

Hydrogen as Fuel – Storage System Simulation in Ultra-Heavy-Duty Applications

Enrico Pasquini*, Filipp Kratschun** and Heiko Baum*

FLUIDON Gesellschaft für Fluidtechnik mbH, Jülicher Straße 338a, D-52070 Aachen, Germany*

NPROXX B.V., Business Trade Center Heerlen Vogt 21, 6422 RK Heerlen, The Netherlands**

E-Mail: info@fluidon.com

Hydrogen as fuel plays a major role in decarbonization of heavy and ultra-heavy duty mobile applications. The energy density of hydrogen and the possibility to quick refuel large amount of hydrogen and, therefore, large amount of energy within a short period of time are the main reasons why hydrogen is a key solution within that specific field of use. In the presented paper main challenges for hydrogen storage systems are presented. A strategy how to cope with these challenges is elaborated and applied to an ultra-heavy duty real world storage system.

Keywords: Hydrogen, Alternative fuel, Fuel cell, Joule-Thomson coefficient, System simulation, Fuel supply, DSHplus, Tank, Conference, Energy management – Hydrogen technology Sustainability assessment,

Target audience: Mobile Applications, Hydrogen Handling, Simulation

1 Introduction

In March 2021, the then minister president of the German state of North Rhine-Westphalia called for Germany to become the world's number one hydrogen country [1]. This national declaration of intent reflects a global trend: while the bulk of the world's hydrogen output is still used for the production of ammonia (mostly fertilisers) and in fuel refining, its use as an emission-free fuel has moved into the focus of cutting-edge research and industry. Regardless of whether it is so-called “green” (i.e. produced with renewable energies) or conventionally produced hydrogen – there are always some special features to be taken into account when using H_2 as a fuel. Carrying larger quantities of hydrogen in vehicles without temperature regulation equipment requires hydrogen to be stored in high-pressure tanks. Due to these high pressures, hydrogen does not behave like so-called *ideal* gases at all. The prominent non-ideal behaviour of hydrogen can cause some unforeseen phenomena to occur in the actual system if they are not properly accounted for during the design phase.

One of the problems arising from this circumstance is the heating up of hydrogen due to pressure drops at resistances (e.g. valves). This is a particular issue for mobile applications since the efficiency of fuel cells drops significantly if the hydrogen they receive is too hot. The temperature rise due to throttling is also a technical barrier when the speed at which hydrogen can be transferred from a reservoir to a vehicle tank is to be increased: If the hydrogen entering the vehicle's tank is already preheated due to throttling, the additional temperature rise within the tank due to compression may exceed temperature thresholds of the thermoplastic diffusion barrier (“liner”) or the CFRP matrix of the pressure vessel. This could lead to reduced life time, increased permeation or leakage of the vessel. Hence, the maximum mass flow rate and thus the required time for refuelling a hydrogen tank is determined by the fluid's temperature rise. Another problem in the context of real gas properties of hydrogen is the determination of the tank content: At the pressure levels typically encountered, a hydrogen tank contains significantly less gas than an estimation based on ideal gas behaviour would suggest.

The present work aims to raise awareness of the above-mentioned problems within the fluid-power engineering community. For this purpose, the essential phenomenological differences between ideal and real gases are elaborated. By introducing the Joule-Thomson coefficient, it is explained why real gases experience a temperature

change at flow restrictions and why this effect does not occur for ideal gases at all. It is also shown why the actual amount of hydrogen stored in a pressurised fuel tank is smaller than the theoretically expected amount.

The practical significance of these phenomena for real hydrogen fuel systems is demonstrated by simulating two real-world examples with the fluid-power analysis software suite DSHplus. The examination of the temperature changes after passing a pressure regulator and the analysis of the filling of a hydrogen tank system illustrate how engineers profit from taking real gas effects into account during the design phase of hydrogen fuel systems. The higher level of detail in the simulation enables the development of measures such that tanks can be filled faster and fuel cells can be operated at a higher efficiency.

Finally, values and equations are provided which can be used for rough estimation of the key real gas effects of hydrogen fuel supply systems. The presented material enables the design engineer to judge whether hydrogen needs to be modelled as a real gas for a particular application.

Currently there are two possible ways to use hydrogen as fuel in heavy duty applications: Fuel cell (FC) and inner combustion engine (ICE). In both applications the storage system consists typically of type 4 vessels connected with valves and pipework leading to a pressure regulator, wherein the tank pressure of 350 bar or 700 bar is reduced down to about 10 bar for a FC application or 30 bar for an ICE application. The technical challenges arising from such a system architecture are the following:

- 1) Fuelling the storage system results in a temperature increase in the type 4 vessels. The quicker the fuelling the higher the temperature. If a certain temperature threshold is exceeded the vessels can be damaged leading to hydrogen leakage or even a vessel disintegration.
- 2) Defueling the storage system i.e., providing hydrogen to FC or ICE causes the temperature in the tanks to drop below a threshold which can also damage the vessel.
- 3) Dynamic interaction between either FC or ICE and the storage system may lead to unexpected high or low pressure at the FC or ICE due to fluidic oscillation within the system.
- 4) Hydrogen at pressure levels of up to 1000bar and the given temperature ranges (-40°C - 85°C) cannot be modelled as ideal gas.
- 5) Calculating a hydrogen storage system “by hand” is rather difficult since in comparison to a diesel tank it consists of multiple vessels with multiple valves and pipes.

The paper is structured as follows to present how to tackle with the challenges listed above: In the second section the thermodynamic background of hydrogen modelling is provided, and a juxtaposition of real and ideal gas is presented. In the third section a system simulation approach by DSHplus is depicted to emphasize how a complex multi-component hydrogen system can be calculated. Section four presents a simple system simulation mainly consisting of a vessel to validate the chosen approach which is validated with experimental results. In section five a real defueling and fuelling process of an Ultra Heavy-Duty application is simulated and compared to test results. A conclusion and a brief outlook of the paper are given in chapter six.

2 Thermodynamic Background

Since most of the problems outlined above arise from thermodynamic phenomena, the underlying fundamentals are briefly reviewed. First, the thermodynamic concept of the thermal equation of state is discussed.

