MONO-DIMESIONAL MODEL VALIDATION OF FAST FILLING HYDROGEN TANKS WITH AND WITHOUT PRE-COOLING

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ABSTRACT

Drivers are accustomed to swiftly refueling their vehicles with traditional liquid and gaseous fuels such as gasoline, diesel or natural gas in a matter of minutes. Similar expectations are now extended to the emerging technology of hydrogen-powered vehicles. The demand for a reasonably quick refueling time presents a new challenge, as the rapid compression of hydrogen inside the tank, for instance, from low pressure to 700 bar, poses a risk to the mechanical properties of the tank material by elevating its temperature. Consequently, the majority of international standards and regulations specify a typical maximum allowable temperature inside tanks, at 85º C.

Furthermore, as the temperature rises, the gas density decreases, resulting in a reduced volume of gas that can be accommodated within the tank. To address the challenge of elevated temperatures, a technological solution, known as pre-cooling, has been conceived to lower the gas temperature before it enters the tank, employing a heat exchanger.

A zero-dimensional (0D) model has been created to evaluate the temperature evolution inside hydrogen tanks during different filling configurations and validated against experimental data and 3D model results.

1 INTRODUCTION

The transition to alternative fuels is strongly needed to reduce greenhouse gas emissions from mobility and to deplete non-renewable energy sources (Sandaka and Kumar 2023). Among these options, hydrogen emerges as a standout candidate due to its high energy density per unit mass, positioning itself as a central component of future energy landscapes. Particularly in the transportation sector, hydrogen-powered fuel cell vehicles (FCVs) offer a compelling alternative to conventional oil-based cars. According to the Intergovernmental Panel on Climate Change report, the transport sector accounted for 23% of total CO2 emissions in 2020 and consumed 28% of the overall energy supply (Ralph and Roberto 2014), with cars and other passenger vehicles contributing by 40% to this emission load (Jean-Paul 2020).

However, the widespread adoption of hydrogen faces significant barriers, including challenges related to production, distribution, refueling infrastructure, and vehicle design (Tashie-Lewis and Nnabuife 2021). Despite these hurdles, if hydrogen production is sourced from renewable energy, hydrogen technologies hold important potential in mitigating key issues associated with energy production and consumption, such as greenhouse gas emissions, pollution, energy security, and sustainability (European Union 2023). Nevertheless, notable technological barriers still need to be overcome for the realization of a comprehensive "hydrogen economy" (Sherif, Barbir, and Veziroglu 2005; Tseng, Lee, and Friley 2005; Brandon and Kurban 2017). One prominent challenge, especially in the transport sector, lies in hydrogen storage, given its low density of 0.09 kg/m³ under standard conditions of temperature and pressure (Ross 2006). Addressing these storage limitations is crucial for the widespread deployment of hydrogen technologies and the realization of their potential benefits (Hassan et al. 2023; Langmi et al. 2021).

