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NUMERICAL SIMULATION OF THERMODYNAMIC GAS TRANSFER PROCESSES IN HIGH-PRESSURE COMPOSITE VESSELS

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ABSTRACT: This paper mainly presents the economic and technical limitations of Compressed Natural Gas (CNG) transportation by ship, particularly the low ratio of gas mass to container weight and the inefficiencies in loading and unloading processes that impact the overall project feasibility. The system validated that CNG loading requires 35–51 hours and unloading 46–55 hours, depending on seasonal hold temperatures. The key objectives were to develop a simulation model to accurately assess process durations, determine the total mass of transported gas, and also calculate the power and energy requirements for high-pressure systems under various operating strategies, including a comparative analysis between methane and hydrogen.

With the development of a MATLAB-based process simulation model designed specifically on the GASVESSEL project, this greatly utilizes the Type III composite vessels.

Keywords: *GASVESSEL Project; Thermodynamics; Composite Vessels; Compressed Natural Gas; CNG transportation.*

Introduction

The use of Natural Gas is becoming more prominent in the transition to a lower-emission global economy, which accounts for approximately 24% of global energy consumption. However, traditional supply systems greatly rely on pipelines or the most common one being Liquefied Natural Gas (LNG). The transportation of Compressed Natural Gases through pressure cylinders offers a viable substitute for the exploitation of small or stranded gas field over distances between 250 and 5000 km. The use of composite materials has significantly improved the safety and weight efficiency of high-pressure storage tanks. The GASVESSEL project is a prominent example, utilizing innovative lightweight cylinders with diameters over 3 meters to transport up to 10,000 tons of CNG. (Cok, Busetto, De Zotti, Dorigo, & Angelini, 2018)

One main obstacle to the general implementation of CNG technology is the low ratio between the mass of transported gas and the weight of the container. Furthermore, the cost-effectiveness of these projects greatly depends on the capability of the loading and unloading cycles. A critical challenge known as the “Fast Filling Process” (FFP), this is where the heat generated by the re-compression of gas leads to “underfilling”, often reducing fill efficiency to approximately 80%. (Taccani, Maggiore, & Micheli, 2020)With the correct anticipation, these thermodynamic transients and the consumption of energy of the plants associated is essential for optimizing system design.

The aim of this project is to develop and implement a numerical simulation model to analyse the thermodynamics of gas transfer for a CNG carrier.

The specific objectives are:

- To develop a system of Ordinary Differential Equations (ODEs) to track gas pressure, temperature, and mass over time.
- To assess the duration and efficiency of loading and unloading processes under different ambient conditions.
- To calculate the power and energy requirements for the on-board compression station.

- To perform a comparative analysis of the transfer dynamics for methane versus hydrogen, assessing the impact on compressor power and final temperatures.

The GASVESSEL specifications highlight the modeling of 272 vertical cylinders, each with a water volume of 175 m³. These vessels feature a 5 mm stainless steel liner and a 35 mm carbon fiber epoxy reinforcement. (Taccani, Maggiore, & Micheli, 2020) The simulation covers the full plant infrastructure: double-stage compressors, regulation valves using the universal gas sizing method, and heat exchangers. For the composition of gas, the main focus is on pure methane using a comparative analysis tested on hydrogen to observe the impact of low molecular weight on compressor power and final temperatures. There are some environmental variables that this model accounts for, such as seasonal variations in hold temperatures, specifically 40 °C for summer loading and 5°C for winter unloading scenarios.

In the midst of modelling this proposed project, there are some mathematical limitations applied to ensure that the model is feasible.

These limitations include:

- A mixing hypothesis, which assumes that there are uniform gas properties within the tank.
- Treating the cylinder wall as a concentrated mass with a uniform average temperature.
- Overlooking potential and kinetic energy of the gas inside the storage vessels.
- Showing the duct flow as one-dimensional and assuming uniform gas properties along the pipe.
- An inherent accuracy margin, as validation against literature shows a temperature prediction error of approximately 5%.