2.1 Thermal Equation of State

If the geometric volume of a tank is known, the mass of hydrogen contained within the vessel can be calculated based on the fluid's density ρ . For a given medium, the relationship between density ρ , thermodynamic

temperature T and pressure p is given through a substance-specific function known as its *thermal equation of state* (EOS).

2.1.1 EOS of an Ideal Gas

The behaviour of many actual gases can be described with sufficient accuracy using the model of an ideal gas. An essential property of ideal gases is that the volume (“co-volume”) of the gas atoms (monatomic gases) or gas molecules (polyatomic gases, e.g., H_2) is negligibly small compared to the volume occupied by the gas. Furthermore, it is assumed that there are no attracting intermolecular forces between the gas atoms/molecules. It can be shown that such a gas obeys the following EOS:

$$\rho = \frac{p}{RT} \quad (1)$$

In the equation above, R refers to the mass-specific gas constant of the respective gas (for hydrogen: $R = 4124 \text{ J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$). This simplified EOS is in good agreement with the behaviour of the actual gas under the following conditions [2]:

- The pressure p is significantly smaller than the critical pressure of the gas (for hydrogen: $p_{\text{crit}} = 13 \text{ bar}$)
- The temperature T is significantly larger than the critical temperature of the gas (for hydrogen: $T_{\text{crit}} = -239.95 \text{ }^\circ\text{C}$)

2.1.2 Compressibility Factor

Even though the model of an ideal gas is useful for many applications (e.g., aerodynamic analysis of commercial subsonic aircraft), its usability is limited for hydrogen supply systems since pressure levels considerably higher than the critical pressure are commonly encountered. Hence, one must resort to more complex EOS which consider the volume of the gas molecules and their interaction, so-called *real gas effects*. A simple and phenomenologically oriented approach is to use the *compressibility factor* (compression factor, gas deviation factor) Z which is defined as follows [2]:

$$Z = \frac{p}{\rho RT} \quad (2)$$

The compressibility factor can be interpreted as a measure by how much the thermal state of an actual gas deviates from what would be expected if it behaved like an ideal gas (i.e., the deviation from eq. 1). Hence, for an ideal gas, the compressibility factor is always equal to unity. For actual gases, the compressibility factor is a fluid-specific function of two state variables, e.g., pressure and temperature.

With respect to the tank filling problem outlined above, the inverse of the compressibility factor provides the ratio of the actual gas content m and the content m_{id} of its “ideal” counterpart at a given pressure and temperature level:

$$\frac{1}{Z} = \frac{\rho}{\rho_{\text{id}}} = \frac{m}{m_{\text{id}}} \quad (3)$$

The mass ratio is plotted against the tank pressure level for three different temperatures in **Figure 1**. As can be seen, for a tank charged with 1000 bar and kept at ambient temperature, the mass ratio roughly equals 0.6. This value indicates that the hydrogen mass contained in the tank is less than 60 % of what would be expected based on the assumption of an ideal gas behaviour. Based on these results, the real-gas properties of hydrogen must be considered during a filling simulation in order to obtain reasonable results that reflect the real-world situation.

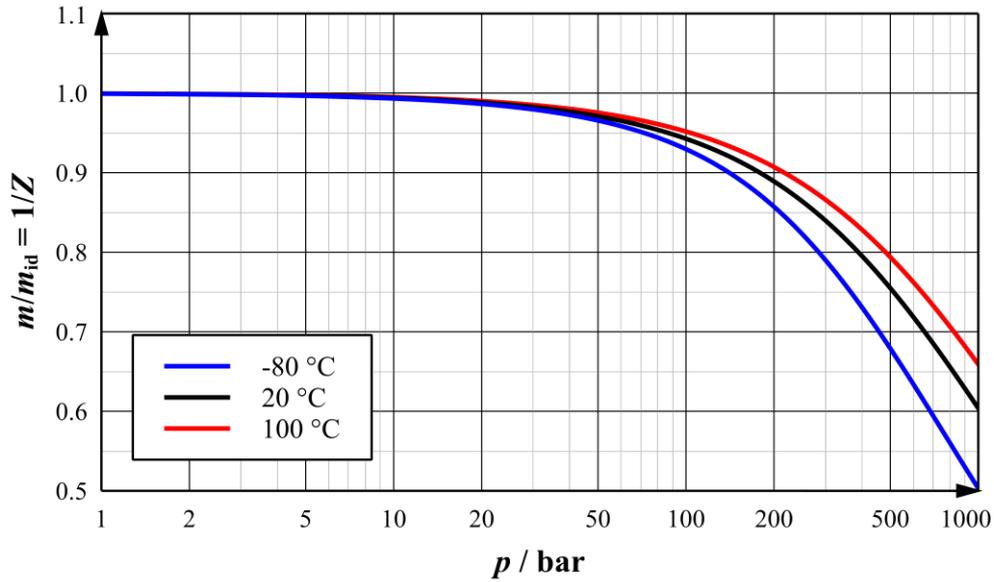


Figure 1: Ratio of actual and “ideal” mass of hydrogen contained in a tank as a function of pressure and temperature [3].

2.2 Isenthalpic Throttling Process

Unlike in the case of liquid flow, pressure losses in gaseous media lead to strong changes in temperature and density: Often, a pronounced heating or cooling of the flowing medium can be observed at valves or other flow resistances. For many technical flows, the heat exchange between the fluid and the environment is negligible compared to the viscous losses at the resistive element. Such a situation corresponds to the thermodynamic concept of an isenthalpic steady flow, i.e., the mass-specific enthalpy h of the fluid remains unchanged across the resistor. Based on this simplification, the temperature changes due to a pressure drop $\Delta p = p_{\text{In}} - p_{\text{Out}} > 0$ can be calculated.

