SIMULATION OF THE FAST FILLING OF HYDROGEN TANKS

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ABSTRACT

High pressure storage of hydrogen in tanks is a promising option to provide the necessary fuel for transportation purposes. The fill process of a high-pressure tank should be reasonably short but must be designed to avoid too high temperatures in the tank. The shorter the fill should be the higher the maximum temperature in the tank climbs. For safety reasons an upper temperature limit is included in the requirements for refillable hydrogen tanks (ISO 15869) which sets the limit for any fill optimization. It is crucial to understand the phenomena during a tank fill to stay within the safety margins.

The paper describes the fast filling process of hydrogen tanks by simulations based on the Computational Fluid Dynamics (CFD) code CFX. The major result of the simulations is the local temperature distribution in the tank depending on the materials of liner and outer thermal insulation. Different material combinations (type III and IV) are investigated.

Some measurements from literature are available and are used to validate the approach followed in CFX to simulate the fast filling of tanks. Validation has to be continued in future to further improve the predictability of the calculations for arbitrary geometries and material combinations.

1.0 INTRODUCTION

The use of hydrogen as a fuel for passenger cars, buses or trucks requires a safe and optimized method to store a sufficient amount of hydrogen. High pressure storage of hydrogen in vehicle tanks is a promising option. Maus [1] gives a very good overview on most aspects of pros and cons of different tank materials and the experimental investigation including modeling of the high pressure storage of hydrogen. The development of a predictable model to calculate the fill process of a high pressure tank occupies a large part of the work of Maus. Dicken and Mérida [2] describe the setup and results of CFD simulations of some fill experiments they carried out. They demonstrate that the knowledge of the spatial temperature distribution during compression is very important to identify the available margin from a maximum allowable temperature in the tank. In practical applications a single representative probe in the tank has to replace the spatial field of temperatures. A typical task for a model is to find the location where the single probe is close to the mean temperature in the tank.

The purpose of this work is to validate a hydrogen tank model developed for the code CFD code CFX against data available from literature and to perform parametric studies. The model may be later used to contribute to the design of new fill experiments at the institute.

2.0 VALIDATION EXPERIMENTS

Dicken and Mérida [3] describe a number of fill experiments which are very well suited for model validation. The experiments are described in detail, cover the fill pressure range of interest and include a fine array of temperature sensors in the test cylinder. This allows a direct comparison of the calculated transient temperature field in the cylinder with the thermocouple readings.

The test cylinder used for the experiments models a type III hydrogen tank (aluminum liner with carbon fiber wrap). It has an inner volume of 74 l and is limited by a design pressure of 350 bar. The inner length is indicated to be 0.893 m and the inner diameter is 0.358 m. The liner has a thickness of 4 mm. The insulation laminate is 15 mm thick. The injection pipe extends 82 mm into the cylinder. All measures of the test facility can be found in [2].

The complete arrangement of the experimental setup is shown in Figure 1. From a high-pressure storage the hydrogen passes a dispenser and flows in the test cylinder. The dispenser measures and controls the mass flow rate. An adjustable pressure control valve in the dispenser sets the pressure ramp to the cylinder. By this means the fill time to the nominal total mass of 1.79 kg (15 C@350 bar) or the maximum allowed pressure of 350 bar in the cylinder can be determined.

Hydrogen mass flow rate and pressure ramp are recorded and can be used as boundary condition for computer simulations. The temperature of the entering hydrogen was also measured.

Dicken and Mérida [3] report a total of 18 experiments from which 7 were used to demonstrate the reproducibility of the measured data. The experiments combine different fill times and initial tank pressures. The fill times used are 40, 190 and 370 s. The initial pressures or masses represent different fill levels of a vehicle tank before refueling. These are 50, 70, 100, 150 and 200 bar.