Literature Review

Compressed Natural Gases commonly known as CNGs, is comprised mainly of methane (CH4), it is often generated from petroleum products and gas wells. Although CNGs are comprised of methane, there are other hydrocarbons also present. This other hydrocarbon includes ethane, propane, butane etc. The characteristic feature of CNG is its odorant nature. (Speight, 2018) . The concept of transporting compressed natural gases was first introduced in the 1960s including the use of vertical steel cylinders. However, this project was abandoned due to the very high cost of pressure vessels. Subsequently, the renewed interest in the technology has led to the development of some alternatives. (Taccani, Maggiore, & Micheli, 2020)

The first and only CNG ship currently in service, is the "Jayanti Baruna". It was first launched in January 2016 in Indonesia and has a capacity of 0.67 MNm3 at 250 bars of gas, that allows East Java to be linked to the island of Lombok. The gas is stored in an 832 vertical cylinder with a height of 12 m, diameter 615 mm, thickness 19 mm. The ratio container/cargo weight is approximately 0.15. Therefore, the currently too low ratio between the mass of transported gas and the vessels–cargo weight can be considered one of the reasons why CNG technology has such a limited diffusion. (Taccani, Maggiore, & Micheli, 2020)

The leading barrier to wider adoption is the low cargo-to-container weight ratio, in which the GASVESSEL project seeks to overcome using Type III composite vessels manufacturing that reduces the weight up to 70%. Since the transition from full metal to composite overwrap technology has become essential for enhancing payload efficiency, it is important to know the different categories of pressure vessels based on their construction. (Kim, Cho, Kim, & Yoon, 2013)

Table 1.0: Categories of pressure vessels based on their construction.

Vessel Type	Construction Method	Weight/Capacity Ratio	Notes
Type I	Full Metal (Steel)	1.1-0.9	Excess Weight
Type II	Metal with Circumferential Reinforcement	0.9-0.75	Insufficient weight reduction for large-scale sea transport
Type III	Metal Liner with Composite Overwrap	0.75-0.55	Standard composite technology
GASVESSEL Type III	Very thin metal Liner (New Technology)	0.45-0.27	Target of the GASVESSEL project 70% lighter.
Type IV	Full Composite (Plastic Liner)	0.55-0.3	Not applicable for >3m diameters or extreme temperatures.

Methodology

The study of this project is primarily based on the GASVESSEL Project; to help develop and implement a numerical simulation model to analyse the thermodynamics of gas transfer processes in composite pressure vessels, a mixed-method design was used to investigate the different behaviours and properties of Compressed Natural Gases (CNGs).

4.1 System Design

The proposed system design of the model represents a complete shipboard plant which will be used for handling compressed natural gases or hydrogen at any pressure amount up to 300 bar. (Cok, Busetto, De Zotti, Dorigo, & Angelini, 2018)

This system design is composed of three main components which are:

i. The Containment System: This is the most important part of the design which consists of specifically Type III composite pressure cylinders. In these vessels, a thin (5 mm) austenitic stainless-steel liner is used, it is wrapped in a 35 mm carbon fibre epoxy reinforcement.

ii. The On-board Plant: In the system there are two double-stage centrifugal compressors working in parallel. The regulation (throttling) valves, a CNG cooler (that is used in loading), and a gas heater (that is used in unloading to prevent freezing).

iii. Duct Network: The manifolds and piping connecting the storage terminal to the ship's vessels are modelled to account for pressure drops and flow resistance.