2.2.1 Joule-Thomson Coefficient

In thermodynamics, the ratio of temperature change dT to pressure change dp for isenthalpic flow is known as the *Joule-Thomson coefficient* μ_{JT} :

$$\left(\frac{\partial T}{\partial p}\right)_h = \mu_{\text{JT}} \quad (4)$$

The Joule-Thomson coefficient of a medium can be expressed in terms of its other thermophysical fluid properties [4]:

$$\mu_{\text{JT}} = \frac{1}{\rho c_p} \left[\frac{1}{v} \left(\frac{\partial v}{\partial T}\right)_p - 1 \right] = \frac{T\gamma_p - 1}{\rho c_p} \quad (5)$$

In the equation above, γ_p denotes the isobaric thermal expansion coefficient (relative change of volume per temperature change at constant pressure), whereas c_p represents the mass-specific isobaric thermal capacity. Both quantities – as well as the density – depend on the pressure and temperature levels the medium is exposed to. Consequently, the Joule-Thomson coefficient is a function of these state variables as well, i.e., $\mu_{\text{JT}} = \mu_{\text{JT}}(p, T)$.

2.2.2 Temperature Change

If the Joule-Thomson coefficient is known, the temperature changes $dT = T_{\text{Out}} - T_{\text{In}}$ due to a pressure drop Δp across a resistor can be calculated. Keeping in mind that a positive pressure drop $\Delta p = p_{\text{In}} - p_{\text{Out}} > 0$ corresponds to a negative pressure change $dp = p_{\text{Out}} - p_{\text{In}} < 0$, one obtains the following relation:

$$T_{\text{Out}} = T_{\text{In}} + \mu_{\text{JT}}(p_{\text{Out}} - p_{\text{In}}) = T_{\text{In}} - \mu_{\text{JT}}\Delta p \quad (6)$$

Hence, for a medium with a positive Joule-Thomson coefficient, a pressure drop across a resistor cools the liquid, whereas a negative μ_{JT} would lead to a temperature rise. This phenomenon is known as the *Joule-Thomson effect*.

For an ideal gas, the product of temperature and thermal expansion coefficient is always exactly equal to unity, i.e., the Joule-Thomson coefficient for such a medium is zero. In this case, the temperature rise due to dissipation is exactly countered by the temperature drop due to expansion. Consequently, a pressure drop across a resistance would *not* change the temperature of the flowing gas if its enthalpy were kept unchanged.

Since the thermal expansion coefficient of actual gases is typically also of the order of T^{-1} , the product $T\gamma_p$ is often close to unity as well. Hence, the sign of the Joule-Thomson coefficient may be subject to change, depending on the exact functional relationship $\gamma_p(p, T)$.

2.2.3 Joule-Thomson Effect in Hydrogen

In order to estimate the strength and direction of the Joule-Thomson effect in hydrogen, the corresponding coefficient is plotted as a function of pressure and different temperature levels in **Figure 2**. It can be seen that the Joule-Thomson coefficient of hydrogen stored in high-pressure tanks is always negative. This implies that the flow through e.g., a pressure regulator in a hydrogen supply system will always lead to a temperature rise of the fluid. As a general trend, the heating up of hydrogen due to isenthalpic throttling gets stronger at higher pressures and higher temperatures – irrespective of the actual pressure drop. Only if the hydrogen is stored at very low temperatures and small pressures, a positive μ_{JT} (i.e., a cooling of the fluid) is experienced at resistances.

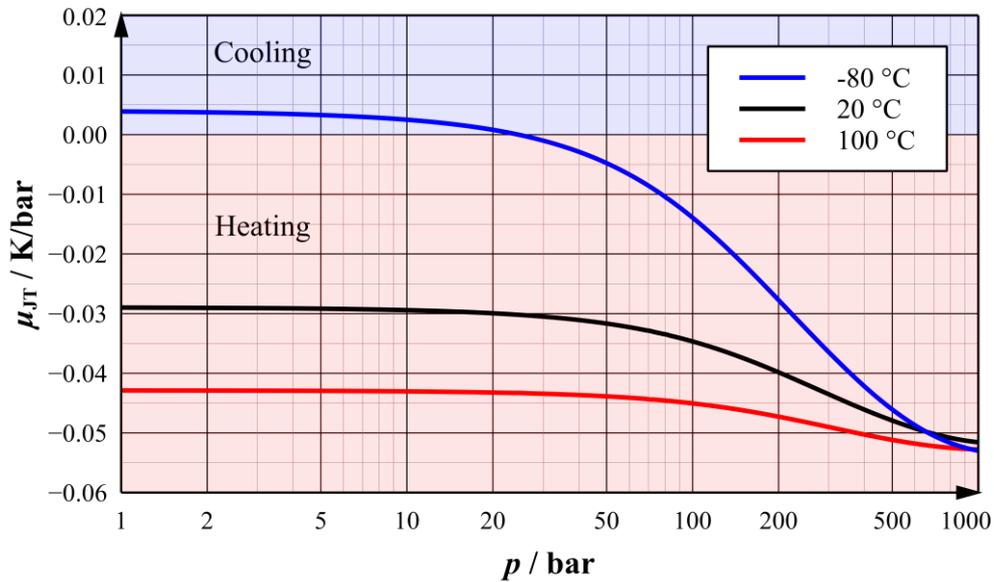


Figure 2: Joule-Thomson coefficient of hydrogen as a function of pressure and temperature [3].

2.2.4 Consideration of Changes in Kinetic Energy

Equation 6 can only be used for the calculation of the downstream temperature if the (mass-specific) kinetic energy $u^2/2$ of the flowing medium is negligible with respect to its enthalpy, i.e., the difference between its enthalpy h and its total enthalpy $h_t = h + u^2/2$ is small. If velocity changes are to be included, the temperature change is given as follows:

$$T_{\text{Out}} = T_{\text{In}} - \mu_{\text{JT}}\Delta p + \frac{1}{2c_p}(u_{\text{in}}^2 - u_{\text{out}}^2) \quad (7)$$

Thus, even a thermally perfect gas with $\mu_{JT} = 0$ might undergo a noticeable temperature change in an isenthalpic flow across a resistor, if the downstream and upstream fluid velocities differ significantly. For real hydrogen, however, the temperature change arising from differing kinetic energies is typically negligible with respect to the Joule-Thomson effect due to its large thermal capacity of $c_p \approx 14300 \text{ J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$.