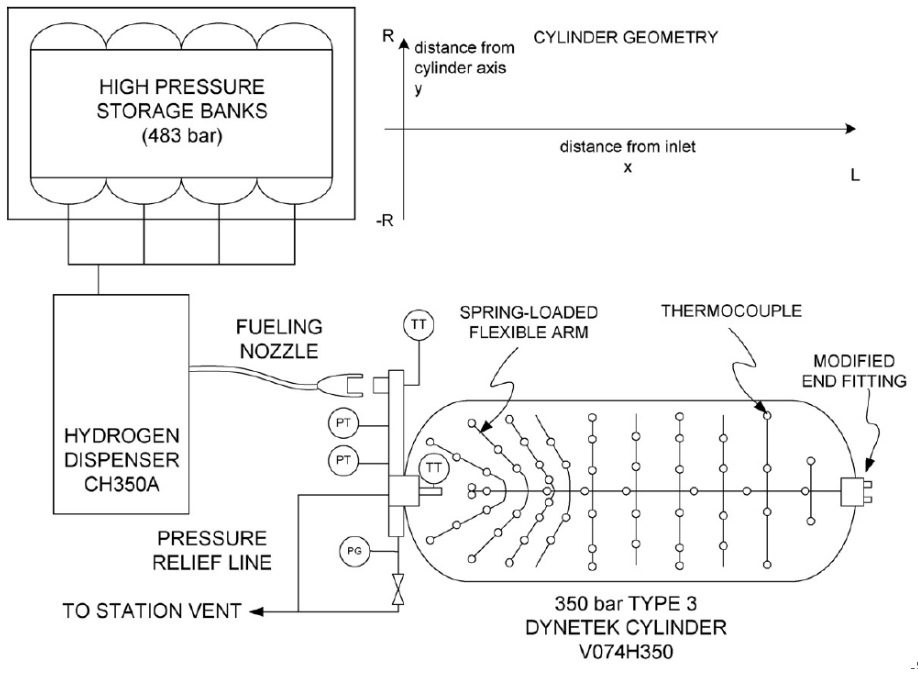

Figure 1. Test arrangement as described by Dicken and Mérida (Fig. 2 from [3])

The test cylinder is very well equipped with temperature probes. A total of 63 thermocouples was installed and are reported to measure temperatures to +/- 1 K. Figure 2 shows the distribution within the test cylinder.

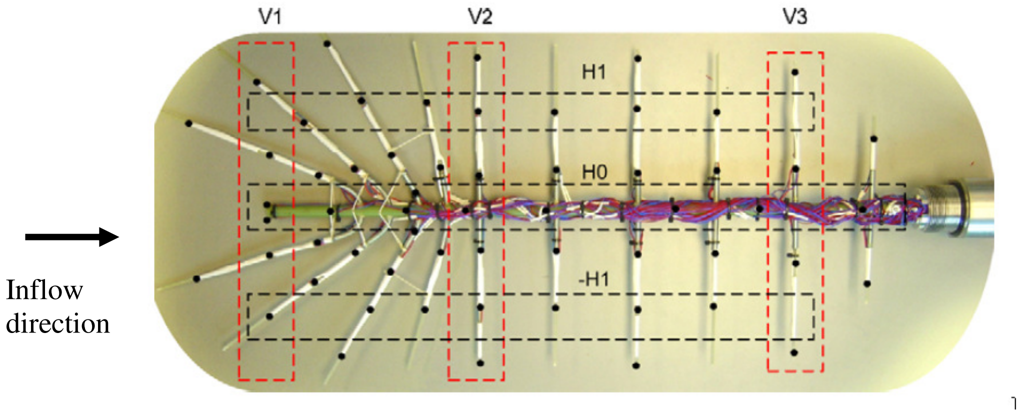

Figure 2. Thermocouple distribution inside the test cylinder (Fig. 4 from [3])

Temperature profiles along horizontal (-H1, H0, H1) and vertical (V1, V2, V3) lines at different times as indicated in Figure 2 can be used to characterize the spatial temperature increase during the fills. A mean temperature is calculated as a weighted average over all installed thermocouples. This mean temperature is provided to identify a single location in the cylinder which shows a representative behavior.

3.0 SIMULATIONS

The calculations discussed next are mainly based on the experiments by Dicken and Mérida [3] roughly described in the paragraph before. Up to now only three of the experiments were simulated because of the limited information available about their boundary and initial conditions.

No dedicated mesh sensitivity studies were carried out at this level of knowledge of the experiments. However the computational mesh was built in accordance with available best practice guidelines. This is reflected e.g. in the fine resolution of mesh cells in the walls of the test cylinder and the fluid adjacent to walls. There cells were chosen with a height of about 1 mm. The next paragraph discusses the mesh in more detail.

3.1 Model setup

The following paragraphs describe the geometrical and physical model which was developed according to the information which was extracted from [1] and [3]. Some uncertainties remain. It is not known to which extent the quality of the calculation results are affected.

3.1.1 Geometry

The computational model was developed based on the dimensions summarized in paragraph 2.0. The curvature of the vessel heads is not exactly known. In order to preserve the total volume when assuming elliptical heads the inner diameter was approximated.

The test cylinder is meshed as a 3D model without simplifications like symmetry planes. This approach involves a higher numerical effort during the simulations but offers a better representation of unsymmetrical phenomena like buoyancy effects which are expected to be important when longer fill times (smaller fill rates) are considered.

