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Modelling the Refuelling of Hydrogen Fuel-Cell Heavy-Duty Vehicles with Multiple Heterogenous Tanks.

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Introduction

Road transport greenhouse gases (GHG) emissions accounts for over one fifth of global CO₂ emissions in the EU. In Europe in recent years, road transport is the only sector whose emissions have unfortunately not stopped rising. This is particularly true for the heavy-duty mobility, such as trucks, city buses and long-distance buses, which account for over 25% of GHG emissions [1]. One of the most promising technologies to decarbonize heavy-duty transport (trucks, buses, trains, boats) is hydrogen fuel cell technology [2]. The development of this technology requires, besides the development of the vehicles, a parallel effort in the advance of hydrogen refuelling infrastructure and the related refuelling protocols.

In terms of vehicle development, the effort required to maintain a range similar to that of fossil-fuelled heavy-duty vehicles is significant. For this purpose, the fuel cell heavy-duty vehicles (FC-HDVs) need bigger onboard storage systems than fuel cell light-duty vehicles (FC-LDVs). To achieve the required hydrogen storage volume, automotive original equipment manufacturers (OEMs) have to exploit any available space in the vehicle by inserting multiple hydrogen storage tanks, often of different sizes, which is not the case for FC-LDVs.

This configuration of the on-board hydrogen storage system could have a significant impact on the derivation of parameters for advanced protocols (such as those defined in the European PRHYDE project [3]), as well as on the evaluation of the vehicle's instantaneous state of charge (SOC). Indeed, due to the different tank sizes of the FC-HDV storage system, the mass flow rate distribution between the tanks, the pressure evolution in each tank size and the temperature rise in the different tanks cannot easily be predicted. Thus, the models used to derive the parameters of FC-HDV refuelling protocols should therefore be updated to consider these effects. Moreover, fine modelling of the evolution of these parameters during refuelling would enable us to accurately estimate the thermodynamic state of each tank in the vehicle hydrogen storage system at the end of each refuelling session. Knowing this thermodynamic state will enable the automotive OEMs to know where to place the sensors needed to assess the vehicle's SOC.

The aim of this work is therefore to propose a thermodynamic model to simulate the refuelling of a hydrogen storage system for HDVs with multiple heterogeneous tanks.

Methodology

The model presented in this paper has been implemented in an internal tool at Lab H₂ within CRIGEN called HyFill. HyFill is developed on MATLAB Simulink (R2021b) [4] from MathWorks[®] and allows to simulate the fast filling of fuel cell vehicle (FCV) hydrogen storage tanks at a hydrogen refuelling stations (HRS) from the dispenser to the vehicle (see Figure 1-a) to predict the final temperature and pressure reached by the hydrogen, as well as the total hydrogen mass transferred to the vehicle storage tanks.

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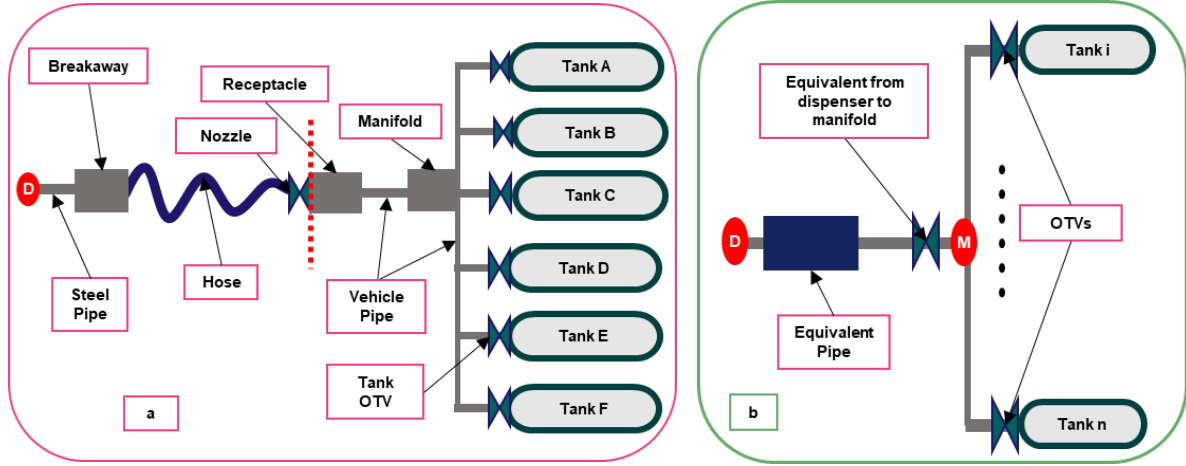