2.3 Isentropic Compression

When analysing the temperature rise during the charging of a hydrogen tank, the assumption of a lossless and adiabatic process provides a conservative estimate. A change of state where friction and heat transfer do not occur implies a constant entropy s , which is why such a process is referred to as *isentropic*. For isentropic compression (or expansion), the ratio of temperature change per pressure change is given by the following expression:

$$\left(\frac{\partial T}{\partial p}\right)_s = \frac{T\gamma_p}{\rho c_p} = \mu_{JT} + \frac{1}{\rho c_p} \quad (8)$$

As can be seen, the temperature rise due to isentropic compression can be expressed through the same thermophysical fluid properties like the Joule-Thomson coefficient. For a thermally perfect gas with constant thermal capacity, it can be shown that the expression above is only a function of the heat capacity ratio (ratio of specific heats) $\kappa = c_p/c_v$ and the current values of temperature and pressure:

$$\left(\frac{\partial T}{\partial p}\right)_s = \frac{T}{p} \frac{\kappa - 1}{\kappa} \quad (9)$$

By separation of variables, this ODE for the temperature can be integrated with respect to pressure. If one denotes the state variables at the beginning of the compression (or expansion) with the index “Init”, the following expression is obtained:

$$T(p) = T_{\text{Init}} \left(\frac{p}{p_{\text{Init}}}\right)^{\frac{\kappa-1}{\kappa}} \quad (10)$$

However, for the practically relevant case of a real gas, the situation is not as straightforward. Even if – for sake of simplicity – a constant thermal capacity c_p is assumed, a closed-form solution for the temperature development during isentropic compression cannot be derived since the density and the thermal expansion coefficient depend on the compressibility factor Z and its derivative:

$$\left(\frac{\partial T}{\partial p}\right)_s = \frac{T\gamma_p}{\rho c_p} = \frac{RT}{pc_p} \left[Z + T \left(\frac{\partial Z}{\partial T}\right)_p \right] \quad (11)$$

Hence, even for the simplified quasi-static analysis of real-gas phenomena, one must resort to numerical software in order to solve the relevant equations. If – as it is most often required – the transient behaviour (e.g., pipe vibrations) or the interaction (e.g., heat transfer) of the involved components should be considered as well, the use of sophisticated simulation tools such as DSHplus is mandatory.

3 Simulation Environment DSHplus

DSHplus is a simulation environment specialised in the dynamic, non-linear calculation of complex fluid-power systems and components.

3.1 1D-CFD vs. 3D-CFD

As a representative of the class of so-called 1D-CFD software, DSHplus closes the gap between lumped-parameter (“0D”) models and elaborate 3D-CFD simulation tools. 1D-CFD tools offer the advantage of easy model set-up and small computational effort while still providing high-quality results comparable to expensive and time-consuming 3D-CFD simulations. Due to the reduced numerical complexity of 1D models, a design engineer can

analyse transient changes in the operation condition of a whole hydrogen supply system in just one simulation run on a standard desktop PC.

3.2 Program Features

To ease the model set-up for the user, DSHplus offers an extensive drag-and-drop library of pipes, valves, resistors, special components (e.g., tanks) and fluids. The most sophisticated pipe models solve the conservation equations of mass, momentum and energy efficiently by combining the Method of Characteristics with a Finite-Difference Scheme. The piping library covers the following physical effects and phenomena:

- Joule-Thomson effect (temperature change due to isenthalpic throttling).
- Dissipative heating of the fluid due to friction
- Pressure- and temperature-dependent fluid properties based on an extensive fluid library
- Steady and unsteady pipe friction (increase of pressure loss due to unsteady flow)
- Convective heat transfer fluid → pipe → environment and vice versa
- Compliant pipe walls and hoses which alter the effective fluid stiffness
- Fluid-structure interaction (bending, torsion, longitudinal stress)

The outlined features make DSHplus a popular choice for...

- Verification of system function
- Analysis of system dynamics
- System revision and re-engineering
- Component selection and design
- Fault diagnosis
- Training purposes

The potential which simulation with DSHplus offers for the analysis of hydrogen supply systems is illustrated by practical examples.

4 Practical Examples

Two common engineering problems associated with hydrogen supply systems are examined by means of numerical simulation. A process which is of particular interest to design engineers in the field of hydrogen supply systems is the filling of tanks.

4.1 Filling of a Hydrogen Tank

Due to the thermal issues outlined above, the filling rate of a tank is limited by the temperature rise in the liner and CFRP layers. Simulating a filling process aids the design engineer in choosing a suitable tank filling strategy: If the simulation shows that the desired filling rate (i.e., refuelling time) would lead to unacceptable temperatures in the tank wall, potential mitigation strategies (e.g., precooling of the hydrogen) can directly be tested and evaluated in terms of their effectiveness. In order to perform the analysis, a simulation model must be set-up.

4.1.1 DSHplus Simulation Model

A suitable DSHplus simulation model to conduct such an investigation is depicted in **Figure 3**.

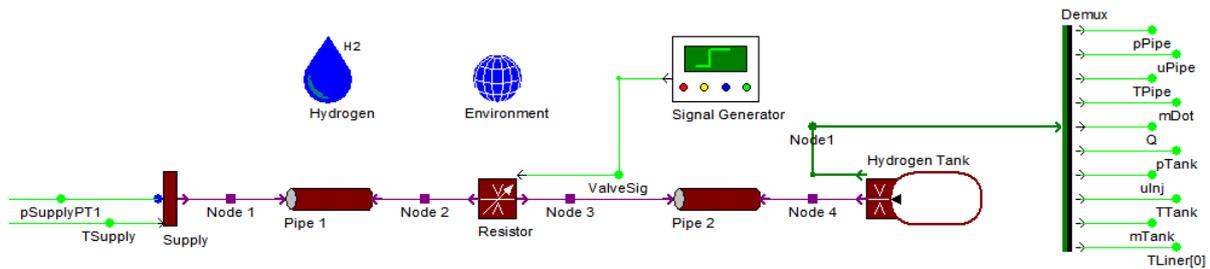


Figure 3: DSHplus simulation model for the analysis of the filling of a hydrogen tank.

