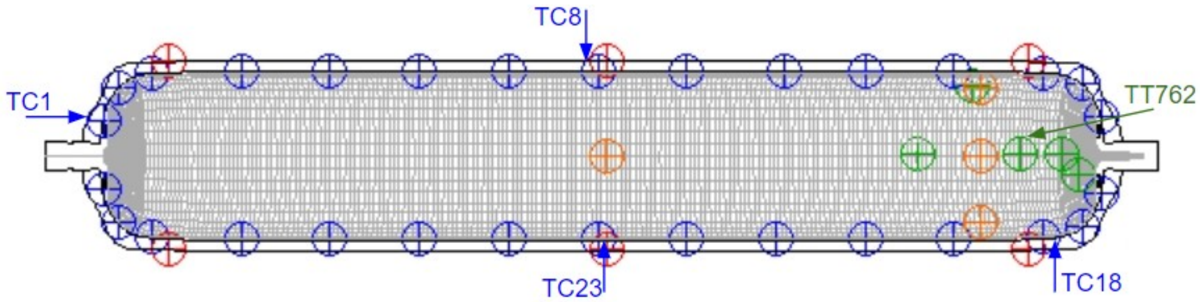

Figure 1. Sketch of the tank with the exact locations of the thermocouples. Green: in the gas. Blue: at liner-wrapping interface. Red: at the external wall surface.

Figure 2 shows the experimental evolution of the temperature for the 5 thermocouples located inside the tank and the 30 thermocouples located at the liner-wrapping interface. One can see that no significant temperature gradient is observed in the gas volume from one thermocouple to another during the entire refueling. The measured values at the liner-wrapping interface show a maximum temperature difference of nearly 10°C at the end of the refueling. This refueling test is therefore considered as a homogeneous case. Note that the highest temperature levels are obtained at the probes located on the top of the tank.

Figure 3 shows the injected gas temperature and the reconstructed mass flow rate. The mass flow rate has been calculated using SOFIL, a transient thermodynamics model, 0D in the gas volume and 1D through the walls, developed by Air Liquide [5, 6]. The measured values of the pressure and temperature upstream and inside the tank permits to reassess the mass flow rate. Figure 3 highlights the fact that the targeted operating conditions are not met. This had already been pointed out in previous studies [12]. The injected gas temperature never reaches the target value of -20°C. It takes about 250s to reach 0°C and about 600s to remain below -10°C. From these observations, it has been concluded that the actually measured operating conditions should be used as inputs of the CFD model for sake of representativeness.

The wind velocity value obviously has an impact on the forced convection at the external wall surface. This parameter is taken into account in the SOFIL model. The wind velocity value has been calibrated so that the experimental evolution of the averaged temperature at the liner-wrapping interface matches with the numerical one obtained with SOFIL. The best match has been obtained for a wind speed of 4m/s. Without wind, the convection coefficient around the tank would be of the order of a few W/m2/K while it is about 12 W/m2/K when the realistic wind speed is accounted for.

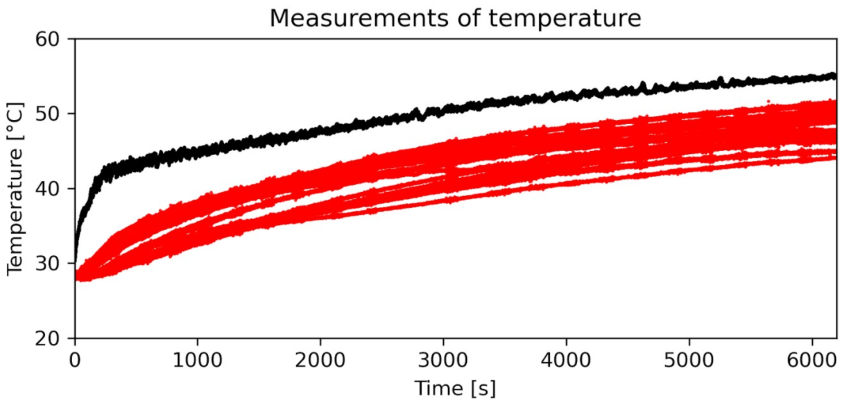

Figure 2. Time histories of temperature measurements. Black: temperature in the gas. Red: temperature at the liner-wrapping interface.

