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Limitations in the Hydrogen Refueling Process of Railway Vehicles

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Abstract

This paper outlines the process of refueling rail vehicles with hydrogen and explores the associated limitations affecting refueling time. For this purpose, simulation models of the refueling process in Dymola are set up. The dispenser of the refueling station, the flow resistances and the heat transfer of the tanks are abstracted and represented in these models. The simulated results are compared with measurement data from the refueling process of the demonstrator train from the FCH2Rail-project and thus validated. The validated model is used to vary various parameters in the refueling process and thus investigate different refueling concepts. It is shown that the temperature in the hydrogen tank in particular limits the refueling time with the given normative limits. The temperature in the tanks can be reduced through better heat transfer in the tanks, pre-cooling, active cooling or modularization and hybridization of the tank modules. Alternatively, the state-of-the-art normative limits for the temperature could be increased by selecting other material parameters in the tank.
Overall, it is shown that a refueling time of 15 minutes for rail vehicles with hydrogen is only possible with considerable process effort, such as pre-cooling.

Keywords: hydrogen, multiple unit, hydrogen refueling, high pressure, simulation, modeling

1 Introduction to hydrogen refueling for rail vehicles

In Europe, only 56% of railway lines are electrified. Conversely, this means that 44% of lines are not electrified and are mainly used by diesel-powered trains [1]. For environmentally friendly rail transport without local CO_2 emissions, hydrogen trains, are currently being used on non-electrified sections in many demonstration and research projects [2]. Such a hydrogen multiple unit is being developed and built as a prototype in the EU-project FCH2Rail (*Fuel Cell Hybrid Power Pack for Rail Applications*) and displayed in Figure 1.

The project is the first in which a hybrid, bi-modal drivetrain has been developed that can draw its electrical power both from the overhead line and from the power pack installed in the train. The power pack in the train is hydrogen powered and consists of fuel cells and batteries which enable catenary-free operation [3].

Figure 1: Demonstrator train (Renfe's Civia commuter unit) and hydrogen refueling station from FCH2RAIL-project

The hydrogen for operating the power pack is stored in the vehicle in gaseous state in pressurized tanks with a working pressure of 35 MPa. The hydrogen is fueled into the train via a prototype of a modular and portable hydrogen refueling station (HRS), which is being built by CNH2 together with Calvera as part of the project. The dispenser container of this HRS is also shown in Figure 1. During refueling, the hydrogen flows from the filling station's intermediate storage tanks into the vehicle tanks. Thanks to the modular design, both the internal storage modules and external storage modules like tube trailers can be used as intermediate storage. In the process, the hydrogen heats up due to the compression in the tanks and the negative Joule Thomson effect [4]. This creates a conflict of objectives between fast refueling and the maximum temperature in the tanks, as the temperature increases with a higher refueling speed.

For a safe refueling process, it must be ensured that a maximum temperature of 85°C is not exceeded. This is defined by the SAE J2601-2 refueling standard [5]. Limits for the hydrogen mass flow of 120 g/s and the maximum pressure in the vehicle storage system of 43,8 MPa are also specified. The pressure level of 43,8 MPa refers to a state at 85°C and a density of 24 g/L. This density corresponds to a state-of-charge

(*SoC*) of 100% at the nominal storage pressure of 35 MPa and a temperature of 15°C. The SoC of 100% is another limitation for the hydrogen storage as no over fueling may occur. During refueling, it is necessary for safety reasons that the system limits shown are adhered to at all times. These system limits for the 35 MPa pressure tanks are shown graphically in Figure 2. Overall, refueling times of 15 minutes are targeted for the commercial operation of hydrogen rail vehicles in local rail passenger transport.