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Specific storage technologies are essential to achieve energy densities comparable to traditional liquid fuels like gasoline or diesel. Currently, the prevalent storage solution adopted by car manufacturers is compressed hydrogen storage (Maus et al. 2008; Rivard, Trudeau, and Zaghib 2019). This method involves storing gaseous hydrogen onboard the vehicle within fully wrapped carbon fiber-reinforced tanks. To achieve high hydrogen densities, the gas is stored under high pressures; hydrogen tanks with nominal working pressures (NWPs) of either 35 or 70 MPa are already available in the market (Barthelemy, Weber, and Barbier 2017). Typically, two types of liners are employed in these tanks: metal liners in type III tanks and polymer liners in type IV tanks (Hua et al. 2011; Cheng et al. 2023).
Reducing refueling times is essential to enhance the convenience of FCVs for consumers, making them more competitive in the automotive market. One of the technological challenges for the successful implementation of FCVs is to reduce refueling times to 3-4 minutes for passenger cars (FCH2 JU Governing Board 2014), which is in line with the technical objectives set by the United States Department of Energy (DoE) for light-duty fuel cell vehicles, aiming to achieve a refueling time of 3.3 minutes for a 5 kg hydrogen onboard storage system (DoE 2017). This objective necessitates progress in hydrogen refueling infrastructure (Aaron Isenstadt and Lutsey 2017), including enhancing the efficiency of hydrogen dispensers and expanding the availability of refueling stations. Moreover, advancements in onboard hydrogen storage systems and fuel cell technology could also help decreasing filling times while upholding safety and reliability standards. During refueling, the compression process leads to a rise in the gas temperature within the tank (Genovese et al. 2023). The ultimate temperature within the tank holds significance for both safety considerations (as the tanks are engineered to function within a range of -40°C to 85°C ("COMMISSION REGULATION (EU) No 406/2010 of 26 April 2010" 2010; "SAE J2579 Standard for Fuel Systems in Fuel Cell and Other Hydrogen Vehicles" 2023)) and the tank's capacity; higher temperatures at the same pressure result in lower gas density. Temperatures outside this range might affect the mechanical properties of the tank materials. The tank's capacity is assessed through the State of Charge (SOC), which denotes the percentage ratio between the hydrogen density inside the tank and its density at the Nominal Working Pressure (NWP) and 15°C (40.2 kg/m³ at 70 MPa NWP). The final temperature of the gas within the vessel directly impacts the tank's SOC, as elevated temperatures lead to decreased gas density and consequently reduce the overall amount of hydrogen in the tank post-filling.
In order to achieve efficient refueling while staying within acceptable temperature thresholds and ensuring satisfactory tank filling levels, the Society of Automotive Engineers (SAE) has implemented the SAE J2601 standard for hydrogen refueling protocols (Society of Automotive Engineers 2014). This standard utilizes a look-up table approach to direct refueling procedures. Variables such as ambient temperature, fuel delivery temperature, size, and initial pressure of the compressed hydrogen storage system (CHSS) determine the operational constraints, including the desired pressure and pressurization rate. The CHSS encompasses all elements constituting the primary high-pressure boundary for containing compressed hydrogen, which may include one or multiple tanks based on storage needs and vehicle design considerations.
Once validated, computational fluid dynamics (CFD) models play a crucial role in modeling hydrogen filling tanks, owing to their capability to accurately replicate the intricate flow and thermal processes inherent in the refueling process (Daniele Melideo et al. 2014a; Zheng et al. 2013; Cui et al. 2024; Daniele Melideo and Baraldi 2015; D. Melideo et al. 2019; 2017; Heitsch, Baraldi, and Moretto 2011; Ebne-Abbasi, Makarov, and Molkov 2024). Through CFD, various aspects of the filling procedure can be analyzed, encompassing gas flow dynamics, temperature distribution, thermal stratification, pressure fluctuations, and heat transfer phenomena within the tank materials. CFD simulations entail solving a series of differential equations, which are discretized and solved iteratively across a computational domain often comprising millions of grid points or elements. The computational time required for CFD simulations can indeed be substantial due to the complex nature of the fluid flow and thermal processes under consideration. In many cases, due to the considerable computational expenses associated with CFD simulations, simplified models are devised and applied; the majority of these reduced models predominantly focus on the thermodynamic state of on-board tanks (Bourgeois et al. 2017; Molkov, Dadashzadeh, and Makarov 2019; Hosseini et al. 2012; Bai et al. 2021; Ramasamy and Richardson 2020; Kuroki et al. 2018; Deng et al. 2023). Nonetheless, despite their comprehensiveness, these simplified models still entail certain limitations, such as the simulation of the thermal dynamics of high-