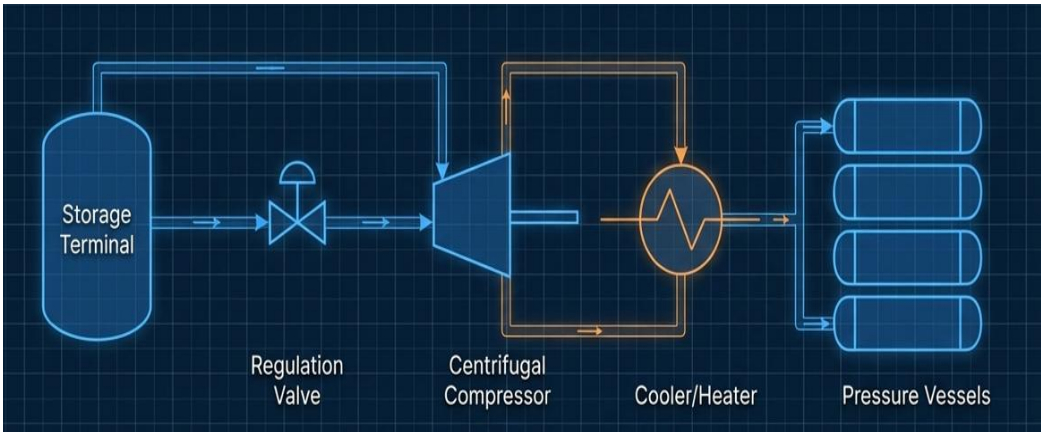

Figure 1: The Physical Component map

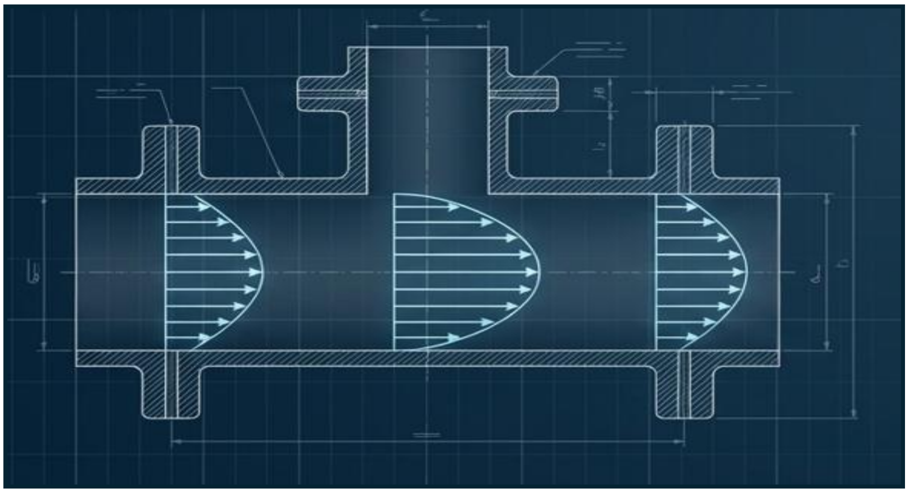

Figure 2: Duct Network Floor Plan to model transient pressure drops across the ship's piping manifold.

4.2 Two-Phase Simulation

The transfer process is divided into two processes to maximize efficiency and minimize energy consumption.

- Free Phase: During this phase, the flow occurs spontaneously because of the pressure difference between the source and the receiver vessels.
- Forced Phase: Once the spontaneous flow rate falls below a threshold, the compressors are then activated to complete the transfer. This phase switches to using compressor characteristic curves to calculate mass flow and power.

4.3 Mathematical Equations

By using various equations, it is possible to track the state of the gas over time.

- Conservation Laws: The implementation of the mass conservation and energy help balance equations. This is due to the kinetic and potential energy being neglected inside the tanks, the energy balance focuses on the internal energy change relative to inlet enthalpy and heat transfer.

Mass Balance: $\frac{dmr}{dt} = m_i$

Energy Balance: $\frac{d(m_i . u_i)}{dt} = m_i \left(h_i + \frac{vi^2}{2}\right) i + \frac{dQr}{dt}$

- Thermal Dynamics: The cylinder wall is treated as a concentrated mass to solve for wall temperature. This accounts for convective heat flux between the gas and the wall, and the wall and the hold's nitrogen atmosphere.

  Wall Temperature and Heat Flux: $\frac{dTw}{dt} = \frac{1}{m_w C_{pw}}(-\frac{dQr}{dt} - \frac{dQ_{amb}}{dt})$

$$\frac{dQ_r}{dt} = -\alpha_i S_i (T_r - T_w)$$

- Real Gas Modelling: Since methane at 300 bar is classified as non-ideal, the ideal gas law cannot be used. A new Equation of State known as the GERG-2008 has to be implemented. This methodology uses the CoolProp open-source library to pull precise thermodynamic properties from the NIST database. (Kunz & Wagner, 2012)

4.4 Numerical Implementation and Validation

In order to model and develop a proper numerical simulation, these physical laws have to be translated into a discrete-time simulation.