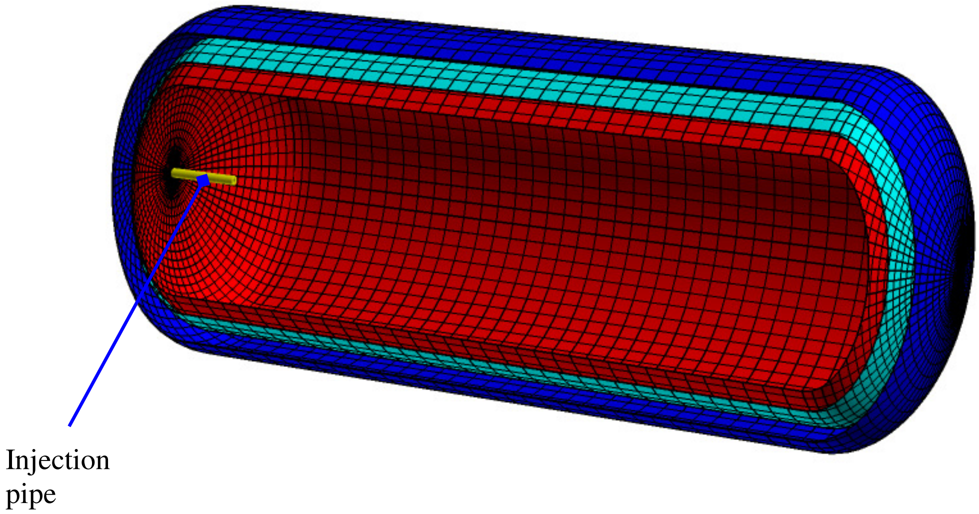

Figure 3. Cut through the modelled test cylinder

The test cylinder consists of a long cylindrical section with elliptical heads. The injection pipe with an inner diameter of 5 mm extends 82 mm into the gas space. Not all information about the geometry is available. Dicken and Mérida [3] mention two ports centered at the elliptical heads of the cylinder but without dimensions. They are neglected in the CFX model. The same applies to the support mechanism of the array of thermocouples as shown in Figure 2. Part of this mechanism is a bundle of instrumentation cables along the central axis of the cylinder. These might influence the flow pattern of the incoming hydrogen in this region. These details are not included in the CFX model.

The test cylinder is composed of three domains. The innermost domain is the gas domain which is connected to the liner as the second domain. The interface between both is shown by a red surface in Figure 3. The second interface is located between liner and the outer insulation of the tank (the third domain, carbon fiber) and is depicted by a light blue surface. The outer boundary of the insulation domain is shown in dark blue color. There is no gap between liner and thermal insulation.

The heat flux in liner and insulation is preferably directed normal to the boundary planes. A hexahedral grid was chosen for these two domains because it reduces the numerical diffusion to a minimum. For the same reason the transitional region between gas domain and inner liner surface is composed of wedges. The main part of the gas domain, however, is unstructured and consists of tetrahedra and pyramids. The total number of nodes over all three domains is 161064 (equivalent to 462846 elements). Figure 4 shows details of the mesh created.

The injection pipe is modeled by about 25 cells across the cross section.