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pressure tanks in Hydrogen Refueling Stations (HRS) during filling, the assessment of the non-uniform distribution of hydrogen temperature within on-board storage tanks, and the computation of temperature differentials across materials within the on-board tank.
A zero-dimensional model has been developed using the AVL CruiseM commercial code to replicate the filling process of a 29-liter type IV tank. The results have been compared with prior CFD and experimental investigations (Daniele Melideo et al. 2014a), (De Miguel et al. 2016), and the model has been adopted to simulate the impact of varying inlet hydrogen temperatures. This study offers a comprehensive analysis of the filling process in compressed hydrogen tanks, providing insights into defining optimal filling strategies based on the desired State of Charge (SOC) and initial hydrogen temperature. While detailed examinations using CFD tools can assess pressure and temperature distributions during tank filling, the computational demand is significant. Hence, it proves advantageous to investigate final configurations that need optimization concerning temperature and filling strategy. Utilizing 0D tools, validated through experimental and CFD analyses, proves beneficial in exploring diverse geometries and tank arrangements to attain high filling rates and SOC.

2 ZERO-DIMENSIONAL NUMERICAL MODEL

The objective of the study is to analyze the temperature evolution inside the tank at different inlet temperatures and imposing a time dependent pressure profile at entrance of the tank. Gaseous hydrogen tanks come in various types, each designed to meet specific requirements in terms of pressure, storage capacity, weight, safety, and application. Type IV hydrogen tanks are high-pressure vessels designed specifically for storing compressed hydrogen gas. They are made of a composite material, typically a combination of carbon fiber and epoxy resin, which provides strength while keeping the weight relatively low compared to traditional metallic tanks (i.e. type III). The type IV classification refers to the tank's construction, where the hydrogen storage vessel is the innermost layer surrounded by layers of composite materials. These tanks are characterized by their lightweight nature, high strength, and resistance to corrosion. They are commonly used in hydrogen fuel cell vehicles and other applications where lightweight, high-pressure storage is required. Type IV tanks are favored for their superior safety characteristics, as the composite materials used in their construction offer better resistance to rupture or failure compared to metal tanks. Additionally, they provide efficient insulation, which helps to maintain the temperature of the stored hydrogen gas. Overall, type IV hydrogen tanks are integral components in hydrogen-powered vehicles and other applications, enabling the safe and efficient storage of hydrogen gas for various uses. A 29-litre type IV has been considered for this study and its main characteristic are reported in Table 1.

Table 1: Characteristic of modelled type IV tank

	TYPE IV tank
Storage volume [L]	29
Vessel mass	32.9
H2 Capacity (at 40.2 kg/m3) [kg]	1.16
External length [mm]	827
External diameter [mm]	279
Internal diameter [mm]	230

The examination of the filling process, considering various influential factors such as pressure increase and duration, has been explored through a zero-dimensional (0D) modeling approach, specifically employing the AVL CruiseM software. The primary characteristic of a 0D model utilized for simulating hydrogen tank filling lies in its simplification of the physical system into a single point or volume with uniform properties. The entirety of the hydrogen tank and filling process is condensed into a singular entity with consistent attributes, including temperature, pressure, and density. This simplification assumes that the system's behavior can be adequately described by average or representative values, without accounting for spatial variations within the tank.

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The 0D model employs mass and energy balance equations to depict the transfer of hydrogen into the tank during filling, considering inflow rates, variations in pressure and temperature, and heat transfer effects to forecast the evolution of system properties over time. A common assumption in 0D models for hydrogen tank filling is the ideal gas law, which relates pressure, volume, temperature, and the number of moles of gas, thereby simplifying the thermodynamic behavior of the hydrogen flow into the tank, while neglecting deviations from ideal gas behavior.

The model defines four volumes, each with related heat transfer among them: a hydrogen gas tank plenum with an initial temperature of 15°C, and three solid domains (liner, carbon fiber, and metallic flange) at an initial temperature of 18°C, as depicted in Figure 1. The pressure of 20 bar, as outlined in the SAE J2601 (SAE International 2016), is designated as the condition corresponding to an almost empty tank, and is chosen as the initial tank pressure. An external ambient temperature of 18°C is imposed for all simulated cases.