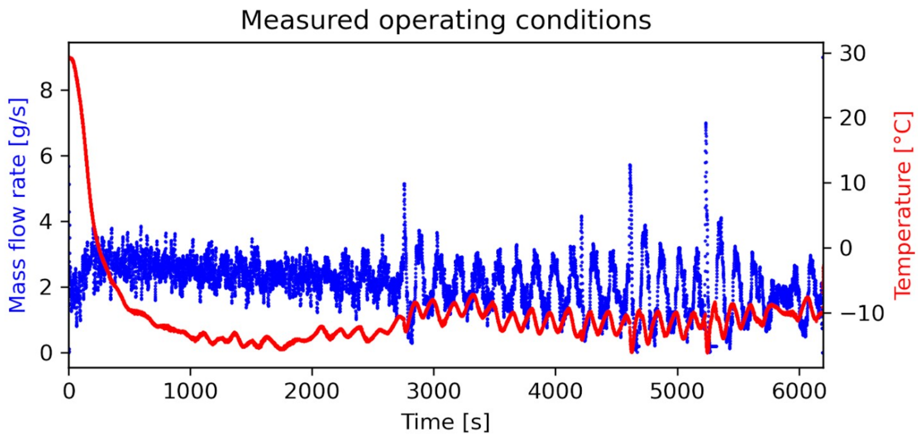

Figure 3. Time histories. Red: measured gas temperature at inlet. Blue: reconstructed inlet mass flow rate.

2.2 Numerical modeling

Heat transfers as well as fluid dynamics are solved in the gas volume and the solid components of the tank.

The choice between 2D axisymmetric and 3D modeling is a common question for this type of simulation. This question makes even more sense when large tanks are considered. Besides, to the best of the authors knowledge, the largest tank ever simulated using CFD found in literature is a 343L tank [15]. The main drawback of 2D axisymmetric simulation is that gravity effect is not accounted for. Zaepffel et al. have shown that such an assumption is not valid anymore for some refueling cases due to the importance of buoyancy [13]. In this study, for sake of representativeness, the tank is modeled as a 3D volume. Making use of the symmetry of the domain, only half of the tank is simulated and a symmetrical boundary condition is applied at the central vertical plane of the tank.

For all the solid components of the tank, namely the wrapping, the liner, the bosses and the injector, temperature dependencies of the heat capacities and thermal conductivities have been accounted for. A polynomial function is used to depict the behavior of each material. It has been obtained by fitting experimental measurements of these properties in the range [23°C; 100°C].

The ambient temperature is set as a boundary condition of the problem. At the external wall surface of the tank, convection and radiation heat fluxes are considered:

$$dFlux = h_{conv}\left(T - T_{amb}\right) + \varepsilon\sigma\left(T^4 - T_{amb}{}^4\right), \quad (1)$$

where σ is the Stefan-Boltzmann constant. The external wall emissivity is supposed to be constant ε = 0.8. The convection coefficient h_{conv} and the ambient temperature T_{amb} are time dependent. h_{conv} is provided by SOFIL results. It slightly varies during the refueling +/- 0.1%. T_{amb} is directly given by the experimental data. T_{amb} varies +/- 1.5 °C during the refueling.

At the inlet of the injector, the mass flow rate and the temperature of the injected gas are set as boundary conditions. It is common to make the assumption of constant boundary conditions during the entire refueling. As already mentioned, it has been observed that these data were not constant during the experimental refueling test under investigation here. Therefore, these boundary conditions have been imposed as time dependent functions in the CFD simulation reported here. Their values are obtained from SOFIL simulation for the mass flow rate and directly from experimental measurements for temperature.