- The main software that will be utilized to run the simulations is MATLAB. MATLAB was the most suitable software to use primarily because of its computational efficiency especially in solving the coupled system of ordinary differential equations that are defined in the thermodynamic transients of the GASVESSEL project.
- Control Logic: The model includes logic for compressor regulation, varying rotational speed to keep the flow between "pumping" and "flooding" limits.
- Validation: By comparing results against experimental data, the sources show that the proposed model can predict final temperatures with an error of just over 5%, which is acceptable in many engineering applications.

Results

5.1 Model Variation

With the use of experimental data, the model was validated and a few comparisons were carried out. Figure 4 depicts an aluminium liner with a reinforcement in composite material (epoxy resin with carbon fibre). The given diameter is 396 mm, the length 830 mm, and the internal volume 70 L. The service pressure is 207 bar, and it is fed by a supply unit of 450 L at a pressure of 400 bar. (Taccani, Maggiore, & Micheli, 2020)

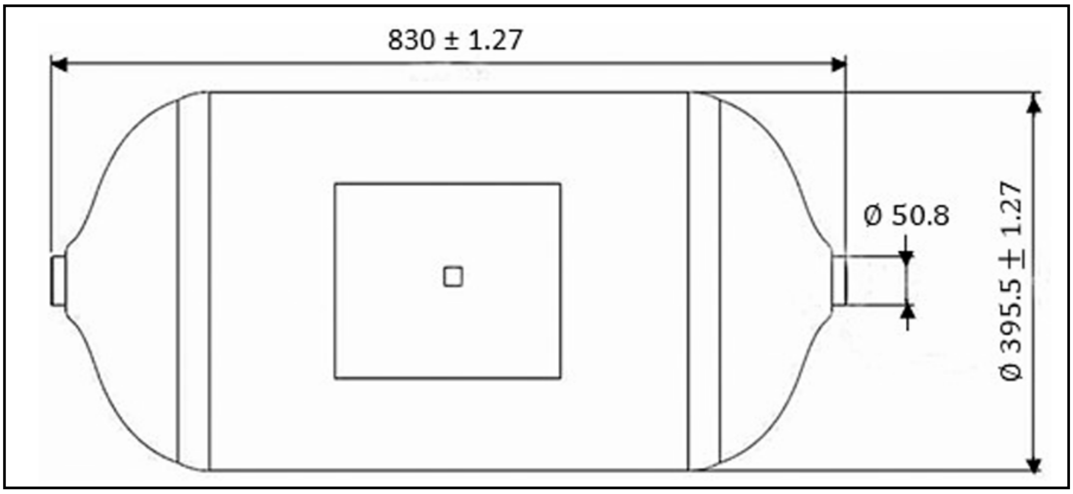

Figure 3: Geometry of the type III CNG cylinder considered for the model validation (Taccani, Maggiore, & Micheli, 2020)

For the safety of cylinders in composite vessel materials, the temperature needs to be taken into consideration. It is important to take note of the temperature rise which occurs in the composition of gas. By assuming that the temperature is 25 ◦C, which is performed in a summer period. The initial cylinder temperature is −8 ◦C, and its initial pressure is 10 bar. Figure 3 shows that the final temperature reached is 41 ◦C, while the experimental temperature is 39 ◦C. The error is just over 5%, but we must consider that not all the errors are traceable to the model.