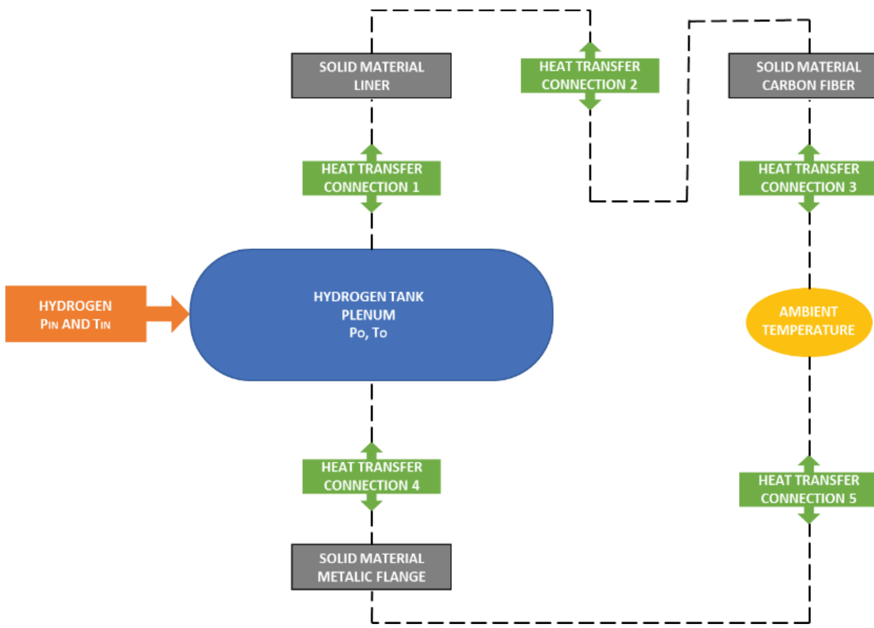

Figure 1: Zero-dimensional model set-up

3 ZERO-DIMENSIONAL MODEL VALIDATION

Model validation holds paramount importance in ensuring the accuracy, reliability, and effectiveness of simulation results and it verifies whether the simulation results align with real-world observations and data. In this study the 0D model was validated by comparing experimental data and CFD results (Daniele Melideo et al. 2014b). The temperature and pressure profile reported in Figure 2 have been imposed at the inlet of the tank. As already mentioned, the simulated tank is a 28-litre type IV, and the filling time is 200 s.

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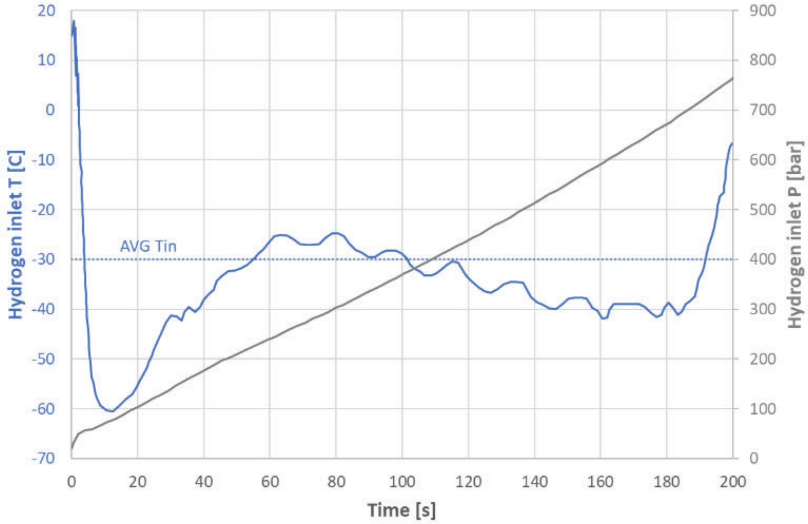

Figure 2: Imposed inlet hydrogen temperature and pressure profile over time

The comparison of average gas temperature profiles during the filling process is illustrated in Figure 3: the AVL CruiseM 0D model is depicted by the solid black line, while the black "x" symbols and the dashed line represent the CFD results and the experimental data, respectively. Additionally, results obtained using a 0D model generated with the H2FillS (T. Kuroki et al., n.d.) software tool are shown with the grey line. The temperature values predicted by the CruiseM 0D model closely match both the experimental and CFD data throughout the entire filling duration. However, the CruiseM 0D model tends to slightly overestimate the experimental values consistently across the simulation period, with the final temperature being 5°C higher than the experimental data. Conversely, while the H2FillS model does not accurately predict the initial pressure peak, it achieves a final gas temperature that closely aligns with the experimental data. An overestimation of the final temperature, despite aligning with experimental and CFD results, has to be considered as a conservative prediction. This conservatism offers a safety margin in estimations, compensating for any potential suboptimal conditions or uncertainties in the modeling process.