This minimal working example for the problem of tank wall heating consists of the following elements:

- Component “Hydrogen” – This element provides the simulation model with the pressure- and temperature-dependent fluid properties of hydrogen.
- Component “Environment” – This element provides the simulation model with the ambient temperature required for calculating the convective heat transfer between tank or pipe walls and the environment.
- Boundary Component “Supply” – This element represents the hydrogen supply reservoir and provides the adjacent pipe with boundary conditions for pressure and temperature level. In our example, the respective values are directly read from a measurement data file. To reduce the impact of measurement imperfections, the pressure values read from the file are smoothed by using a first-order lag element (“PT1”).
- Components “Pipe 1” and “Pipe 2”: These elements represent the piping system which connects the individual constituents of the hydrogen supply system. The pipes are characterised by their length, inner diameter, wall thickness and material properties.
- Component “Resistor” – This element represents an adjustable valve. This component is used to expose the tank to the supply reservoir pressure or to cut it off it after the filling is completed.
- Component “Signal Generator” – This element provides the resistor component with the current valve stroke (0 – 100 %). The valve stroke may be a function of time.
- Component “Hydrogen Tank” – This element represents a hydrogen tank. The model of the hydrogen tank itself features several sub-components:
 - On-tank valve
 - Injector
 - Gaseous tank content
 - Liner layer
 - CFRP layer
- Component “Demux” – This element enables the user to access internal variables of the tank component. Thus, values like the fluid velocity at the injector exit u_{Inj} , the temperature of the inner surface of the liner $T_{Liner}(0)$ or the mass of the tank content m_{Tank} can be analysed.

4.1.2 Detailed Description of the Tank Model

In order to represent the non-linear discharge behaviour of the on-tank valve, the component is modelled as a compressible resistor (formula of de Saint-Venant and Wantzel): If – for a given upstream pressure – the downstream pressure is lowered below a certain value, the flow rate across the resistor will not increase further (“choking”).

The gaseous tank content is modelled as a real gas which exchanges heat with its environment, i.e., the liner layer. The gas temperature rises if the rate at which enthalpy enters the tank with the flow supersedes the heat flux to the liner and vice versa.

For the design engineer to be able to analyse the temperature distribution within the temperature-sensitive pipe wall materials, both the liner and the CFRP are modelled as continuous media with distributed thermal capacities and thermal conductivities. The resulting energy equations for both domains are solved through a Finite Volume Scheme.

The heat transfer between the inner side of the liner material and the gaseous tank content is modelled through a heat transfer coefficient. The value of this coefficient greatly depends on the flow situation within the tank: During the filling process, hydrogen is injected into the tank at a high velocity through the injector pipe. The impacting hydrogen jet induces a strong mixing of the tank content, thus enhancing the heat transfer between tank content and liner (forced convection). However, after the filling has been completed, the tank content is almost at rest. In this case, the only remaining macroscopic movement of gas particles within the tank is due to local temperature differences, so-called natural convection. Compared with the filling process, this leads to a greatly reduced heat transfer coefficient.

The heat transfer between the outer surface of the CFRP layer and the environment is modelled through a heat transfer coefficient as well. Here, it is assumed that this heat transfer is always governed by natural convection, i.e., externally induced flow fields due to e.g., ventilators are not considered.

4.1.3 Description of the Filling Process

Before the start of the simulation ($t < 0$), the resistor valve is closed. Thus, the pressure levels of pipes 1 and 2 are independent of each other. Whereas pipe 1 is exposed to the pressure from the supply reservoir (initial gauge pressure $p_g \approx 515$ bar), pipe 2 shares the pressure level of the tank content (initial gauge pressure $p_g \approx 17.5$ bar). At $t = 0$, the valve is opened, thus establishing hydraulic communication between the reservoir and the tank. Due to the pressure difference, a flow from the reservoir to the tank is initiated, leading to an increase of the tank pressure. After the tank has reached the desired pressure level (i.e., a particular state of charge), the valve is closed again at $t \approx 220$ s.

4.1.4 Results & Discussion

The results of the simulation run are plotted in **Figure 4**. The graph shows the development of the (gauge) pressures and temperatures of both the supply reservoir and the tank under investigation. Experimentally determined values are shown as dashed curves, whereas the simulation results are presented as solid curves.

As can be seen, the opening of the valve at $t = 0$ (and thus the loss of hydrogen mass in the reservoir) leads to a sudden drop in the supply pressure level. The pressure drop in the pressure-regulated reservoir causes a compressor to start up which attempts to restore the initial pressure level through compression of the remaining hydrogen. The compression of hydrogen within the reservoir leads to a noticeable increase of the reservoir temperature. Achieving the initial pressure level through compression is hampered by the fact that hydrogen is continuously leaving the reservoir. Only after the filling of the tank has stopped at $t \approx 220$ s, the compressor is able to slowly return the reservoir to its initial pressure level. During the filling process, the pressure level in the tank rises due to accumulation of hydrogen mass and subsequent compression. As can be seen, the simulated and measured tank pressures are virtually indistinguishable, indicating that the discharge behaviour of the on-tank valve and other resistive elements was modelled properly.