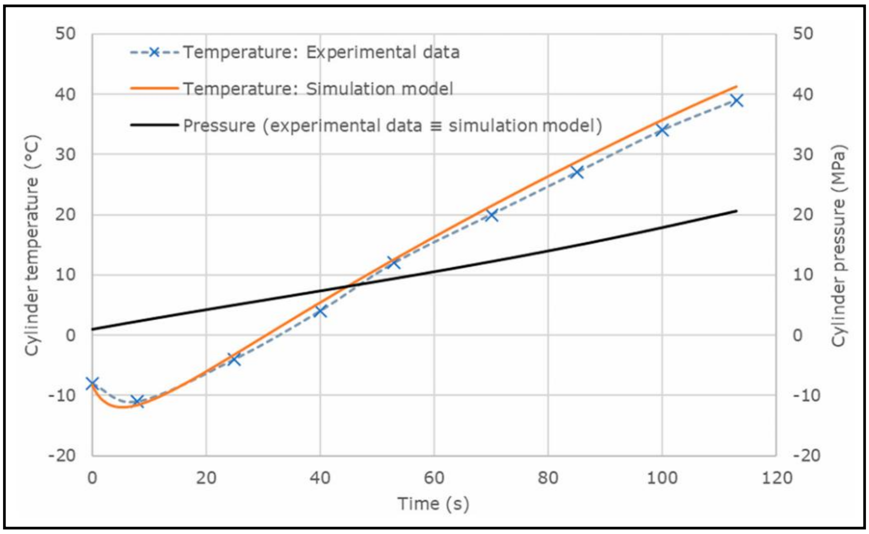

Figure 4: Comparison between experimental and numerical results

5.2 Process Duration

The numerical simulation calculates the required time for a complete cargo transfer; this identifies the transition point between the free phase and the forced phase. The development of the numerical simulations was done using MATLAB. The simulations were split up into two different types: Adiabatic simulations and non-adiabatic simulations.

Adiabatic Simulations

The loading process has a total loading time of 35 hours. However, since the Joule-Thompson effect is seen to be more dominant initially, this results in a temperature drop of 10 °C, before being superseded by internal energy conversion as cylinder pressure increases.

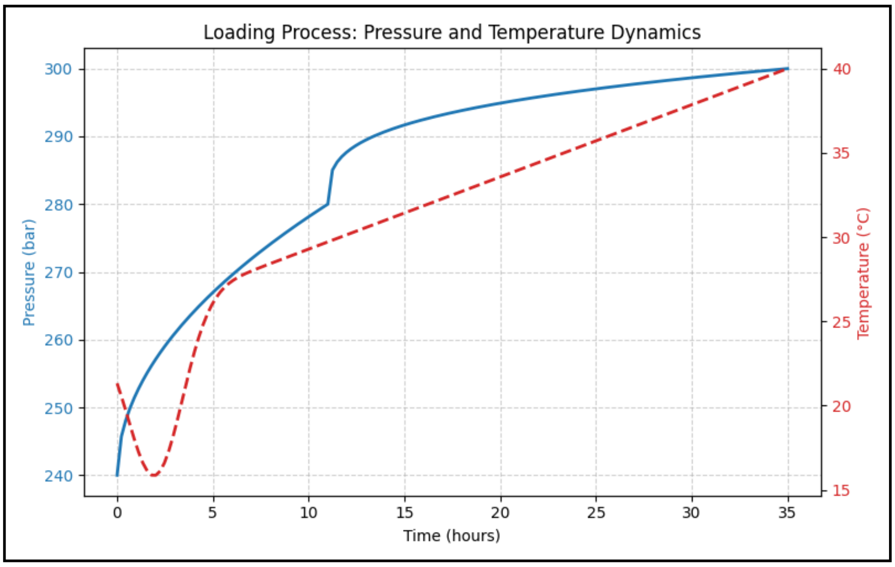

Figure 5: Illustration of the dynamics of the loading Process.

Loading Phase

During the loading process, the free phase lasted for the first 11 hours, this was driven by the pressure difference between the terminal (>240 bar) and the ship's vessels. As for the forced phase, it started at the 11-hour mark when the flow rate falls below the operational threshold, which required 24 hours of active compression to in order to reach the 300-bar design pressure.