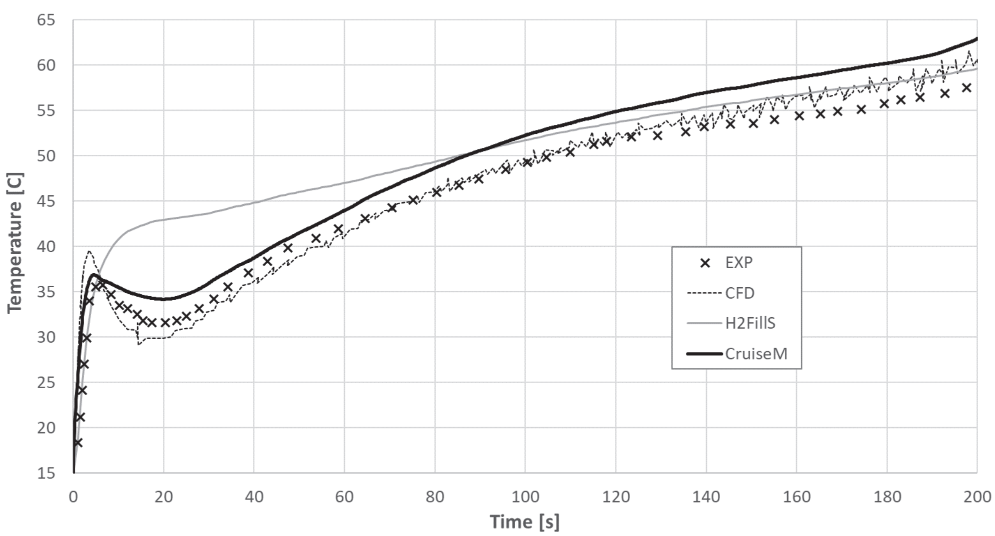

Figure 3: Average gas temperature during the filling, a comparison among OD models, CFD model and experimental data

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4 THE EFFECT OF DIFFERENT HYDROGEN INLET GAS TEMPERATURE FOR TYPE IV TANK

To evaluate the impact of varying inlet gas temperatures on tank temperature, four different scenarios were examined. Figure 4 illustrates the tank gas temperature profiles during filling corresponding to inlet hydrogen temperatures of 15°C, 0°C, -20°C, and -40°C. A comparison with CFD results (Daniele Melideo et al. 2014b) indicates that, similar to the previous case, the 0D model tends to overestimate the CFD results. Moreover, the discrepancy between the final temperatures calculated by the two models increases with higher inlet gas temperatures. These differences may stem from the geometrical approximations made in the 0D model, which could affect the precision of heat transfer predictions between the gas, the tank, and the ambient surroundings. Additionally, the CFD model can discern variations in temperature distribution within the tank and at different heights, influencing the internal mixing of zones with differing temperatures and between the gas and the tank.
As shown in
Table 2, concerning final temperatures, the 0D model consistently predicts higher values than the CFD model across all cases, with a maximum percentage difference of 9.84%. The mass flow rates and densities exhibit close similarity between the two models, with variances not exceeding 1.54%. At the conclusion of the filling process, the hydrogen mass calculated using the 0D model is at most 6.03% greater than that computed by the CFD model.
Because of the increased gas temperature resulting from compression within the tank, the temperature of the external wall also rises. The initial material temperature remains consistent at 18°C across all four cases. As illustrated in Figure 5, the external wall temperature rises by 18°C, 16°C, 12°C, and 8°C for inlet hydrogen temperatures of 15°C, 0°C, -20°C, and -40°C, respectively.