The simulations are performed using the commercial software ANSYS Fluent V19.3. Several turbulent models have been tested in different studies in the past years such as k-epsilon ones (standard, realizable, modified, RNG), k-omega (SST), Reynolds Stress Models (RSM). Suryan et al. have compared some of these models in one of their works [9]. They concluded that results were similar and they advised to use the realizable k-epsilon model. In the past years, the SST k-omega model has shown good performance [13-15]. In this study, it has been decided to use the SST k-omega model. A coupled scheme is used for pressure-velocity coupling. Time integration is performed following a first order implicit method and spatial discretization is achieved by a second order upwind scheme.

Ideal gas model is not a relevant choice for the range of pressure considered in this refueling process. Several equations of state have been tested in previous studies, such as Redlich-Kwong [7, 9, 12, 14], Peng-Robinson [8], NIST [10,13,15]. The NIST real gas tables [17] recommended by Bourgeois et al. [16] is chosen in this study.

The mesh is refined in 2 particular fluid zones, namely at the outlet of the injector where the main activity of the turbulent flow is concentrated and close to the walls to accurately represent the heat transfer at the thermal boundary layer level. The mesh contains about 300 000 cells.

The time step is set through a User Defined Function that ensures a maximum Courant number of 50. The maximum time step allowed is 0.01s. Pre-studies have been performed to validate this method. It was found to provide an optimal trade-off between the accuracy and the computational time.

It has been checked that the simulation is conservative. The error in mass slightly increases during the calculation but remains lower than 1e-4. The order of magnitude of simulations is approximately two months, using 64 cores in parallel.

3. RESULTS

3.1 Validation of the results

Only the first 4000s of the refueling have been computed yet.

The averaged pressure in the tank is in close match with the experimental results.

In Figure 4, the profiles of average temperature in the fluid, at the liner-fluid interface and at the liner-wrapping interface are plotted. The plots in red, blue and black show the results obtained respectively with the 3D CFD model, the SOFIL model and experimental measurements. Note that the experimental average temperatures are averaged among the total number of probes, namely 5 in the fluid in the rear part of the tank and 30 at the liner-wrapping interface. In Figure 4, the equivalent averaged values among the probes obtained for the CFD results are also shown.

It can be seen that the CFD average fluid temperature as well as the average temperature among the 5 probes in the fluid follows the same trend as the experimental measurements. The later definition is closer to the experimental value as expected. In addition, the CFD model reproduces the experimentally measured oscillations of temperatures, which would not have been the case with imposed constant mass flow rate and temperature at the inlet. The average fluid temperature has also been compared to the value predicted by SOFIL. The agreement is satisfactory: differences between CFD and SOFIL remain below 2°C.

The average temperature at the liner-wrapping interface obtained with the 3D CFD simulation is also in good agreement with both the experimental value averaged among the 30 thermocouples surrounding the tank and the value predicted by SOFIL. For both comparisons, temperature differences remain below 1°C.

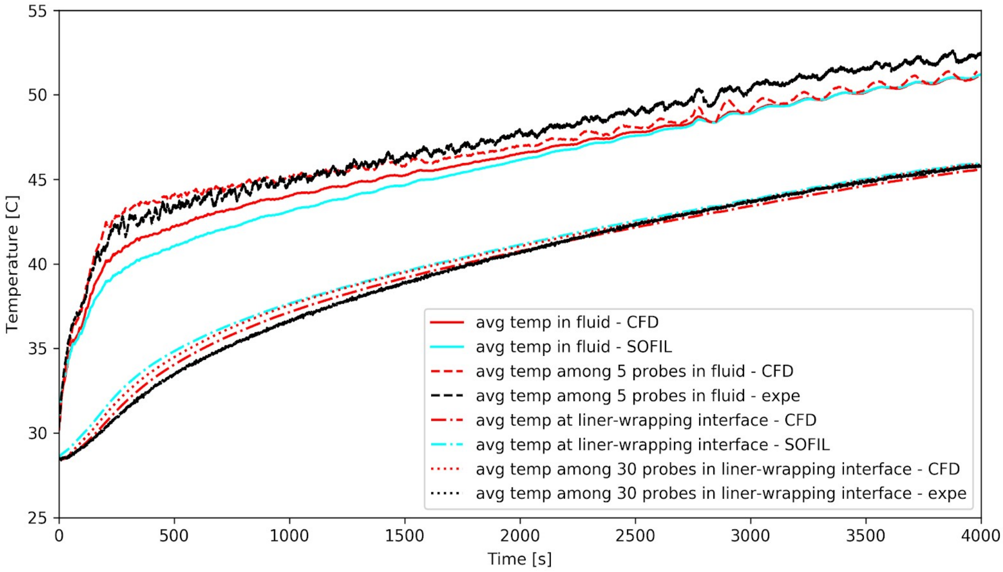

Figure 4. Time histories of average temperature. Red: CFD results. Blue: SOFIL results. Black: experiments.