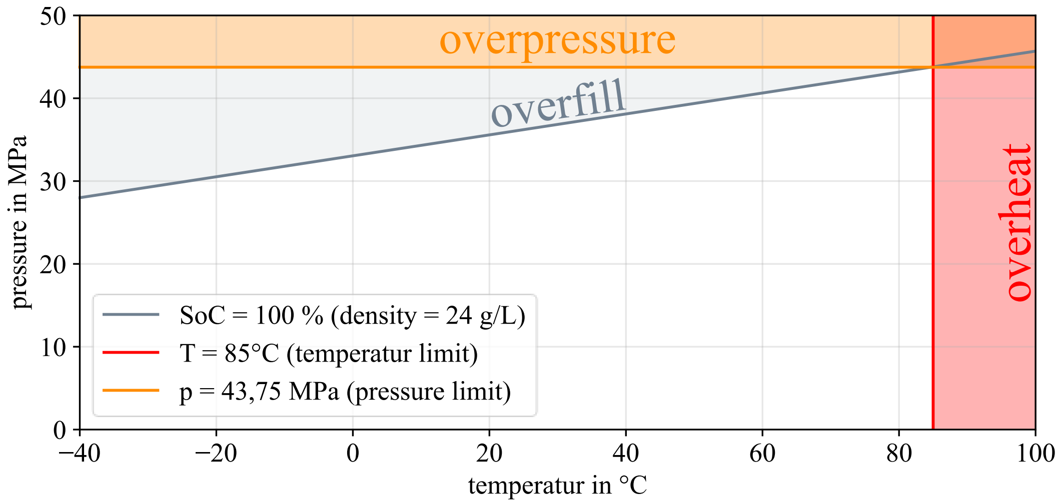

Figure 2: Temperature and pressure limits for a 35 MPa hydrogen refueling process according to SAE J2601-2 (changed presentation of [5])

In order to comply with these and more specifications, the refueling process was examined in more detail in this publication. Models were set up and simulations of the refueling process were carried out to identify the limiting factors for refueling in rail vehicles. The structure of the models and simulations as well as the identified limitations of the refueling process are presented in the following chapters.

2 Methodical approach for modeling the refueling process

Various modelling approaches were considered for the creation of the simulation models. The modelling activities for hydrogen refueling can be divided into different methodologies. In addition to CFD analyses (*computational fluid dynamics*) and the development of thermodynamic models (e.g. H2Fills [6]), the refueling process has also been investigated using machine learning methods since 2020. Genovese et al [7] provide a detailed summary of research activities on hydrogen refueling in their review published in 2023.

It should be noted that most studies focus on 70 MPa storage technology and low hydrogen capacities of less than 10 kg per vehicle. The reason for this is that the focus of these studies is mostly on passenger cars. The refueling of rail vehicles, which often use 35 MPa storage technology with hydrogen capacities of over 150 kg per vehicle, has been investigated less.

To create the simulation models, the refueling process and the components involved must be abstracted. For this purpose, an abstraction level was selected which identifies the components which have an influence on the refueling process (see Figure 3). The state of the hydrogen in the dispenser at the filling station serves as one boundary condition for the refueling process. This is followed by breakaway, hose, receptacle, piping and valves. The flow resistance of all these components can be summarized in a single flow resistance K_V. Finally, the state of the hydrogen in the tank is determined, which also depends on its geometry and the heat transfer with the environment.

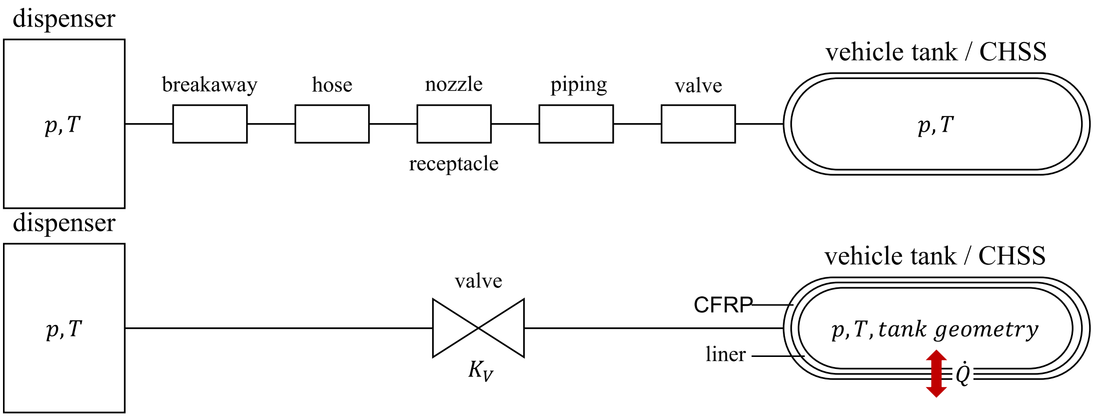

Figure 3: Abstraction levels of the hydrogen refueling process and the involved components (changed presentation of [8])

There are two main approaches to model the abstracted refueling process shown in Figure 3. A distinction is made between lumped-parameter or CFD models. Compared to a CFD model, a lumped-parameter model is characterized by a significantly faster computing time. However, it should be noted that the computing time is accompanied by a lower resolution of the system. Spatial effects, such as the temperature distribution in the vehicle tank, are not considered. The temperature determined in the vehicle tank is available as a scalar. A CFD analysis, on the other hand, makes it possible to resolve the problem in the three spatial directions so that, for example, temperature fields in the vehicle tank can be analyzed. However, such a resolution of the system is very complex and involves a high computing time.