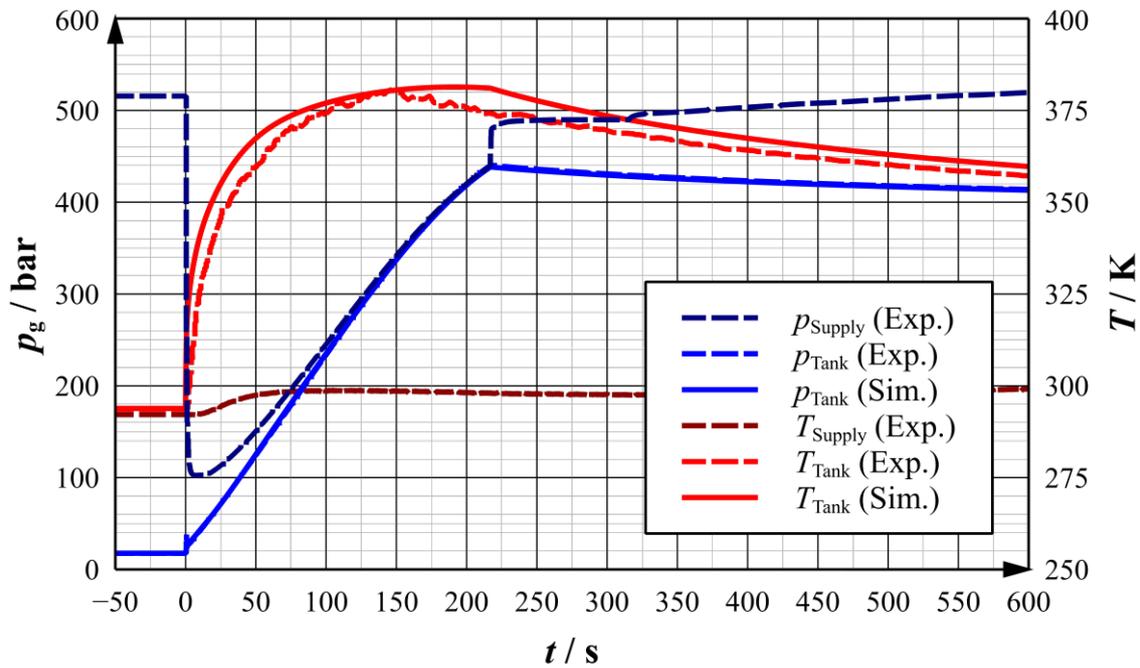


Figure 4: Measured and simulated gauge pressures and temperatures for the charging process.

The simulated tank temperature deviates visibly from the measured value, even though the agreement is still acceptable for engineering purposes. The observed deviations arise from two independent factors: Firstly, the temperature of the gaseous tank content is not spatially uniform, i.e., there is a temperature distribution within the tank. Depending on the sensor position, the measured gas temperature might vary significantly, whereas the tank model assumes a lumped gas mass of uniform temperature. Secondly, the simulated temperature of the gas content is strongly affected by the heat transfer to the tank wall. Since simplified strategies were used to calculate the internal (gas \leftrightarrow liner) and external (CFRP \leftrightarrow environment) heat transfer coefficients, the simulated heat transfer rates will differ from the actual ones.

5 System Simulation for an Ultra-Heavy-Duty Application

A real-world use case where the model of isenthalpic throttling can be applied is the flow through a pressure regulator of a hydrogen supply system. The pressure regulator ensures that the high-pressure hydrogen stored in the tanks can be fed to fuel cells an acceptable pressure level.

5.1 DSHplus Simulation Model

The simulation model of the hydrogen supply system under investigation is depicted in **Figure 5**.

The system consists of four hydrogen storage tanks, each with a nominal capacity of 340 l each. The four tanks are connected through a manifold consisting of pipes and T-junctions. Attached to the manifold is a pressure regulator which is set to a target (gauge) pressure of 10 bar on the low-pressure side. The downstream port of the pressure regulator is connected to the fuel cell through a pipe (“Pipe 13”).

Other than the element already introduced and described in section 4.1.1, the DSHplus model consists of the following component models:

- Component “Closed End” – This boundary element provides the simulation model with the condition of a closed pipe end.
- Component “Outlet” – This boundary element provides the simulation model with the mass flow rate (“mDotOutlet”) consumed by the fuel cell.

- Component “Sum” – This element is used to calculate the deviation “dp” of the actual pressure on the downstream end of the pressure regulator (“pLow”) from the respective target (gauge) pressure (“pLowTarget”).
- Component “PIDT1 Controller” – This simple controller element is used in conjunction with an adjustable resistor (“Pressure Regulator”) to dynamically represent the pressure regulator under investigation. Based on the value of “dp”, a suitable value of the “ValveOpening” (ranging from 0 to 100 %) is calculated.