The local temperature time histories given by the thermocouples in the gas and at the liner-wrapping interface have been compared with the numerical results, see Figure 5.

For all the thermocouples located in the fluid, as can be seen for the TT762 probe, the experimental and numerical profiles are really close, with less than 2°C difference in the worst case. The numerical model is able to reproduce the temperature oscillations locally monitored.

For the thermocouples located at the liner-wrapping interface, the numerical results are really good for probes located in the central bottom and top regions of the tank, see the plots for TC8 located at the center of the top interface and TC23 located at the center of the bottom interface. At the extremities of the tank, i.e at the bosses, the agreement is not as good as in the region described above. One can observe it for the probe located close to the inlet, see results for probe TC1, and at the rear part of the tank, see results for probe TC18. It can be seen that the numerical results overestimate the temperature measurements up to 5°C. This can be explained by the fact that the CFD turbulent model overestimates the turbulent mixing process at this location where a very weak residual turbulent activity is expected.

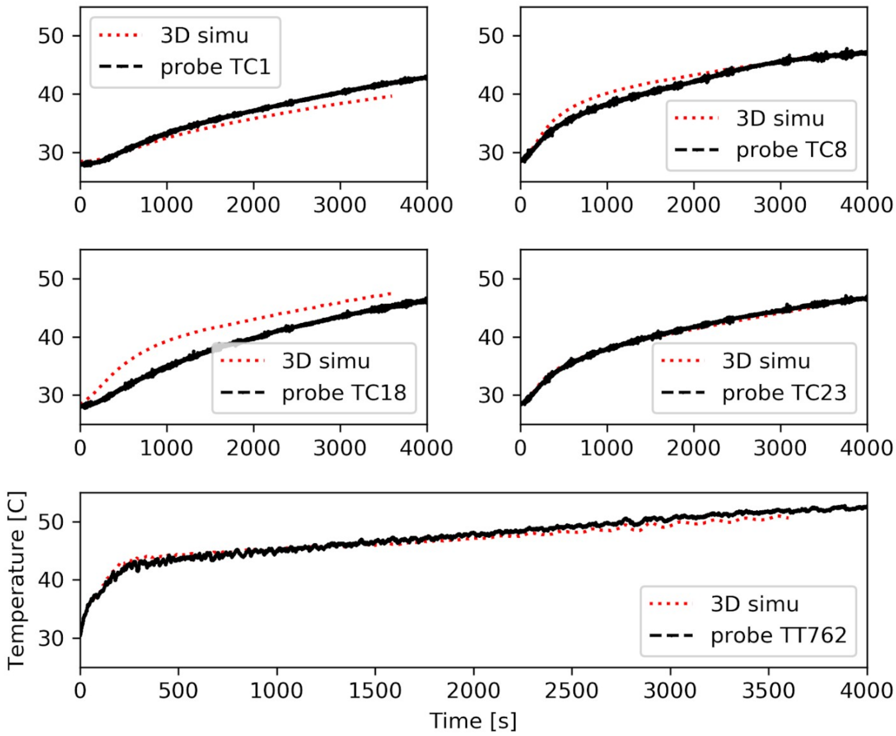

Figure 5. Comparison of local temperature profiles in the fluid at probe TT762 and at different liner-wrapping interface locations TC*. Black: experimental data. Red: CFD results. Refer to Figure 1 to see the exact locations of the probes.