Due to the large number of planned parameter variations, a lumped parameter model was set up in the Dymola simulation environment (Modelica based) for this publication. The user interface of this model is shown in Figure 4.
The model essentially consists of the termination conditions (black), the fluid model including heat transfer (blue) and the system logic for control (red). In addition, a display of the simulation time is built into the simulation model (see Figure 4). The termination conditions are based on the limits presented in Figure 2. In the fluid model, the state of the hydrogen is calculated using real gas equations from the

External Media Library, which implements them from the open-source tool CoolProp [9].

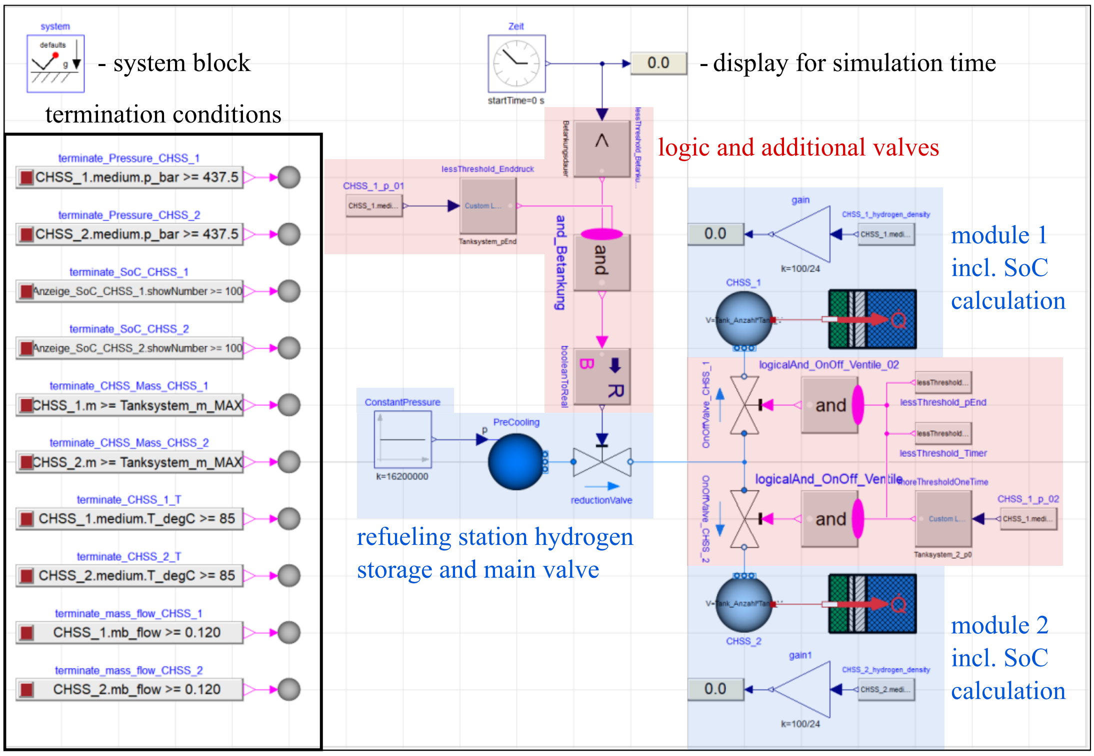

Figure 4: Surface of the main simulation model in Dymola

The sub- model for the heat transfer describes the heat exchange of the tank system with its environment and is shown in Figure 5. It consists largely of blocks from the "Thermal" library of the "Modelica Standard Library". Blocks from the "Modelica Buildings Library" [10] are also used to model the transient heat conduction in the tank wall.

The heat exchange of the tank system consists of a convective heat transfer between hydrogen and the inner tank surface, the (transient) heat conduction through the two-layer tank wall, the convective heat transfer between the outer tank surface and the room air as well as the thermal radiation of the outer tank surface. The areas in heat transfer are calculated for a single tank. In order to be able to use the heat transfer model for the tank system, these are multiplied by the number of individual tanks in the tank system.