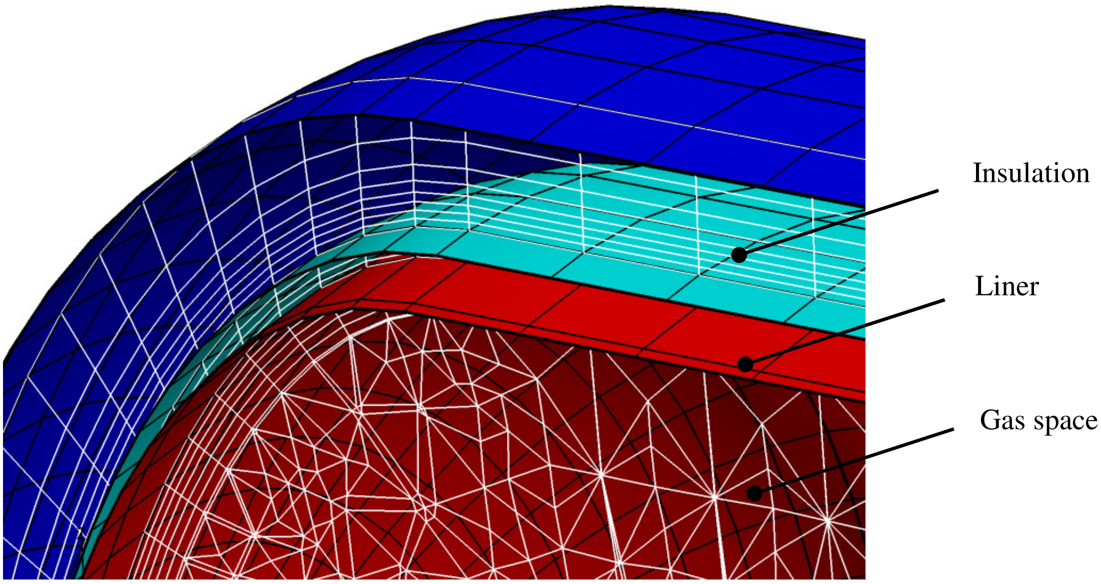

Figure 4. Details of the mesh in fluid, liner and insulation

This figure gives some idea about the relations in thickness between liner and outer insulation. The cells close to the interfaces (gas space to liner and liner to outer insulation) have an average height of about 1 mm.

3.1.2 Code options

The code applied was CFX 11 SP1 [4]. The following options were selected:

- A single component gas (hydrogen) is modeled. Air is not included e.g. as a background fluid because the tank is always held at overpressure to environment.

- The “Redlich-Kwong” real gas behavior instead of the ideal gas law is activated to calculate the density. Absolute gas pressures up to 350 bar require this. The real gas formulation calculates about 15 % smaller densities compared with the ideal gas law. A built-in library in CFX for hydrogen provides all the necessary input required by the “Redlich-Kwong” equation of state. The specific heat capacity of hydrogen is calculated using the “Redlich Kwong Polynomial” to build a table depending on pressure and temperature. The thermal conductivity is calculated based on the “Modified Eucken Model” and the dynamic viscosity follows the “Rigid Non Interacting Sphere Model”.

- The SST (Shear Stress Transport) turbulence model is used for all simulations. This model includes an automatic treatment for wall functions. If regions with sufficient high mesh resolution near walls are found then wall functions are not activated otherwise a combination of linear and logarithmic wall function (blending factors allow user interference) is applied. Production and dissipation terms for buoyancy are activated.

- The computer model consists of three domains. These are the gas domain, the liner as a solid domain and the outer insulation as a second solid domain. Interfaces which provide a conservative heat transport between the three domains of the model are defined. 3D heat conduction in the solid domains is activated.

- The expression language of CFX (CEL) is used to calculate time dependent values of the cylinder mass and the average temperatures in gas space and liner.

3.1.3 Boundary and initial conditions

Boundaries of the test cylinder to the environment exist at the outer wall of the insulation and the hydrogen inflow opening:

- An inlet is defined to allow inflow of hydrogen through the pipe in Figure 3. In order to allow the formation of a realistic velocity profile over the cross section of the injection pipe the inlet is placed sufficiently far upstream of the pipe mouth in the cylinder. Two options are available to generate a flow. If known a mass flow rate can be directly specified as a function of time. The second option is based on the absolute pressure outside of the tank. During the experiments discussed here the pressure outside of the test cylinder was controlled to achieve a subsonic flow rate into the cylinder and to fill the cylinder in a pre-defined time. The pressure option at the inlet is consequently the preferred option. Inflow temperature and pressure histories were directly imported from the experimentally measured curves given in [2].

- The outer wall of the insulation around the test cylinder can be either considered to be adiabatic or can have a certain heat transfer coefficient to the surrounding air. Because of the low conductivity of the insulation material and the relatively short fill times the adiabatic option was chosen.

- Quiescent flow conditions in combination with very low values of turbulent kinetic energy and energy dissipation are set as initial state in the cylinder. Walls and the gas space of the cylinder are at the same temperature. The total pressure is set according to the desired hydrogen fill degree to start from.

3.2 Results

As a first step to validate CFX for filling processes under high pressure one experiment from the series described in [3] is simulated and compared to selected measurements. The test was carried out with a fill time of 40 s starting from an initial tank pressure of 100 bar.

In addition to the validation calculation results of two studies with a higher initial pressure of 200 bar and in one case a different liner material (type IV instead of type III) are discussed.