As a conclusion, the 3D CFD model accurately estimates the average temperatures in the fluid and at the different solid interfaces. Locally, it is found that the model well depicts the temperature variations in the gas and at the liner-wrapping interface, apart from the extremities of the tank. It is interesting to note that the slight measured oscillations are also represented by the numerical model, thanks to the time-dependent boundary conditions that are imposed at the inlet.

3.2 Phenomenological study of the refueling process

The temperature is uniformly initialized in the tank and the solid components. The compression induced by the injection of the gas causes an increase of the gas temperature. The heat is transferred by convection from the gas to the internal tank wall and then conducted through the solid components of the material.

The jet momentum is maximum during the first hundreds of seconds, with an inlet velocity higher than 100 m/s. Figure 6 shows that the jet is straight and that the temperature is almost uniform in the region of influence of the jet. Conversely, at the rear part of the tank, vertical gradients appear. Actually, the greatest vertical temperature gradients at the rear part of the tank are obtained between t=100s and t=300s. The maximum gradient between the top and bottom of the tank along a vertical line at 0.35cm from the back of the tank has been estimated at 5°C. This vertical line is represented in Figure 1, see orange dots. Globally, the rate of increase of average temperature is maximum during this phase as shown in Figure 4, mainly due to the relatively high levels of injected gas temperature during the first hundreds of seconds, see Figure 3.

While the refueling keeps going, the jet momentum decreases. This is due to the increase of the pressure inside the tank and hence the related increase in the gas density. Globally, the jet remains straight. The region of influence of the jet becomes narrower and narrower. The temperature remains cold in the jet while it is increasingly hotter in the rest of the tank. Both vertical and horizontal temperature gradients decrease. At t=3600s, the vertical gradient at the rear part of the tank, and the horizontal gradient between the middle of the tank and the rear part of the tank are respectively 0.9°C and 0.3°C. One can refer to the orange dots in Figure 1 to see the exact location where the temperature has been assessed to calculate these gradients.

A high frequency post-treatment of the simulation permits to observe that the non constant mass flow rate imposed at the inlet significantly impacts the jet momentum during the refueling. These fluctuations may play a significant role in the overall mixing process and have to be accounted for in the CFD simulation.

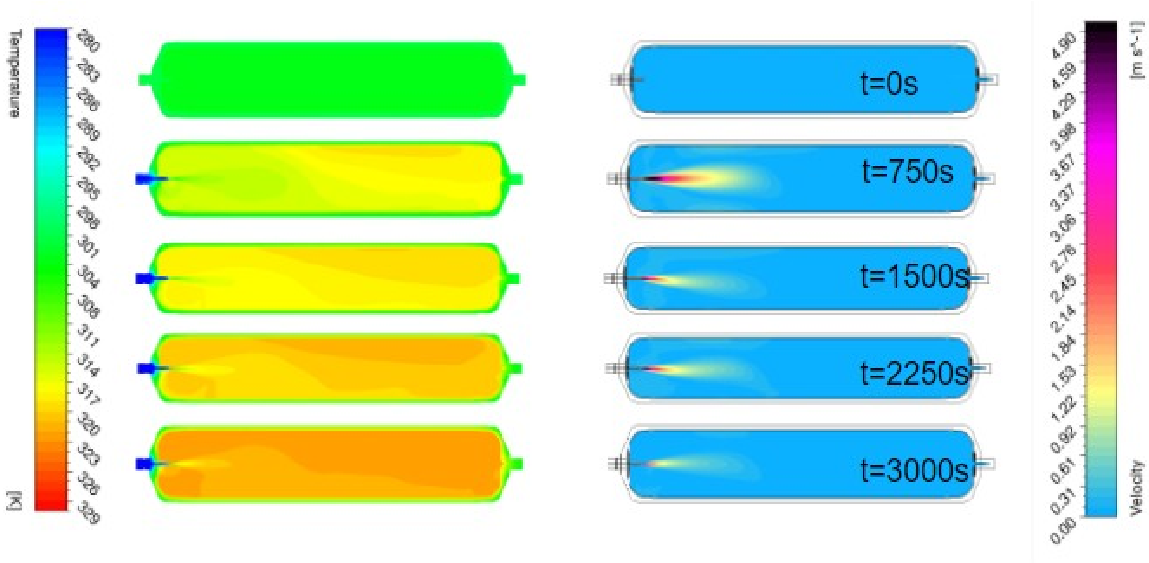

Figure 6. Temperature (left) and velocity profiles (right) at different times of the refueling obtained by 3D CFD simulation.