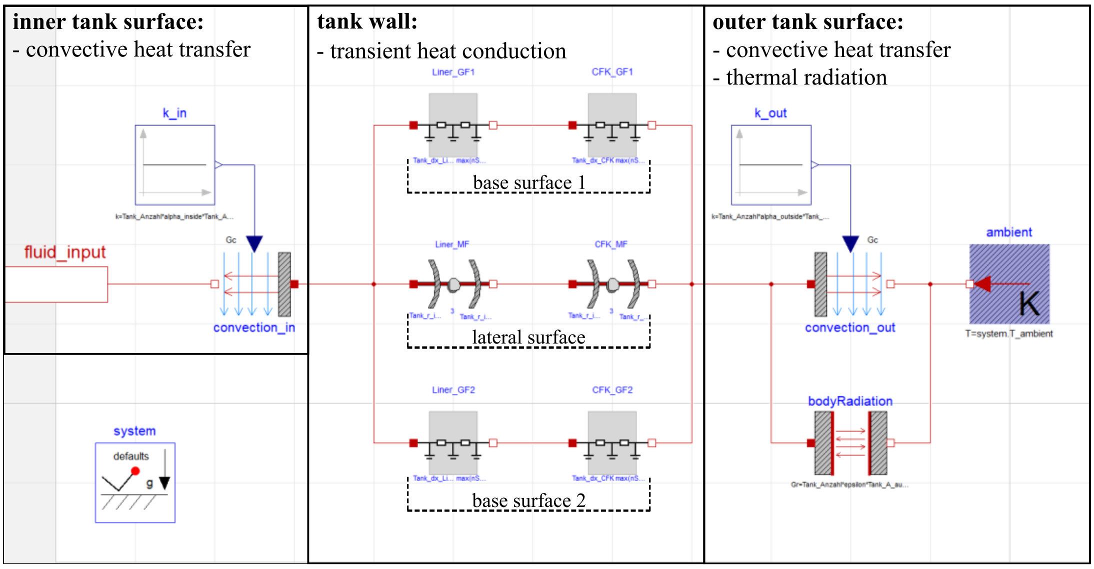

Figure 5: Surface of the heat transfer sub-model in Dymola

The tank system of the demonstrator train consists of a total of 4 tank modules, of which 2 are connected and refueled together. Each tank module in turn consists of 8 individual tanks, each with 5 kg of hydrogen and a nominal pressure of 35 MPa. These are type 3 tanks whose outer wall consists of an aluminum liner and a carbon fiber reinforced polymer layer (*CFRP*). The liner acts as a diffusion barrier for the hydrogen molecules, while the CFRP layer ensures the stability of the tank. The dimensions of the tanks and the heat transfer coefficients for the parameterization of the model are summarized in Table 1.

Table 1: Parameterization of the refueling model

Parameter tanks	Value	Source	Parameter heat transfer	Value	Source
Tank volume	0.205 m^3	[11]	CFRP specific heat	1120 J/(kg K)	[8]
Diameter of the tanks	0.396 m	[11]	Liner specific heat	1106 J/(kg K)	[8]
Length of the tanks	2.11 m	[11]	CFRP thermal conductivity	0.74 W/(m K)	[8]
Thickness of CFRP layer	0.01 m	[8]	Liner thermal conductivity	164 W/(m K)	[8]
Thickness of liner layer	0.005 m	[8]	CFRP material density	1494 kg/m^3	[8]
			Liner material density	2700 kg/m^3	[8]
			Inner heat transfer coefficient α_{in}	250 W/(m^2 K)	[12]
			Outer heat transfer coefficient α_{out}	10 W/(m^2 K)	[12]

Various refueling simulations are carried out with the models set up in order to identify the limiting factors for the refueling time. Based on literature research, the factors and concepts presented in Table 2 will be examined within parameter variations. The focus of the concepts is on the materials of the tanks, the overall hydrogen capacity, the average pressure ramp rate (*APRR*) of the refueling station, the resulting time-dependent curves of the hydrogen mass flow and the ambient and pre-cooling temperatures.