Figure 1 -Scheme of the refuelling station on the left (a) and its simplification on the right (b).

The modelling approach is pseudo-1D. It considers that the gas temperature is uniform at each instant in the tank. The heat transfer between the gas and the ambient is modelled by the unsteady one-dimensional radial heat conduction equation. To calculate the temperature, mass, and pressure of the gas in the tank, a system of three equations is solved at each time step during the whole filling or emptying simulation; these are the mass balance, the energy balance for a control volume and the equation of state here given by [5]:

$$\begin{cases} \frac{dm}{dt} = \dot{m}_{in} - \dot{m}_{out} \\ \frac{dm u}{dt} = \dot{m}_{in} h_{in} - \dot{m}_{out} h_{out} - \dot{Q}_{g-w} \\ \frac{P}{\rho} = ZRT \end{cases} \quad 1$$

In this equation system (Eq. 1), m is the hydrogen mass in the tank, \dot{m}_{in} and \dot{m}_{out} are the inlet and outlet mass flow rate respectively, u is the specific mass internal energy, h is the specific mass enthalpy, P , T and ρ are hydrogen pressure, temperature and density respectively, Z is the hydrogen compressibility factor depending on thermodynamic variables, R is the gas constant. The hydrogen compressibility factor as well as all other thermodynamic properties of hydrogen are calculated in HyFill using a fundamental equation of state (GERG-2008 equation of state [5]). The heat flow from the gas to the tank wall ($\dot{Q}_{g-w}[kW]$) is given by Eq. (2):

$$\dot{Q}_{g-w} = S_{in} H_{in} (T - T_{w,r=r_{in}}) \quad 2$$

Where S_{in} is the inner wall surface of the tank, H_{in} is the inner film mass heat transfer coefficient determined from the correlation for internal turbulent flow [7], $T_{w,r=r_{in}}$ is the temperature of the inner wall of the tank. It is obtained by solving the unsteady one-dimensional radial heat conduction equation (assuming azimuthal symmetry as the tank wall temperature is the same along its entire length for a given radius) given by [9], in Eq. (3):

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\lambda}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T_w}{\partial r} \right) \quad 3$$

Where $c_p [Jkg^{-1}K^{-1}]$ is the specific heat at constant pressure, and $\lambda [Wm^{-1}]$ is the thermal conductivity of the tank wall material. The boundary condition necessary to solve this equation is the mass heat flow from the outer tank wall to the ambient air:

$$\dot{Q}_{w-a} = S_{out} H_{out} (T_{w,r=r_{out}} - T_{amb}) + \varepsilon_w \sigma S_{out} (T_{w,r=r_{out}}^4 - T_{amb}^4) \quad 4$$

where H_{out} is the outer film heat transfer coefficient considered constant (natural convection assumption), S_{out} is the outer wall surface of the tank, $T_{w,r=r_{out}}$ is the temperature of the outer wall of the tank, T_{amb} is the ambient temperature, ε_w is the emissivity of the external wall of the tank, σ is the Stefan-Boltzmann constant.