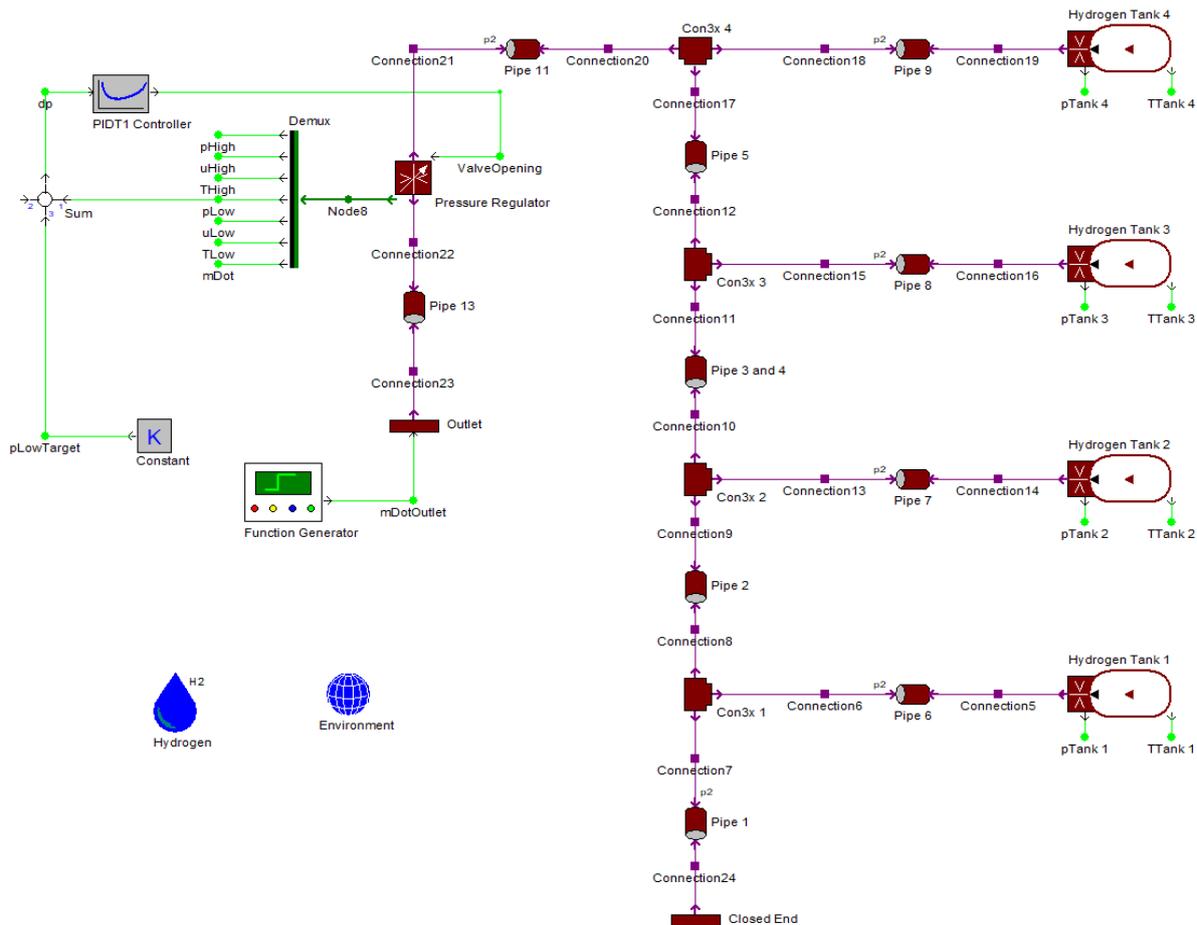


Figure 5: DSHplus model for the analysis of the temperature change across the pressure regulator of a hydrogen supply system.

5.2 Results System Discharging

The experimental set up is chosen such way, that the output mass flow rate is controlled to constant value of 5.6 g/s. Pressure inside the main high-pressure line, which connects the vessels as well as temperature inside the vessels is measured. The initial pressure in the tanks is roughly 390 bar and the temperature is roughly 70°C. The simulation results in comparison to test results are shown in Figure 6.

It is apparent that simulated pressure, mass flow rate as well as temperature match the test results very well and therefore this approach is suitable to calculate a defueling process of hydrogen storage system.

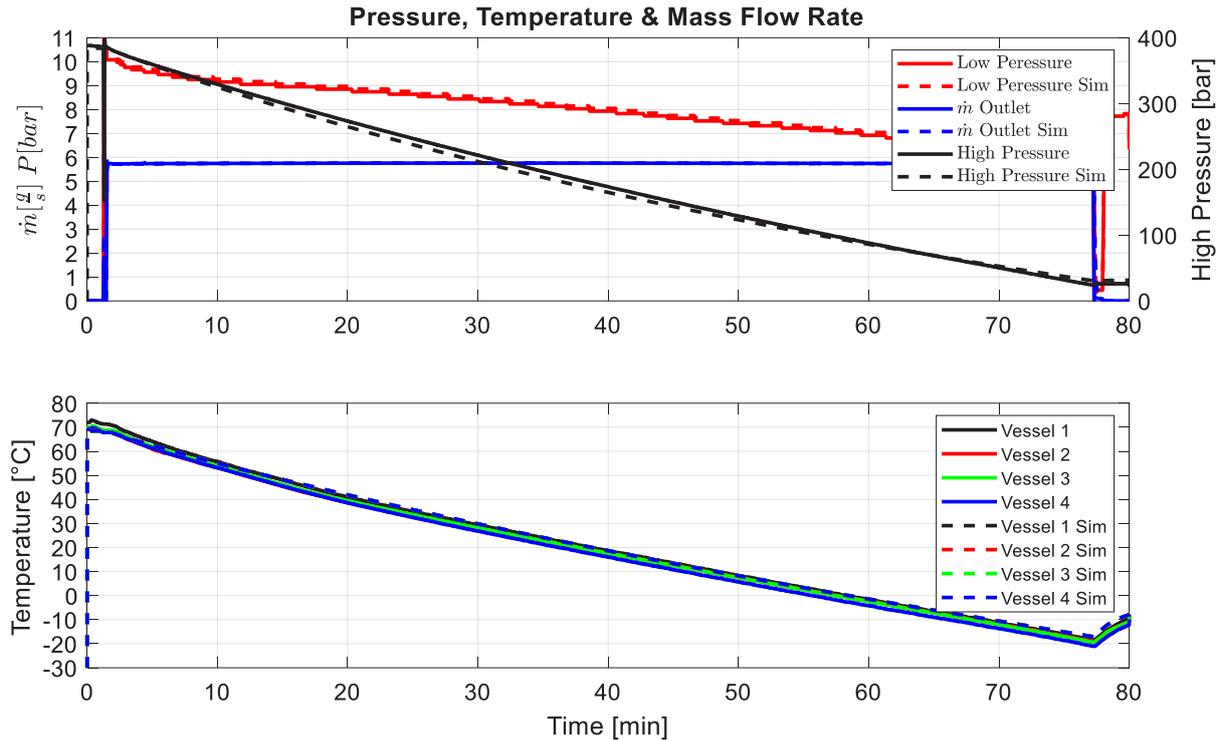


Figure 6: Simulation and measurement results system defueling.

5.3 Results System Fuelling

Fuelling of the system was carried out with -10°C precooled hydrogen at an environment of 20°C . The mass flow rate entering the system is measured. Moreover, temperature in each vessel as well as in the high-pressure line connecting the vessels is measured as well. The results are depicted in the figure below.