Table 2: Possible limiting factors of hydrogen refueling time

Factor	Influence on refueling process	Reference
Tank type and material	Material parameters of tank type influence heat transfer, e.g. aluminum liner for type 3 and polymer liner for type 4	[8]
Hydrogen capacity	Higher capacity leads to higher massflows	[13]
APRR	Higher APRR leads to higher temperatures	[14]
Hydrogen massflow	Different massflow curves lead to different temperature curves	[15], [16]
Ambient and pre-cooling temperature	Increased ambient and pre-cooling temperatures increase the hydrogen temperature in the storage	[7], [8]

In order to be able to investigate the various factors from Table 2 for the hydrogen refueling of rail vehicles, measurements of the refueling process are carried out in addition to the simulations. Measurement data is recorded both in the vehicle and at the HRS.

The data recorded in the vehicle are the temperatures in the individual tanks and the pressures in the individual tank modules. The SoC is also recorded, which is calculated based on the pressures and temperatures. At the HRS, the hydrogen pressure, temperature and mass flow are measured in the dispenser. The ambient temperature is also recorded as a measured value. The recorded measurement data is compared with the results of the model simulations in order to evaluate and validate them.

3 Results of model validation and limiting factors for the refueling process

To validate and evaluate the models presented in the previous section, the calculated simulation results were compared with the measured data. The comparison of dispenser pressure in simulation and measurement is shown in Figure 6. The measured pressure at the dispenser is shown in red. The dots mark measured values every 10 seconds. The increase in pressure during the refueling process is clearly visible. This takes place in 4 cascades in Figure 6. These are caused by the structure of the connected tube trailer, as different storage sections of the trailer are used during the refueling process. As soon as the pressure in one section has dropped due to the overflow into the vehicle tanks, the next cascade is switched on for overflow into the vehicle tanks. Certain outliers in the measurement data can also be seen, which are probably caused by electro-magnetical interference in the measurement system. However, as this only relates to very few points, the measurement data quality is still sufficient to be used as input for the simulation models. The simulation data fitted to the measurement data is shown as a blue curve Figure 6 and used as input for the refueling process in the simulation models. It is important to note that the refueling processes investigated and measured here are prototype refuelings used to validate the thermodynamic models and do not reflect the targets for refueling time in the FCH2RAIL-project.

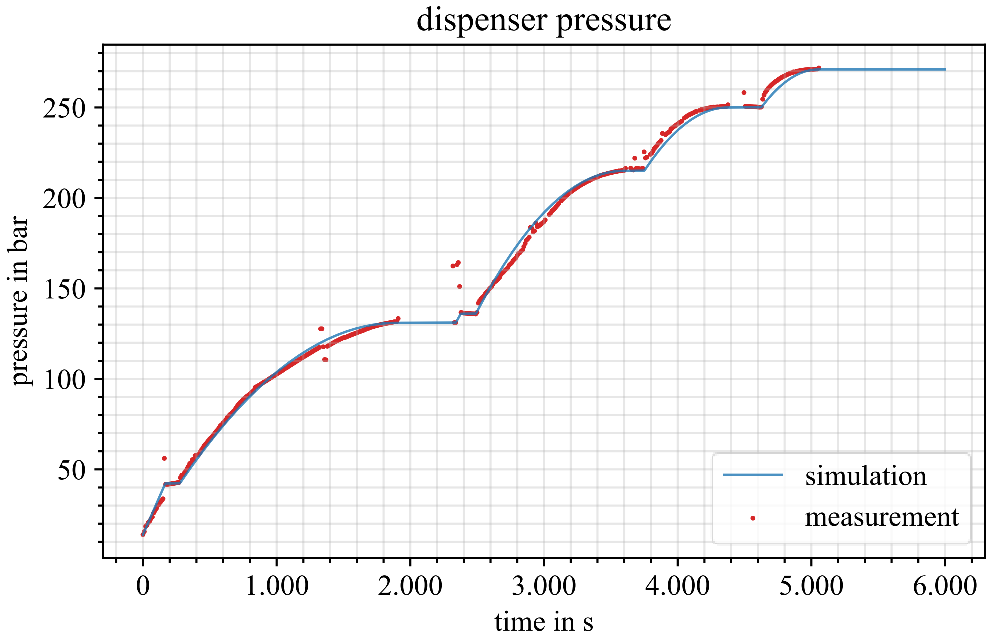

Figure 6: Dispenser pressure in the simulation and measurement from the 28th November 2023

The hydrogen mass flow into the vehicle is set from the pressure specification of the HRS, which causes the pressure and temperature rise in the vehicle tank. The calculation of those values is the relevant indicator for validating the simulation model. As an example, the relative deviations between the calculated and measured temperature and pressure in the vehicle tanks are shown in Figure 7 for the refueling process of Figure 6.