One of the major outputs obtained from the CFD simulations and which is not available with 0D models is the maximal temperature information. In Figure 7, the maximum temperature reached in the gas, liner and wrapping volumes are plotted. One can observe that the maximum temperature in the gas quickly increases at the beginning of the refueling. It increases by 15°C in a few hundreds of seconds which corresponds to an average rate of 0.04°C/s then it keeps increasing but much slower at an average rate of 0.002°C/s. The temperature fields show that the maximum temperature in the fluid is reached in the top rear part of the tank. One can observe a delay and attenuation of the maximum temperature in the solid parts compared to the fluid part. From t=2000s, the maximum temperature in the liner and in the wrapping follows almost the same rates of increase as the one in the gas. Globally, the maximum temperatures in the liner and in the wrapping are respectively about 1°C and 5°C lower than the one in the gas.

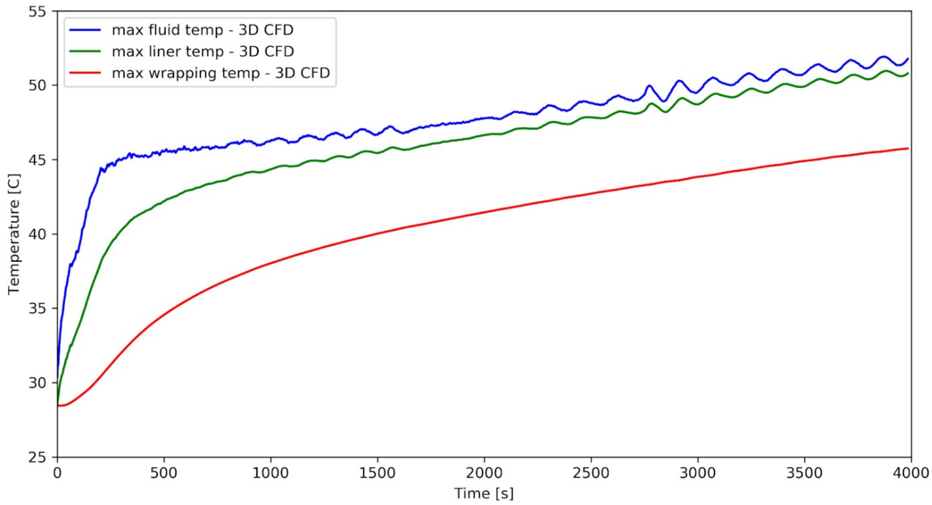

Figure 7. Time histories of maximum temperature. Blue: in the gas. Green: in the liner. Red: in the wrapping.

3.3 Methodologies towards faster simulations

3.3.1 2D axisymmetric simulations

In parallel to the 3D simulation presented in this study, it has been tried to solve the problem as a 2D axisymmetric problem with the aim to drastically decrease the numerical cost of the simulation. The underlying assumption is that buoyancy forces play a negligible role during this filling process and that gravity can be legitimately neglected. As a result, the free convection is not accounted for. The hypothesis is maintained by the fact that no significant vertical gradients of temperature had been experimentally observed under the considered filling conditions. In addition, the 3D simulation results show that the jet remains straight during the refueling.

The results of the 2D axisymmetric simulation are very different from the one obtained by the 3D simulation as can be seen in Figure 8. The average gas temperature inside the tank is significantly higher and the temperature fields are largely different too. With the 2D axisymmetric simulation, a significant horizontal temperature gradient is observed.

Another 3D simulation without gravity has been launched. The results obtained were similar to the results obtained with the 2D axisymmetric simulation as it can be seen in Figure 8. Therefore, it can be concluded that the difference observed between the 3D simulation accounting for gravity and the 2D axisymmetric simulation are due to buoyancy effects. The limitations of a 2D axisymmetric simulation had already been pointed out for refueling cases with higher temperature stratification [13]. These results demonstrate that natural convection cannot be neglected inside the tank. As a conclusion the 2D axisymmetric strategy cannot be used for the accurate estimation of the average temperature in the gas and hence in the walls.