3.2.1 Validation test

Dicken and Mérida [2] analyzed the same experiment with a 2D model implemented in the code FLUENT. They included the pressure and temperature history of the flow entering the test cylinder in their paper. These two curves were also used as boundary conditions for the CFX calculation. As a result of the calculation the maximum allowed mass in the tank of 1.79 kg is not reached exactly at the end of the fill process but only 1.65 kg. This may be due to uncertainties in the pressure history used to calculate the flow into the test cylinder. The mentioned mass difference in the cylinder is also due to compression of hydrogen in the cylinder which causes the maximum tank pressure to be reached before the nominal mass is filled in. Once the fill process is finished the tank would cool down to environmental conditions and would tend to cause the well known under-fill situation with less mass in the tank than possible. Purpose of experiments and numerical simulations is therefore the reliable prediction of the temperature field in the tank and to create eventually a fill strategy which minimizes the compression heat-up at acceptable fill times. The limitation of the temperature increase during the fill (ISO 15869) is also necessary to maintain the safety of the hydrogen tank.

Figure 5 shows two results of the CFX simulation. The temperature field is quite uniform with slightly lower temperatures in the lower section of the cylinder and along the head on the injection side. The incoming hydrogen is colder than the compressed hydrogen inside the tank; consequently the plume is directed downwards.

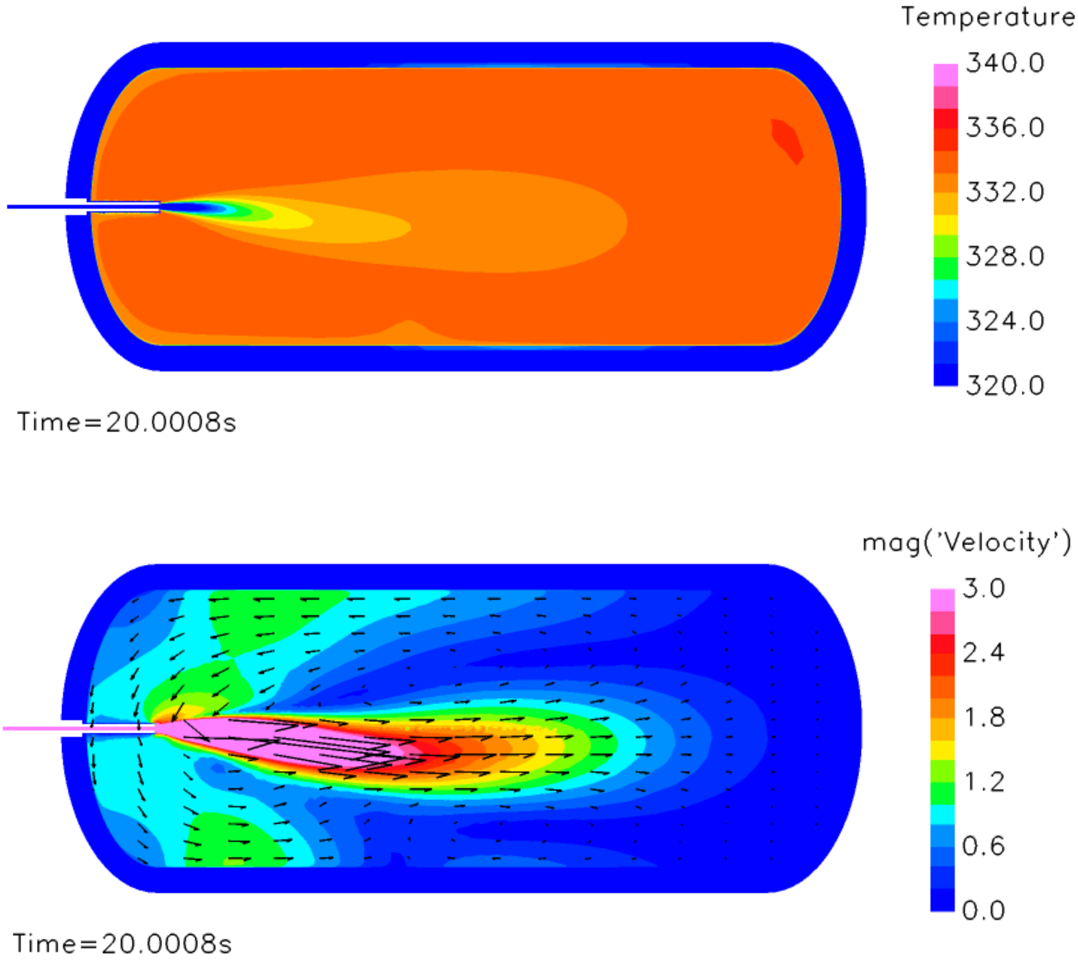

Figure 5. Temperature [K] and velocity [m/s] distribution in the test cylinder after 50 % of fill time

The flow in Figure 5 is a three dimensional field from which only a projection in the vertical center plane is visible. Backflow is observed in the upper part of the cylinder which is directed towards the space behind the injection pipe.