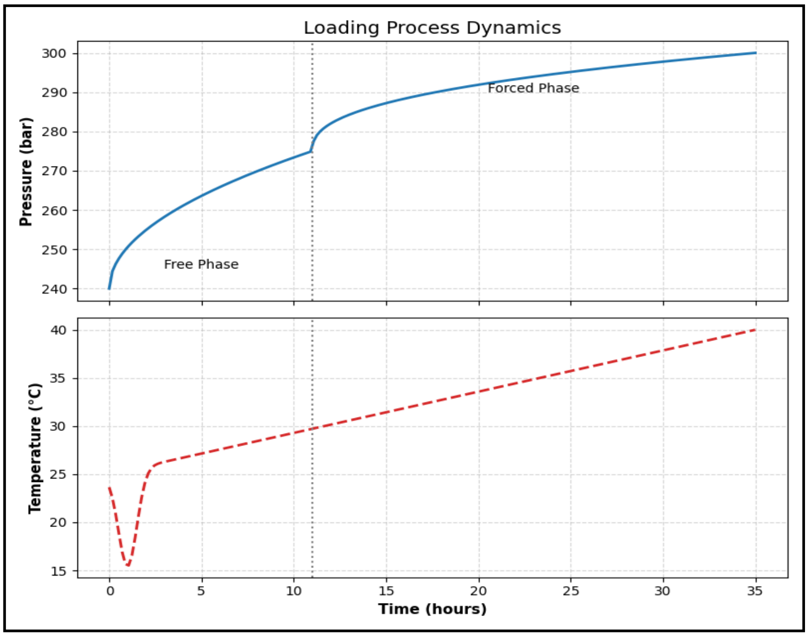

Figure 6: Illustration of the loading process, in correspondence with the pressure and temperature over a 35-hour duration.

Unloading Phase

During the unloading process, the total duration took much longer requiring approximately 46 hours. The free phase accounts for 12 hours and where as the forced phase required about 34 hours, due to the compressors requiring operation to be performed at a much higher compression ratio in order to move gas into the 120-bar destination pipeline.

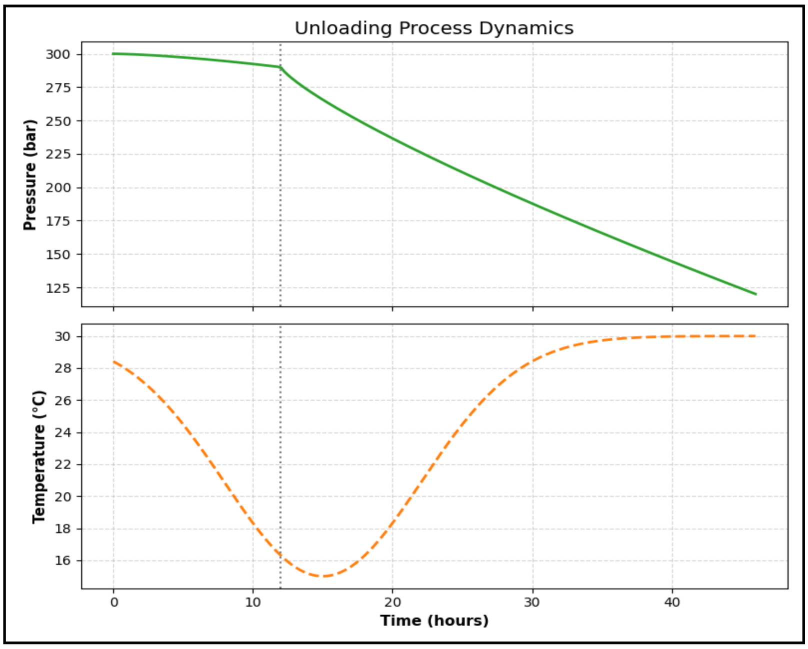

Figure 7: Illustration of the unloading process, this graph represents a 46-hour duration and the transition from free phase to forced phase.