A very high relative deviation of 15% can be seen for the pressure curve, especially at the beginning, which, however, only represents small absolute deviations due to the low absolute pressure values at the start of refueling. In the further course of refueling, the deviation is rarely outside +- 3%. The temperature shows relative deviations of up to 4%. This behavior was also confirmed during validation in many other refueling processes. The deviations between measurement and simulation were always less than 5% for the temperature and always less than 15% for the pressure in the vehicle tank. The temperature is always overestimated so that the model is a conservative modeling approach for determining the temperature.

All in all, this represents a sufficient accuracy for the selected lumped-parameter approach, meaning that the simulation model has been validated. It is therefore suitable for investigating the approaches presented in Table 2 for limiting the refueling process.

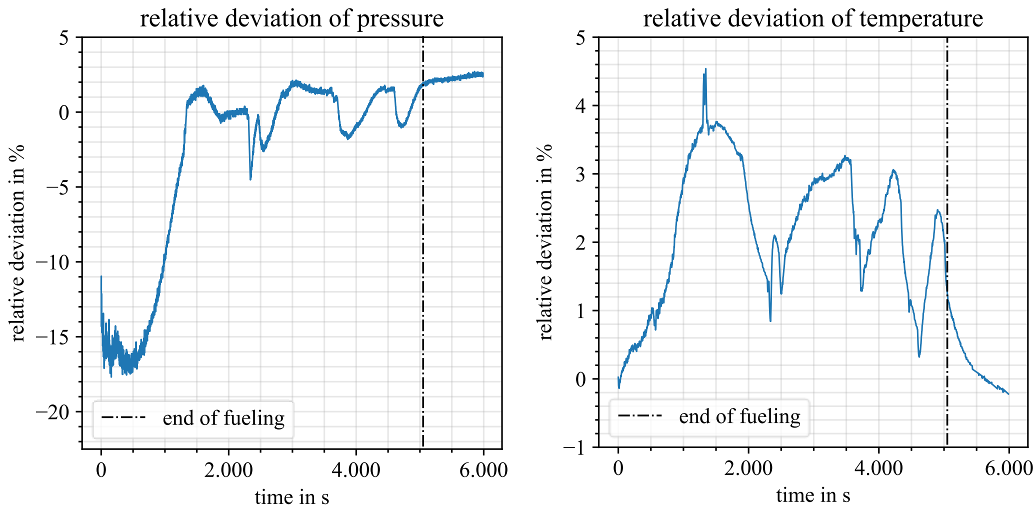

Figure 7: Relative deviation of pressure and temperature between simulation and measurement data

Parameter variations were carried out with the validated simulation models in order to investigate the limiting factors for the refueling time. The parameters hydrogen capacity, APRR, hydrogen mass flow, ambient and pre-cooling temperatures and tank type as described in Table 2 were varied.

The variation of the hydrogen capacity shows that the refueling time increases with the capacity. Modularization of the tank system brings advantages here if several dispensers are available and different module can be refueled in parallel. When looking at the APRR, it becomes apparent that steeper linear pressure ramps increase the refueling speed, whereby the hydrogen temperature in the vehicle tanks also increases. If a progressive pressure ramp is selected instead of the linear pressure ramp as shown in Figure 8, the refueling time is extended and the tank heats up considerably towards the end of refueling.

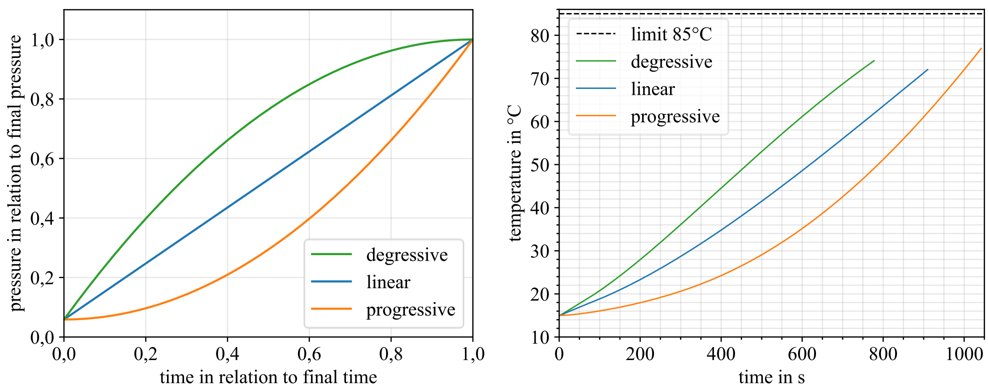

Figure 8: Progressive, linear and degressive pressure ramp rates (left) and temperature during the refueling (right)