Figure 6 provides a comparison of the simulation with measured data. At three different fractions of the total fill time temperature profiles along the horizontal line H0 (see Figure 2) are extracted and compared with data from [3]. This figure and following normalize the temperature in the cylinder with a mean temperature. The simulated mean temperature in the test cylinder is a volume weighted average over the cylinder volume. The experimental mean temperature was calculated from the available 63 thermocouple readings weighted by the vertical distance from the central axis in the cylinder and an area factor. Figure 6 illustrates that temperature differences from the mean value are below 10 K.

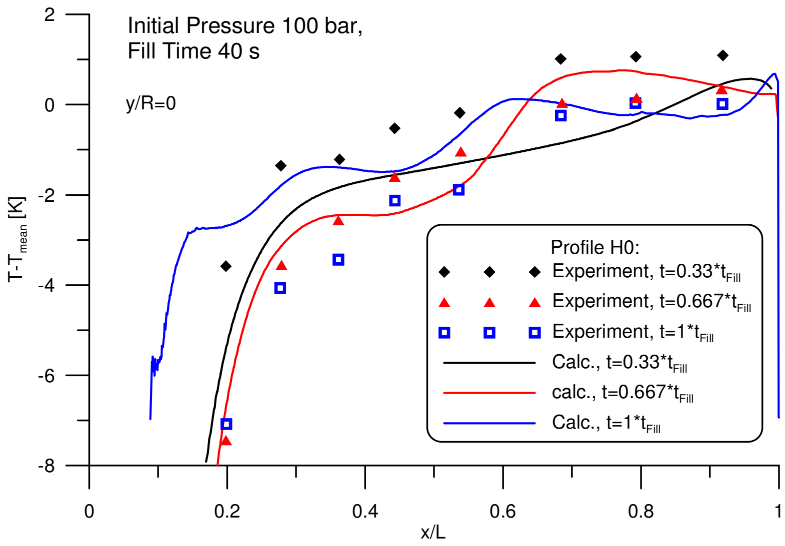

Figure 6. Horizontal temperature profiles during the fill, data from [3]

This figure shows a generally higher temperature at the opposite end of the test cylinder measured from the injection pipe. This behavior can be also seen in the calculation. At one third of the fill time there is some underestimation of the measured temperatures along H0. This tendency reverses towards the end of the fill process to a slight over-prediction. Possible reasons might be found in uncertainties of the conditions at which hydrogen enters the cylinder and in the heat transfer of pure hydrogen to the liner.

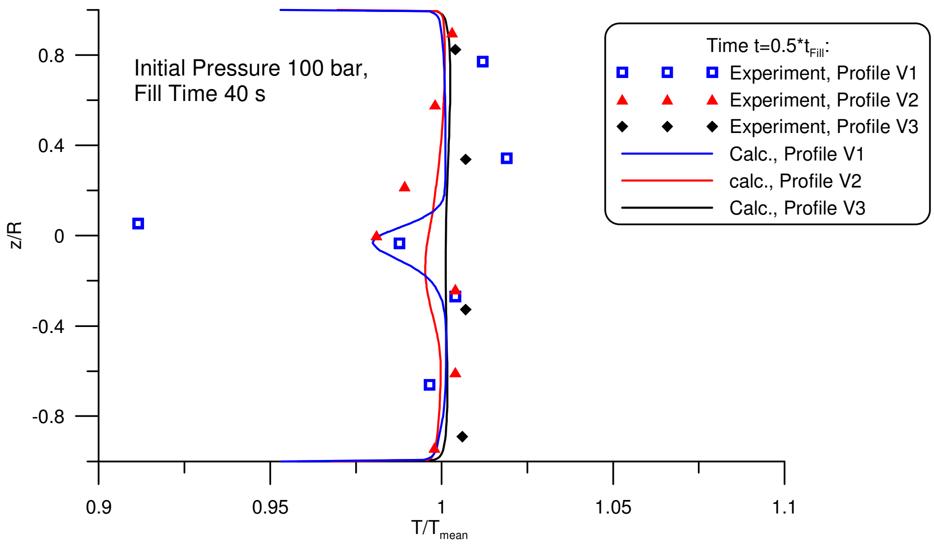

Figure 7. Vertical temperature profiles after 50 % of the fill time (20 s), data from [3]

Figure 7 provides some vertical temperature profiles after 20 s (50 % of fill time) at lines V1, V2 and V3 (compare Figure 2). At position V1 which is closest to the inflow pipe the calculated temperature does not show a distinct decrease compared to the measured value. In the test cylinder there are measurement cables located along the center axis. It is not known to which extent the flow and consequently also the temperature distribution is influenced. It is also observed that the calculated temperatures have a more symmetrical pattern in relation to the horizontal axis of the cylinder. The tendency that the profiles become flat towards the opposite end of the cylinder is calculated correctly.