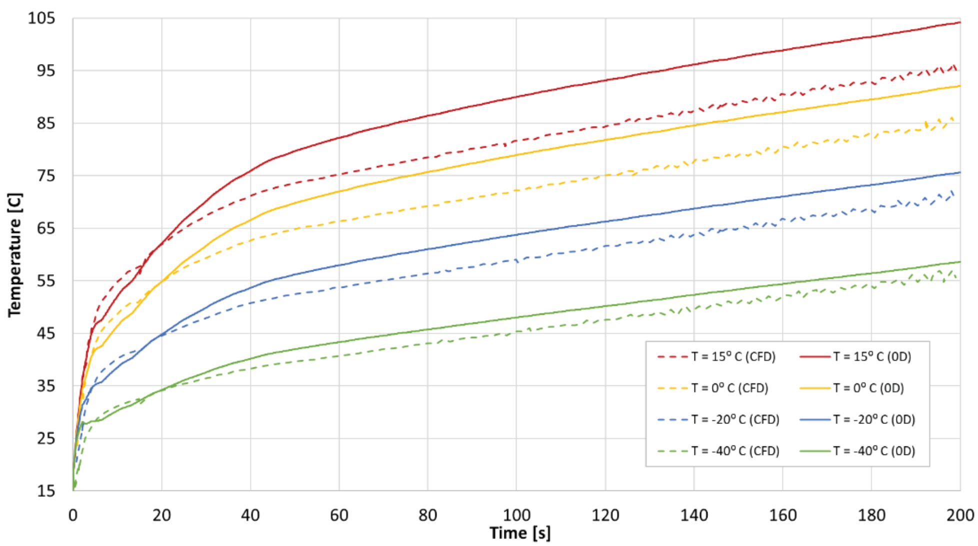

Figure 4: Average tank gas temperature profile for different inlet gas temperature (0D and CFD results)

Table 2: Comparison among OD model and CFD model: some relevant characteristics

	REF			-40 C			-20 C			0 C			15 C		
	CFD	CruiseM	diff	CFD	CruiseM	diff	CFD	CruiseM	diff	CFD	CruiseM	diff	CFD	CruiseM	diff
Final T [C]	57.32	62.59	9.19%	55.7006	58.75336	5.48%	70.2423	75.77328	7.87%	84.5807	92.26055	9.08%	94.9977	104.3484	9.84%
AVG Mass Flow [kg/s]	0.00522	0.005299	1.51%	0.00531	0.005355	0.85%	0.00516	0.005158	-0.03%	0.00497	0.004981	0.22%	0.00485	0.004858	0.17%
Total Mass [kg]	1.045	1.108	6.03%	1.062	1.119	5.41%	1.031	1.080	4.76%	0.994	1.045	5.09%	0.971	1.020	5.05%
Density [kg/m3]	38.280	38.350	0.18%	38.650	38.735	0.22%	37.490	37.371	-0.32%	36.430	36.144	-0.79%	35.700	35.295	-1.13%
SOC	0.952	0.954		0.961	0.964		0.933	0.930		0.906	0.899		0.888	0.878	