In HyFill the fuelling line is modelled in a separate Simulink block. The fuelling line is composed of stainless-steel pipe, breakaway, hose, nozzle, receptacle, on-tank valve (OTV) and it is modelled as a cylindrical pipe. The geometric model of the pipe conserves the fuelling line thermal mass. Distributed pressure drops along the pipe length are neglected and (hydrogen is not considered as compressible as the Mach number is lower than 0.3 in the piping ($Ma < 0.3$)), thus there is mass and momentum conservation between input and output of the pipe. To consider the effect of the thermal mass, the model consists of the energy balance of the gas in the pipe and of the pipe wall:

$$\begin{cases} \frac{dmu}{dt} = 0 = \dot{m}(h_{out} - h_{in}) + \dot{Q}_{g-w} \\ \frac{dU_{pipe}}{dt} = \dot{Q}_{w-a} + \dot{Q}_{g-w} \end{cases} \quad 5$$

Where \dot{m} is the hydrogen mass flow rate the pipe, h_{out} and h_{in} are the mass enthalpy entering and exiting the pipe. U_{pipe} is the internal energy of the pipe wall. \dot{Q}_{w-a} is the heat flux from the ambient to the pipe wall and it is calculated as Eq. 4. \dot{Q}_{g-w} is the heat transfer from the pipe wall to the gas and it is estimated by assuming constant wall temperature along the pipe length. Consequently, the pipe transfers heat while maintaining a constant wall temperature along its length and radius. This can be motivated by the fact that the Biot number, defined as:

$$Bi = \frac{H_{in}}{\lambda_w/t_w} \quad 6$$

Where t_w is the wall thickness in first approximation the radial distribution of temperature can be neglected [9], thus $dT_w/dr = 0$. As seen in the experimental work by Kuroki et al [10], the temperature varies along the length only at the start of the refuelling, but the variation becomes smaller in the last part of the refuelling, therefore the longitudinal distribution of temperature can be negligible, thus $dT_w/dx = 0$. The hydrogen properties along the pipeline are also considered as constant.

The refuelling is a process regulated with pressure, thus the mass flowing in the system depends on the pressure differential between the high-pressure storage of the station and the storage tanks of vehicle. On the other hand, the pressure drop depends on the gas mass and temperature in each tank, and both change depending on the mass flow rate. Thus, it is a complex problem determined by a non-linear equations system that must be solved simultaneously.

The system can be simplified as shown in the scheme in Figure 1-b, because two main hypotheses are applied:

- as the heat transfer is already considered in the pipe model, and the expansion through the valves is adiabatic, thus isenthalpic, the energy is conserved.
- The pressure drops of the piping section that share the same mass flow rate can be modelled as a single valve with a flow coefficient ($k_v [m^3 h^{-1}]$) representing the pressure drops of all the correspondent section. The distributed pressure drops are neglected.

Thus, the system can be described by associating a mass balance and the characteristic equation of each valve. The characteristic equation chosen is derived from the IEC 60534 standard [11]:

$$\dot{m} = \begin{cases} \rho_1 N k_v \frac{2}{3} \sqrt{\frac{P_1}{2\rho_1}} & \text{if } P_1 > 2 P_2 \\ \rho_1 N k_v \left(1 - \frac{2 P_1 - P_2}{3 P_1}\right) \sqrt{\frac{(P_1 - P_2)}{\rho_1}} & \text{if } P_1 \leq 2 P_2 \end{cases} \quad 7$$

Where subscripts 1 and 2 refers respectively to upstream and downstream conditions, and N is a constant equal to 31.6.

Results and discussion

Generally, for a range of around 1000 km, the FC-HDV storage system needs to carry around 100 kg of hydrogen [12]. To maintain the same refuelling time as a diesel truck, it needs to be refuelled in around 10 minutes. For this reason, the model was tested in this study on a storage system with a total volume of around 2.5 m³, composed of Type IV tanks with a nominal working pressure of 70 MPa. This storage system is composed of two 500L tanks, four 300L tanks and three 100L tanks.

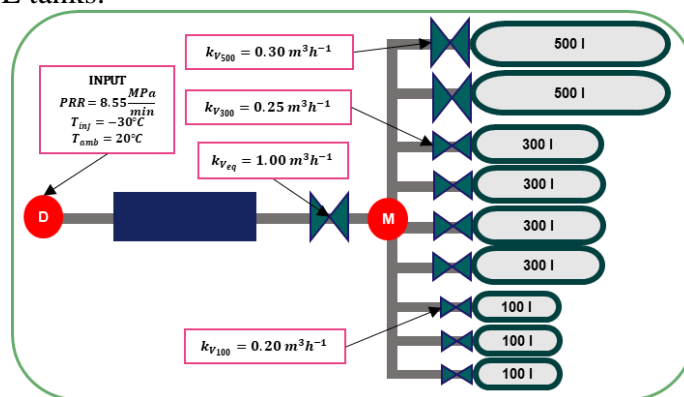


Figure 2 – Scheme of the model with the simulation inputs and parameters of the main components.