Further investigations on the heat transfer to the liner might identify if the calculated temperature profiles could be improved.

3.2.2 Applications

Two applications are presented to show tendencies if either the initial pressure in the tank (partial fill condition before refueling) or the liner material are changed.

An initial pressure of 200 bar instead of 100 bar in the tank means that during the fill the mass of hydrogen would increase only by a factor of 1.6 instead of 3 as from 100 bar. With the same fill time a lower temperature rise is expected.

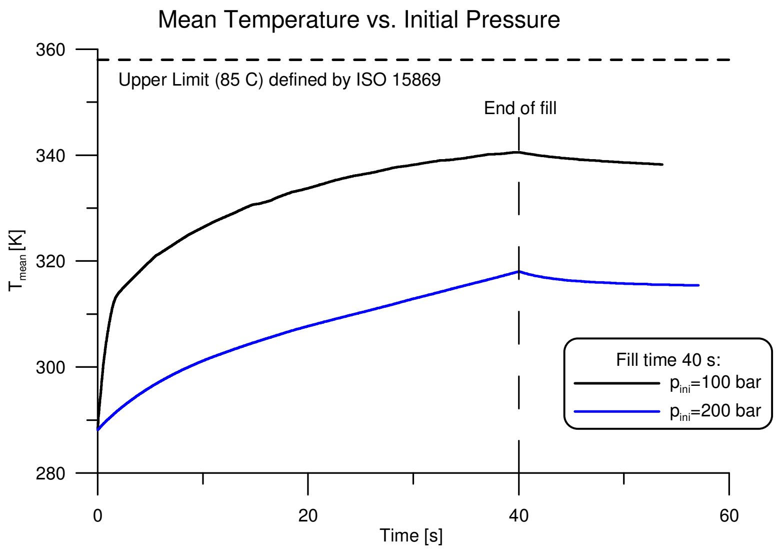

Figure 8. Mean temperature history in the test cylinder depending on the initial pressure

This behavior confirmed by the calculated mean temperature history shown in Figure 8. This figure includes also the upper temperature limit for hydrogen tanks (358 K or 85 C defined by ISO 15869) which must not be exceeded during the filling process. With an initial pressure of 100 bar this temperature limit is not reached. However with lower tank pressures before refueling and a short fill time it appears possible to come close to the maximum allowed temperature limit.

Figure 8 shows that the simulations also include the beginning of the relaxation phase after the end of the fill. However, measurements beyond the fill process were not published and an assessment of the heat transfer from the cylinder remains to be dealt with.

A second parametric study was carried out to identify temperature differences in the tank if a different liner material is used.

Table 1. Summary of property data of liner materials used

	Thermal conductivity	Density	Specific heat capacity
	W/mK	Kg/m^3	J/kgK
Aluminium [2] (type III)	167	900	2730
Polyamide [1] (type IV)	0.3	1140	1500

The type III liner material in Table 1 was used in the experiments by Dicken and Mérida [3]. The type IV liner was chosen as a generic material of this group of liner materials. Another material could have been HDPE (high density poly ethylene).