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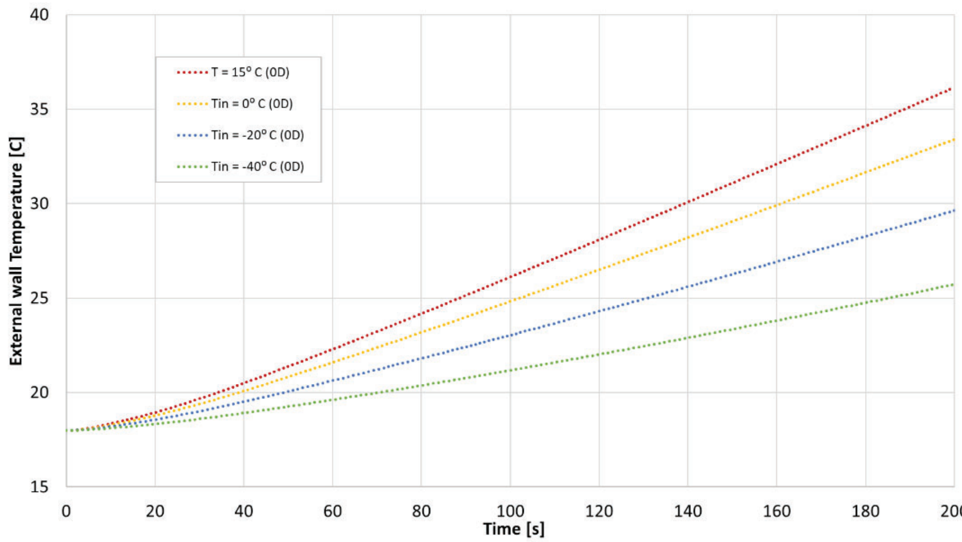

Figure 5: External wall temperature profile for different inlet gas temperature calculated with the 0D model

Within a Type IV hydrogen tank, heat diffusion occurs within the plastic liner and carbon fiber material, driven by temperature differences across these layers. Understanding this heat transfer process is crucial for ensuring the safe and efficient operation of tanks designed to store high-pressure hydrogen gas. In such tanks, the diffusion of heat within the plastic liner and carbon fiber composite layers significantly impacts the overall temperature distribution. Effective thermal management is essential to prevent temperatures that could compromise the tank's structural integrity or impact hydrogen storage performance. The rate of heat diffusion in the plastic liner depends on various factors, including the type of plastic, its thermal conductivity, thickness, and the temperature gradient across the material. Similarly, for the carbon fiber, factors such as fiber orientation, volume fraction of fibers, matrix type, and temperature gradient across the material influence the heat diffusion rate. For the scenario where the inlet hydrogen temperature is 15°C, the evolution of the internal liner wall and the boundary between the liner and carbon fiber throughout the filling process has been calculated and presented in Figure 6.

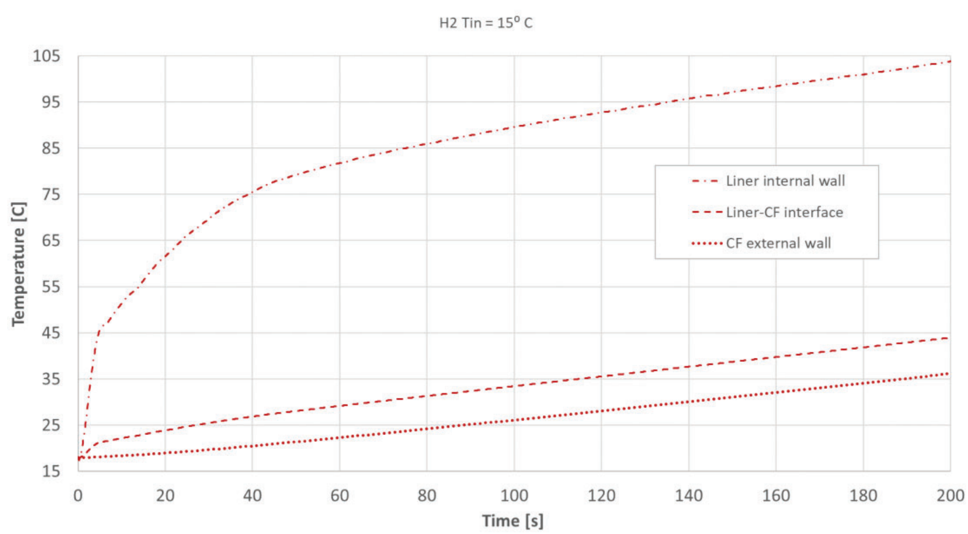

Figure 6: Material temperature profile for the case with inlet hydrogen temperature of 15ºC