The refuelling simulation is performed at constant pressure ramp rate (PRR) of 8.55 MPa/min imposed at the dispenser. This PRR is calculated to satisfy 10 minutes refuelling from the lowest acceptable pressure (2 MPa) to the maximum operating pressure (MOP) of each tank (87.5 MPa). The equivalent flow coefficient (k_V) of the fuelling line is equal to 1 m³h⁻¹. For the three tank sizes, the flow coefficients of the OTVs are 0.30, 0.25, 0.20 m³h⁻¹ respectively, in decreasing order of tank volume. As there is no thermodynamical difference in the tank parameters and input for each tank of the same size, only one tank for each size considered is simulated to evaluate temperature and pressure evolution, but all the tanks are considered in the total mass balance. The refuelling is simulated with ambient temperature set to 20°C, initial pressure of the tanks 2 MPa, initial thermal equilibrium between the system and the ambient. The initial gas temperature at the dispenser outlet is set at the ambient and it decreases linearly at -30°C in 30 seconds as recommended in the SAE J2601 protocol [13].

In Figure 3 are presented the results of the refuelling simulation considering different tank sizes. the top left graph presents the average gas temperature evolution in the in these conditions, none of the tanks reaches the critical temperature of 85°C. On the right the pressure is represented at different points of the station, it can be noted that the highest pressure drops are during the first part of the refuelling and are mainly concentrated in the fuelling line. On the bottom there is the mass flow rate on the left (total in black). The total mass flow rate does not exceed the maximum value of 300 gs⁻¹ allowed by the new protocols for FC-HVD refuelling [14]. In the graph only one curve I represented for each tank size not each tank has been simulated as identical tank have identical input conditions (with the applied hypothesis), thus the sum of the three curves do not add up to the total mass flowrate, as each curve should be multiplied for the correspondent number of tank. On the bottom right there is the SOC of each tank. The simulation ended when a SOC of 100% was reached in the smaller tank. From the results of the refuelling in Figure 3 we can see that temperature, pressure and mass flow rate evolve differently for the three tank types. More in detail, the larger the tank, the higher the mass flow rate. This could be explained by the higher-pressure difference and higher flow coefficient. The pressure increases faster in the smallest tanks even if it has lower mass flowrate when compared to the other tanks, this may be related to the low volume, as in small volume tanks the pressure increases more than in bigger tanks for the same amount of gas injected, ad

to the lower flow coefficient, which consents more mass flowrate to pass with a smaller pressure difference. It can also be noted that the temperature at the start is higher in the smallest size tank, due to the fastest compression, but by the end of the refuelling, it is the biggest tank the one with the highest temperature. This may be caused by the combined effects of the higher mass flow rate and the lower ratio of the internal surface over volume of the largest tank. This represents a first limiting factor when deriving the protocols, as the biggest tanks limit the refuelling speed. On the other hand, the state of charge (SOC) within small tanks increases faster than in bigger tanks, meaning that the smaller tanks will reach the maximum SOC earlier during the refuelling, thus imposing the premature end of the refuelling to avoid over pressures, even if the overall SOC is lower than 100%.