A degressive pressure ramp is suitable for implementation here, as it rises sharply at the beginning of the refueling process and flattens out towards the end. This means that lower refueling times are calculated in the simulation model compared to the linear characteristic curve. The degressive characteristic curve results in a high mass flow at the start of refueling, which also has a positive effect on the refueling time when the mass flows are varied.

The investigations also show how sensitive the hydrogen refueling time reacts to ambient temperatures and pre-cooling. If these temperatures are decreased, the refueling time can also be reduced. Table 3 shows refueling at -10°C, 15°C and 30°C for tank systems with type 3 and type 4 tanks and a total capacity of 160 kg of hydrogen. The 160 kg are divided into 2 modules of 80 kg each, which are refueled individually. The refueling time for the modules increases from -10°C to 30°C to almost 3 times the value. The modules were refueled in such a way that a maximum hydrogen temperature of 85°C and a SoC of 100% was reached but not exceeded. A starting pressure of 60 bar was selected for refueling. The investigations show that the ambient temperature, the pre-cooling temperature of the hydrogen and the temperature limit in the tank are limiting factors for the refueling time.

However, the effects of these factors can be influenced by the choice of tank materials, which can be seen in the variation of tank types. Modules with type 3 tanks can be refueled faster due to the higher thermal conductivity of the aluminum liner compared to the polymer liner in type 4 tanks, if the same temperature limit is applied. Table 3 shows that the refueling time of type 4 modules is 26% to 39% longer, depending on the ambient temperature. A hybrid tank system consisting of type 3 and type 4 tanks represents a compromise here. If, for example, half of the tanks are designed as type 3 and the other half of the tanks as type 4, the refueling times in the column on the right in Table 3 can be expected. When hybridizing, however, the system weight must be taken into account, as type 4 tanks are lighter than type 3 tanks. The use of both tank types in the same vehicle therefore produces a tank module that is lighter than a pure type 3 system and can be refueled faster than a pure type 4 system.

Table 3: Simulated refueling time for a storage with 160 kg* of hydrogen capacity under variation of ambient temperature ϑ_{amb}, pre-cooling temperature ϑ_{PC}, start temperature $\vartheta_0$and tank types

	Type 3	Type 4	Hybrid
Refueling time for $\vartheta_{amb}, \vartheta_{PC}, \vartheta_0 = -10°C$	13.5 min (± 0%)	17.1 min (+ 26.1%)	15.3 min [a] (+ 13.1%)
Refueling time for $\vartheta_{amb}, \vartheta_{PC}, \vartheta_0 = 15°C$	21.9 min (± 0%)	29.5 min (+ 34.7%)	25.7 min [a] (+ 17.3%)
Refueling time for $\vartheta_{amb}, \vartheta_{PC}, \vartheta_0 = 30°C$	36.2 min (± 0%)	50.4 min (+ 39.1%)	43.3 min [a] (+ 19.6%)

* sequential refueling (2 x 80 kg) with a starting pressure of 60 bar

[a] calculated using the refueling time for 80 kg of type 3 and type 4 tanks

Overall, it can be seen that a refueling time of 15 minutes for hydrogen rail vehicles can only be achieved with considerable cooling effort. The energy costs of this effort must be clearly weighed against the benefits of faster refueling. If the fastest possible refueling is to be achieved, the following recommendations must be observed:

- Use of type 3 tanks
- Modularization and simultaneous refueling of several independent tank systems
- Maximization of the average mass flow and the fastest possible increase in mass flow at the start of refueling
- Refueling with maximum pre-cooling (-40°C)
- Refueling at the lowest ambient temperature
- Cooling the tanks (active cooling at outer surface and/or lowering the initial temperature of the tanks)
- Increasing the hydrogen gas temperature limit
- Setting a component temperature limit instead of a hydrogen gas temperature limit