2D results are much more conservative in terms of temperature in the gas. For instance, from t=1000s, the average gas temperature remains about 7°C higher with the 2D simulation than with the 3D simulation as shown in Figure 8.

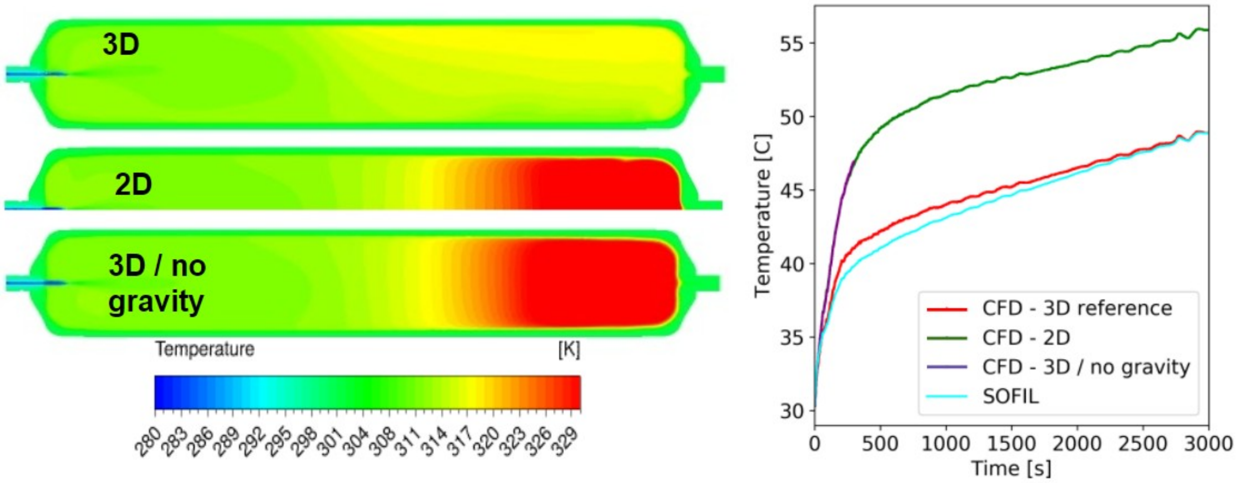

Figure 8. Temperature distributions after 250s of refueling obtained with the 3D simulations and time history of average fluid temperature.

3.3.2 Two-step methodology: switch from 0D to 3D modeling

The SOFIL model permits to quickly (~1 min) simulate refueling of a tank, providing among others the following physical quantities: average gas temperature and pressure, average temperature at the solid interfaces. It has been tried to initialize the 3D CFD simulation 2500s after refueling start-up using these SOFIL data. This simulation will be referred to as “accelerated 3D simulation” hereafter.

At the initialization of the accelerated 3D simulation, the average temperature in the gas is the same as the one obtained with the 3D reference simulation. In the liner and in the wrapping, the accelerated 3D simulation is initialized with less than 1°C and 2°C overestimated average temperature respectively. However, in the boss through which the gas is injected, the differences between the two simulations at t=2500s are more significant: a 15°C difference in average temperature is observed. This difference is illustrated in Figure 9.

The simulation has been run up to 4000s of refueling. The average temperature in the fluid and at the liner-fluid and liner-wrapping interfaces are well described by the 3D accelerated simulation. The average temperatures are slightly overestimated (~1°C) but it does not increase during the refueling.

Locally, the temperature is overestimated by ~1°C with the accelerated simulation at the location of thermocouples in the gas as well as for the thermocouples located in the bottom and top regions of the liner-wrapping interface. For the thermocouples located in the extremities of the liner-wrapping interface, the difference in temperature between the 2 simulations can be higher, i.e close to 5°C. This might be due to the initialization of the solution in the solid bosses which is too far from the 3D reference solution, as it can be shown in Figure 9.