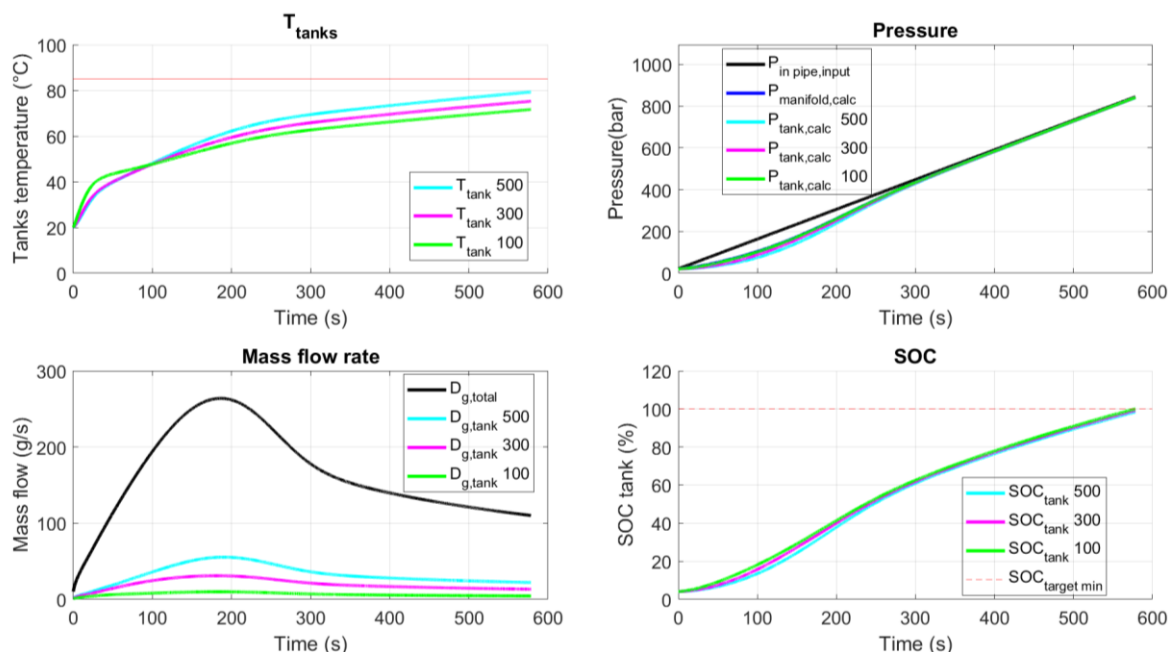


Figure 3 – Results of the refuelling simulation considering different tank sizes (light blue 500 l, pink 300 l, green 100 l) during the simulation. On the top left graphs presents the gas temperature inside the tank. On the right there the pressure is represented at different points of the station, in black is the pressure at the outlet of the dispenser, in blue the pressure at the manifold and then the pressure in the different tanks. On the bottom the mass flow rate on the left (total in black) and the SOC of each tank on the right.

Conclusions

A new model capable of predicting the behaviour of vehicle storage systems composed by multiple heterogeneous tanks during the refuelling, has been developed. This model can give a clear insight on the thermodynamical evolution of the gas in the hydrogen storage tanks system that will be commonly used in heavy-duty vehicles. A refuelling simulation has been conducted to analyse the evolution of the thermodynamical variables during the refuelling of a 100 kg storage system capacity.

Some critical aspects have been identified, such as the limitation to reach the complete filling of the system without exceeding the maximum allowable SOC of smaller tanks, and the correlation between the maximum tank size and final gas temperature that limits the refuelling time in the derivation of the protocol parameters. The identified behaviour shows trends in the refuelling of HDVs storage systems that can only be predicted by simulating all the tanks. Another consideration is that protocols with communication will need to communicate to the station pressure and temperature of the vehicle that in case of multiple heterogeneous tanks is not unique. From this first analysis, it seems that the correct pressure sensor to use is the one in the smallest tank, to avoid over pressure, while the correct temperature sensor is the one in

the biggest tank, to avoid overheating. The model could be used in the future to better define the sensors position.

Further perspectives to the work here presented are the experimental validation of the model and the integration of the distributed pressure drops in the fuelling line and in the pipe sections between the manifold and the tanks, alongside with a more precise estimation of the heat transfer between the hydrogen and the vehicle piping system. Once validated the model could be used to derive filling protocols adapted to vehicles with different tank sizes. As the model also gives information on the performances of the stations in terms of complete refuelling, it can be foreseen that this tool could be used in to test or compare stations designs, for example in terms of the cooling power required.

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