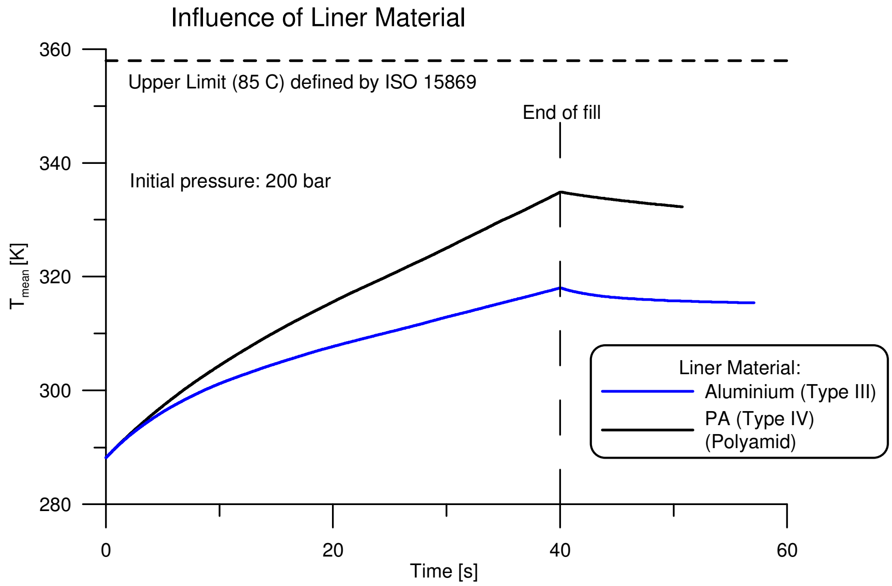

Figure 9. Influence of liner material on the mean tank temperature

Figure 9 depicts the calculated mean hydrogen temperatures in the test cylinder. At the end of the fill process the mean temperature is about 17 K higher when the specified liner type IV is used. This means with plastic liners which have advantages in the production process the temperature control inside the tank becomes even more important than with liners of type III. An option to avoid too high mean temperatures is to extend fill times.

3.3 Summary

Dicken and Mérida [3] derived from the series of experiments they performed a general relation between the normalized mean temperature increase and the normalized mass in the tank. The coefficients of the curve fit change if the fill time is modified. For a fill time of 40 s the dependency is shown in Figure 10. The equation coefficients are indicated in [3]. Results of the two experiments with liner type III calculated in this work (100 and 200 bar initial pressure) were normalized with the initial mean temperature and mass and put in comparison to the general relation. Figure 10 shows a good agreement to the curve fit. This indicates that as long as only global information from a fill process like the mean temperature is required, then more detailed calculations are not necessary. CFD calculations are useful if the spatial distribution of temperature or details of the flow field are asked for.

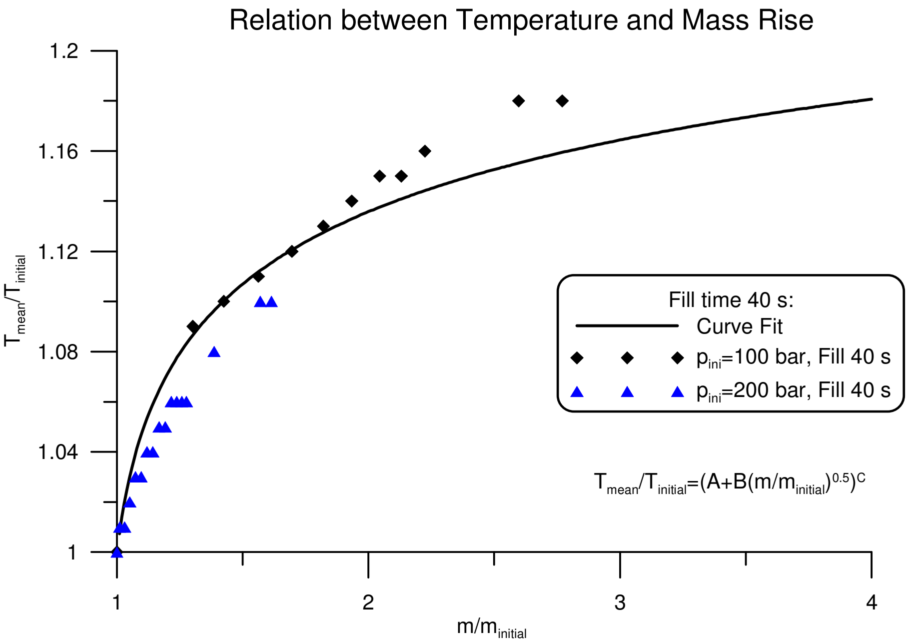

Figure 10. Generalised relation between temperature and mass in comparison with the two tests analysed

4.0 CONCLUSIONS

The precise prediction of the temperature distribution inside a hydrogen tank during refueling is important. It contributes to a safe handling of hydrogen as vehicle fuel. It also allows minimizing the fill time without exceeding maximum allowed temperatures.

A first step in the validation of the CFD code CFX for fast filling processes based on literature data was carried out. The fill of tanks is a complex process. The high final fill pressure requires the application of a real gas description rather than the ideal gas law. A 3D geometrical model as opposed to a 2D approach was used in the calculations in order to properly simulate buoyancy effects when longer fill times are of interest.

The numerical results obtained are encouraging. Improvements become possible with a better knowledge of the experimental conditions. On the numerical side the mesh resolution near the inner liner wall in combination with the heat transfer from pure hydrogen should be further investigated.

Two studies on the influence of the initial pressure in the tank before refueling and the influence of the liner material on the temperature growth in the tank were presented. The tendencies observed are in agreement with literature data.

ACKNOWLEDGEMENT

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