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The impact of the initial inlet gas temperature on the final temperature has been examined and illustrated in Figure 7, where the same pressure profile is applied at the tank inlet. Typically, when comparing delivery temperatures, type III tanks achieve lower final temperatures than type IV tanks. In both scenarios, elevated fuel delivery temperatures lead to higher final temperatures upon filling completion. However, irrespective of delivery temperature, the final temperature rises proportionally with the increase in initial temperature and maintains a consistent slope. Given the current emphasis on Type IV tanks to diminish overall weight and size for onboard hydrogen storage, it is evident that their thermal efficiency is inferior, resulting in higher final charge temperatures. Future exploration of innovative solutions to regulate final temperatures is essential, enabling higher pressures and filling temperatures.

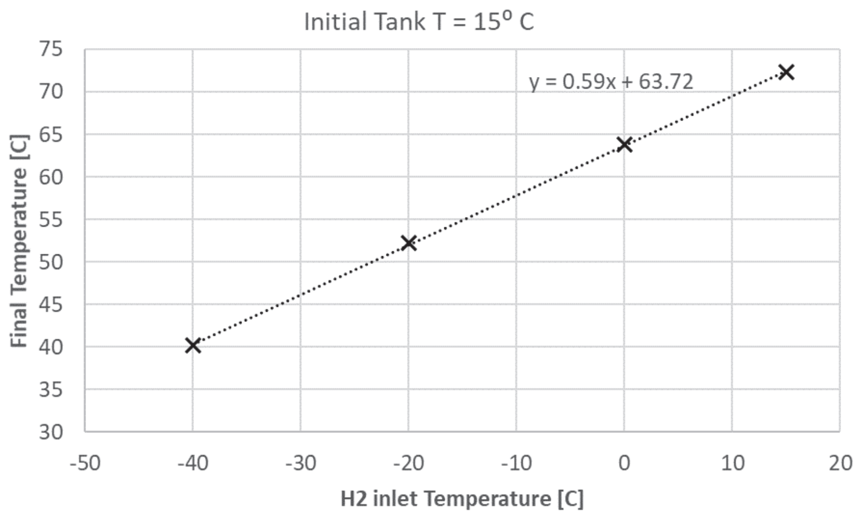

Figure 7: Final gas temperatures reached at the end of the filling versus the initial temperature for fillings for several delivery gas temperatures

5 CONCLUSION

The transition to alternative fuels, particularly hydrogen, shows promise in addressing critical challenges like greenhouse gas emissions, pollution, energy security, and sustainability within the transportation sector. Despite significant hurdles, such as those pertaining to production, distribution, and refueling infrastructure, hydrogen technologies hold substantial potential if derived from renewable energy sources. However, substantial technological obstacles persist, particularly in hydrogen storage, which is pivotal for the widespread adoption of hydrogen technologies.

This study employs a 0D numerical model developed using AVL CruiseM to analyze the filling process of hydrogen storage tanks, with a focus on type IV tanks commonly utilized in fuel cell vehicles (FCVs). The objective is to examine the influence of factors like inlet gas temperature and tank design parameters on temperature evolution during filling. Results suggest that while the 0D models, though simplified compared to CFD simulations, offer valuable insights into temperature profiles within the tanks, discrepancies between the two models were observed. The 0D models tend to overestimate temperatures, particularly at higher inlet gas temperatures, potentially due to geometrical approximations.

The results of this study underscore the significance of considering factors such as inlet gas temperature and tank design parameters in optimizing hydrogen storage systems for future transportation applications. Further research in this domain is imperative to surmount technological barriers and unlock the full potential of hydrogen technologies in realizing sustainable energy solutions.

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NOMENCLATURE

0D	Zero-dimensional
CFD	Computational Fluid Dynamics
CHSS	Compressed Hydrogen Storage System
DoE	United States Department of Energy
FCV	Hydrogen-Powered Fuel Cell Vehicles
FCVs	Fuel Cell Vehicles
HRS	Hydrogen Refuelling Stations
NWPs	Nominal Working Pressures
SAE	Society of Automotive Engineers
SOC	State of Charge

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