Regarding the maximum temperatures in the gas and at the different solid interfaces, the 3D accelerated simulation overestimates by at most 2°C the values all along the simulation time. The trends during the refueling are globally the same with the 2 CFD simulations.

Figure 9 shows the temperature fields obtained with the 2 CFD simulations at different times. One can see that after a few hundreds of seconds, the temperature fields almost ‘forgot’ its initial conditions. The flow dynamics in the gas phase is quickly recovered after a few seconds. The memory effect is more pronounced from the heat transfer perspective, in particular in the solid components. For instance it can be qualitatively estimated in Figure 9 that it takes about 1000s for the solid boss crossed by the cold injected gas to recover its actual temperature field.

Overall, the accelerated simulation methodology provides reliable results when compared with the reference 3D simulation, while decreasing the computational time from two months to two weeks for this study. The main phenomena are well described and the key outputs of the model such as the average and maximum temperatures can be predicted with a moderate margin of error. Owing to the gain in simulation duration, it is a promising methodology. This methodology should be further assessed on other refueling conditions and tank geometries.

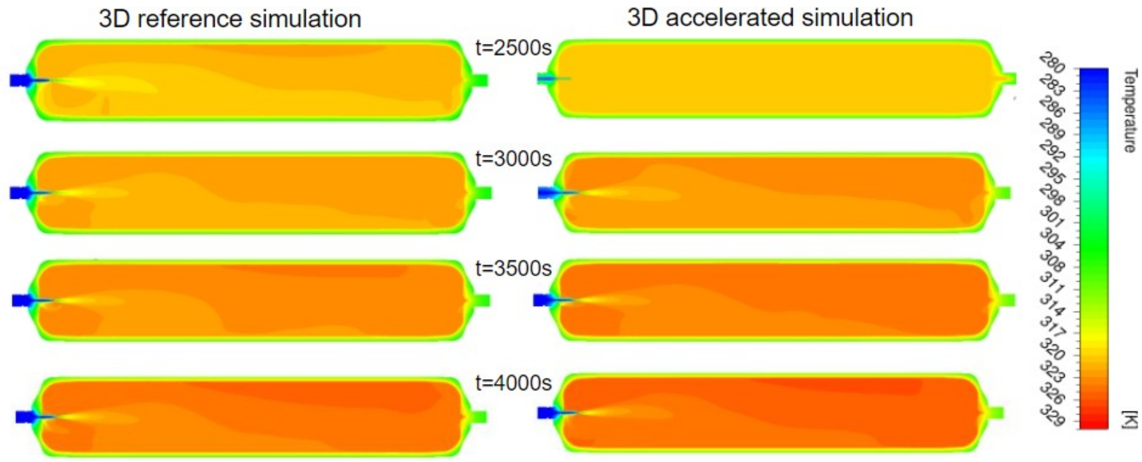

Figure 9. Temperature fields at different refueling times obtained with the 3D reference simulation (left) and 3D accelerated simulation (right)

4. CONCLUSIONS

The 3D reference CFD strategy applied in this work gives results in good agreement with the experimental data. This comparison validates the model applicability for tank refueling simulations. In addition, this study permits to further prove the interest of CFD strategy versus 0D/1D modeling, especially when investigating thermal stratification. The model now needs to be tested and validated for other ranges of operating conditions, in particular the ones for which vertical stratification has been experimentally reported.

The 2D axisymmetric strategy has shown its limits for the considered operating conditions and tank design. Despite the fact that no significant stratification was experimentally observed, buoyancy forces play a major role during the refueling and hence they should not be neglected in numerical models. As a conclusion the 2D axisymmetric strategy is not recommended.

Another modeling strategy has been tested in this work to accelerate simulations. It consists in initializing the 3D CFD simulation after refueling start-up using results provided by a 1D thermodynamics model. For the considered operating conditions and tank size, the methodology has provided results in good agreement with the reference CFD with reasonable errors while significantly decreasing the computational cost. Hence, it can be seen as a promising methodology. More efforts are still needed to validate this method in a larger range of operating conditions and sizes of tanks.

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