5.3 Thermal Trends and Energy Consumption

Non- adiabatic Simulations

By utilizing non-adiabatic simulations in the model, the results show that the heat exchange with the nitrogen hold (T_{hold} = 5-40 °C) significantly tend to improve fill efficiency. During the summer loading, the loaded mass was increased by 8% over the adiabatic phase, however this resulted un the duration extending to 51 hours. The specific energy consumption varied between 96 kJ/kg (adiabatic loading) and 183 kJ/kg (winter loading). (Taccani, Maggiore, & Micheli, 2020)

Discussions

The development and implementation of a numerical simulation have successfully reproduced the thermodynamic transient of the GASVESSEL project with a high degree of accuracy. The results reflect that this proposed project has an error margin of just over 5% when compared to experimental benchmarks for Type III cylinders.

One of the contributing factors to the results was the impact of temperature variations. Such temperature variations often control the operational envelope. In order to prevent the condensation of propane and butane during the unloading process, heaters are required to maintain the gas temperature at least above 4 °C. However, during the winter seasons, it was observed that the gas reached 0 °C even with heat exchange taking place, which means it is very necessary to ensure thermal management of the compressor intake.

Furthermore, another factor to consider is optimizing the efficiency and payload. The concept used by the GASVESSEL Project brings in a fuel consumption of 1.14% - 1.45% of total cargo. With this efficiency it has allowed the choice of AISI 304/304L stainless steel to be used as the liner. Austenitic Stainless steel is the most common stainless-steel category; it is characterized by a face-cantered cubic crystal structure. Due to their excellent properties, they were utilized as they permit massive increases in yield strength through hydroforming without becoming brittle. At break, the material used remains elongated at break which exceeds 15%, a critical state for the autofrettage process. All these elements induce the compressive stresses in the liner that stabilizes it against the composite wrap. (Taccani, Maggiore, & Micheli, 2020)

A comparative analysis of the transfer dynamics for methane versus hydrogen was perform specifically to asses the impact the respective gases had on compressor power and final temperatures. According to the results, the thermodynamic behaviour of hydrogen differs significantly due to its low molecular weight.

Table 2.0: This table shows the comparison between hydrogen(H_2) and methane (CH_4).

Metric	Methane (CNG)	Hydrogen(H_2)
Loading Time	35h	21h
Loaded Mass	7609 ton	724 ton
Stored Energy (20°C)	130,278 MWh	31,136 MWh
Energy Consumption	96 kJ/kg	954 kJ/kg

According to Table 2.0, hydrogen has a much higher energy consumption than methane. With hydrogen's energy consumption at 954kJ/kg, this makes it almost 10 times higher than methane's. A number of factors contribute to this increase include:

- Molecular Weight: Hydrogen's low molecular weight affects the performance of compressors. Like for instance, in volumetric compressors, this leads to higher valve power losses which results in more work required move the same mass of gas compared to the heavier methane molecule.
- Efficiency Drop: The maximum adiabatic efficiency of the compressor drops from 93% (methane) to 70% (hydrogen) at low compression ratios.
- Thermal Limits: With thermal limits, the hydrogen loading temperatures can exceed 120 °C, approaching the glass transition temperature (T_g) of traditional resins. This necessitates more energy-intensive thermal management. This can greatly compromise the structural integrity of the vessel.

Conclusion

In summary, the proposed project has proven the techno-economic viability of the GASVESSEL project. There was a 70% reduction in the weight of the vessel therefore enabling an increase in payload. The model demonstrates that implementation of unloading and loading, they can be achieved within viable maritime windows.

By performing the numerical simulations, there were critical operational benchmarks established for the GASVESSEL Configuration. The time required for loading was observed to vary between 35 and 51 hours, whereas the unloading time required a bit longer which was between 46 and 55 hours. All these were highly dependent on factors such as the temperature. The identification of the "underfilling" effect in which the re-compression heating causing gas temperatures to peak at 78°C, this resulted in the restriction of fill efficiency to almost 85%. (Taccani, Maggiore, & Micheli, 2020)

The summarized results have yet again validated the applications of mathematics in engineering specifically thermodynamics. With proper mathematical approaches, the design of compressed gas transport systems was optimized. Recommendations for future research include, performing a full-scale experimental test to make the model more efficient and integrate various thermodynamic techniques into comprehensive ship-wide energy frameworks.

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