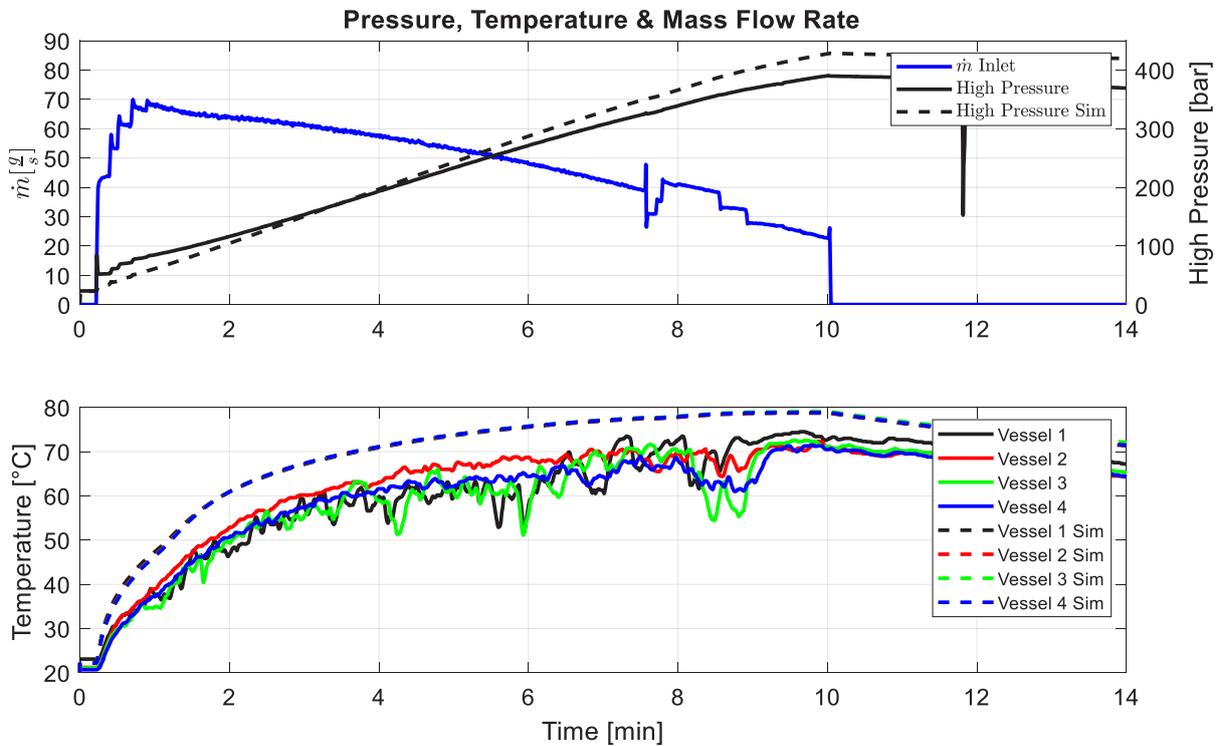


Figure 7: Simulation and measurement results system fuelling.

For the fuelling process the deviation in the temperature as well as in pressure is greater than for the case of defueling. The deviation in pressure can be explained with an erroneous and noisy mass flow rate signal, since the pressure in the system is strongly connected to the mass flow rate entering the system. However, a deviation of roughly 20 bar and 10°C indicates that also for the fuelling process the simulation approach is suitable and gives accurate results.

6 Summary and Conclusion

The transformation of CO₂ emitting engines into emission-neutral drives is one of the major challenges of the 21st century.

Using hydrogen as fuel poses several challenges to the fuel supply system design engineer. As has been demonstrated, the throttling of high-pressure hydrogen down to pressures acceptable for e.g., fuel cells is associated with a strong heating of the medium. Another associated problem is the heating of hydrogen due to compression, e.g., in tanks or cooling down due to expansion. Since many components of hydrogen systems (e.g., diffusion barriers) or their performance (e.g., fuel cells) are highly temperature-sensitive, it is imperative to consider thermal aspects at an early stage of the design process. Due to the pronounced non-ideal behaviour of hydrogen and a complex multi-component storage system, the use of numerical system simulation is mandatory. As could be demonstrated through two practical real-world examples, the 1D-CFD simulation approach by the software DSHplus offers a suitable environment to successfully perform thermal analyses and the subsequent design reiterations.

Nomenclature

<i>Variable</i>	<i>Description</i>	<i>Unit</i>
γ_p	Isobaric thermal expansion coefficient	K ⁻¹
κ	Heat capacity ratio	1
μ_{JT}	Joule-Thomson coefficient	K·Pa ⁻¹
ρ	Density	kg·m ⁻³
c_p	Mass-specific heat capacity at constant pressure	J·kg ⁻¹ ·K ⁻¹
h	Mass-specific enthalpy	J·kg ⁻¹
h_t	Mass-specific total enthalpy	J·kg ⁻¹
m	Mass	kg
\dot{m}	Mass flow rate	kg·s ⁻¹
p	Thermodynamic pressure	bar
R	Mass-specific gas constant	J·kg ⁻¹ ·K ⁻¹
s	Mass-specific entropy	J·kg ⁻¹ ·K ⁻¹
T	Thermodynamic temperature	K
u	Area-averaged fluid velocity	m·s ⁻¹
v	Mass-specific volume	m ³ ·kg ⁻¹
Z	Compressibility factor	1

References

- [1] N, N., *CDU startet Arbeit an Wahlprogramm - Laschet will "Aufbruch"*, In: reuters.com, <https://www.reuters.com/article/deutschland-cdu-laschet-idDEKBN2BM15V>, visited on March 16th, 2022.
- [2] Baehr, H. D. and Kabelac, S.: *Thermodynamik – Grundlagen und technische Anwendungen*, 14th corrected edition, Springer Verlag, Heidelberg, Germany, 2009.
- [L] Lemmon, E. W., Bell, I. H., Huber, M. L. and McLinden, M. O., *Thermophysical Properties of Fluid Systems*, In: NIST Chemistry WebBook, NIST Standard Reference Database Number 69, Eds. P.J. Linstrom and W.G. Mallard, National Institute of Standards and Technology, Gaithersburg MD, 20899, <https://doi.org/10.18434/T4D303>, (retrieved March 16th, 2022).
- [4] Knoche, K. F. and Bošnjaković, F.: *Technische Thermodynamik Teil 1*, 8th corrected edition, Steinkopff Verlag, Darmstadt, Germany, 1998.