4 Conclusions

The hydrogen refueling process for rail vehicles has so far been less studied than the refueling process in passenger cars due to the large quantities of hydrogen involved. The refueling time is an important factor for the operation of hydrogen rail vehicles precisely because of the high quantity of hydrogen. This refueling time is mainly limited by the thermodynamic behavior of the hydrogen in the refueling process. To overcome these limiting factors, either the process control in the refueling station or the material parameters of the tanks in the vehicle can be adapted. In the filling station, a rapid increase in the mass flow through the pressure ramp rate must be achieved. In addition, the temperatures in the tanks must be kept as low as possible or the temperature limits of the corresponding standards must be increased in order to refuel as quickly as possible. This was determined both in measurements and simulations as part of the FCH2Rail-project. By further recording measurement data in the test operation of the demonstrator train, further findings on reducing the refueling time are to be collected in the future in order to ensure a safe and fast refueling process with hydrogen rail vehicles.

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References

[1] A. Chamaret, P. Manney, P. Clément, J. Ernst and H. Flerlage, "Analysis, trends and expectations for low carbon railway," *Transportation Research Procedia,* 2023.

[2] M. Böhm, A. Fernández Del Rey, J. Pagenkopf, M. Varela, S. Herwartz-Polster and B. Nieto Calderón, "Review and comparison of worldwide hydrogen activities in the rail sector with special focus on on-board storage and refueling technologies," *International Journal of Hydrogen Energy,* pp. 38003-38017, 2022.

[3] H. Dittus, "FCH2RAIL project: First hydrogen train on the Spanish railway network," Clean Hydrogen Partnership, 2023. [Online]. Available: https://www.fch2rail.eu/en/projects/fch2rail.

[4] R. Caponi, A. Monforti Ferrario, E. V. G. Bocci and M. Della Pietra, "Thermodynamic modeling of hydrogen refueling for heavy-duty fuel cell buses and comparison with aggregated real data," *International Journal of Hydrogen Energy,* 2021.

[5] SAE International, "SAE J2601-2: Fueling Protocol for Gaseous Hydrogen Powered Heavy Duty Vehicles," 2023.

[6] T. Kuroki, K. Nagasawa, M. Peters, D. Leighton, J. Kurtz, N. Sakoda, M. Monde and Y. Takata, "Thermodynamic Modeling of Hydrogen Fueling Process from High Pressure Storage Tanks to Vehicle Tank," *International Journal of Hydrogen Energy,* 2021.

[7] M. Genovese, V. Cigolotti, E. Jannelli and P. Fragiacomo, "Hydrogen Refueling Process: Theory, Modeling, and In-Force Applications," *Energies,* 2023.

[8] A. Charolais, F. Ammouri, E. N. Q. Vyazmina, T. S. C. D. Guewouo, A. Ruiz, L. Gambone, A. Grab, S. Quong and S. Darvish, "Deliverable D4.1 - Report on Preliminary Simulations," *PRYHDE,* 2020.

[9] I. H. Bell, J. Wronski, S. Quoilin and V. Lemort, "Pure and Pseudo-pure Fluid Thermophysical Property Evaluation and the Open-Source Thermophysical Property Library CoolProp," *Industrial & Engineering Chemistry Research,* 2014.

[10] W. Wetter, W. Zuo, T. Nouidui and X. Pang, "Modelica Buildings library," *Journal of Building Performance Simulation,* 2014.

[11] Luxfer Gas Cylinders, "Specification Tables (W205H35)," 2024. [Online]. Available: https://www.luxfercylinders.com/specifications/.

[12] M. Monde, P. Woodfield, T. Takano and M. Kosaka, "Estimation of temperature change in practical hydrogen pressure tanks being filled at high pressures of 35 and 70 MPa," *International Journal of Hydrogen Energy,* 2012.

[13] M. Greisel and M. Gebhard, "Technical Report: Minimum Ambient Precooling (MAP) Hydrogen Refueling Protocol for 35MPa Heavy Duty Vehicles (20-42.5 kg)," *Clean Energy Partnership (CEP)*, 2022.

[14] M. Striednig, S. Brandstätter, M. Sartory and M. Klell, "Thermodynamic real gas analysis of a tank filling process," *International Journal of Hydrogen Energy*, 2014.

[15] SAE International, "SAE J2601: Fueling Protocols for Light Duty Gaseous Hydrogen Surface Vehicles," 2020.

[16] Q. Li, J. Zhou, Q. Chang and W. Xing, "Effects of geometry and inconstant mass flow rate on temperatures within a pressurized hydrogen cylinder during refueling," *International Journal of Hydrogen Energy*, 2012.