

Thermodynamic modelling of cryo-compressed hydrogen storage tanks for trucks

Master's thesis in Automotive Engineering

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Cover: Thermodynamic model of Hydrogen storage

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0.1 Abstract

Currently today's transportation is either by conventional ICE driven vehicles, fully electric vehicle or hybrid vehicle. Based on environmental impact with increasing concentration of greenhouse gases in the atmosphere such as Carbon dioxide and nitrogen dioxides emerged partly as a bi-product from combustion, there has been a rising initiative to electrify transportation and cut down on tail pipe emissions. However, driving range in electrified vehicles may be short for long haul truck applications and in general, transition towards electrification has been too quick for a proper charging infrastructure to be implemented. Fuel Cell driven vehicles with hydrogen is a concept that has been initiated as an alternative fuel which during energy conversion in fuel cells will produce water as the only bi-product and with higher possibilities to achieve longer driving range than battery electric vehicles.

In this thesis, study is focused on storage of hydrogen for automotive applications. Simulation of different truck operations that could possibly take place in a real life to observe how the truck operations would affect the overall storage performance in terms of thermal aspects such as pressure, temperature and density in the tank. Key state properties of storage tank in this study is fill density of hydrogen storage, boil-off losses and external heat required during hydrogen consumption. Initial tank temperature and pressure, fuel temperature and truck operation are the parameters affecting the state properties. Results from simulation in form of plots will help to visualise the evolution of state properties with change in mentioned parameters. Simulation is run with the help of GT SUITE by Gamma Technologies, which has a high computation power with predefined library of information of many fluids with a possibility to run simulations for hydrogen storage with the latest version of software.

Keywords: Fuel cell, hydrogen storage, cryogenic storage, cryo-compressed hydrogen, fill density, GT SUITE

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List of Acronyms

Below is the list of acronyms that have been used throughout this thesis listed in alphabetical order:

<i>CcH₂</i>	Cryo-compressed hydrogen
<i>CGH₂</i>	Compressed gaseous hydrogen
<i>LH₂</i>	Liquid hydrogen

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1

Introduction

A brief introduction about the fuel used for transportation energy needs, advantages and disadvantages of using various fuels and a potential solution for a sustainable future transport.

1.1 Background

The automotive industry and its ever-changing technology for transport has been revolutionised since the invention of internal combustion engine, and the significant role of transport in the industrial era has been important for improving the transportation technology in terms of energy conversion efficiency and harmful emissions such as carbon dioxide from internal combustion engine due to the dependency of fossil fuels. According to EU norms, emission standards have been modified over the years and they have been made strict in terms of fuel efficiency of internal combustion engine and its tailpipe emissions such as carbon dioxide and nitrogen oxides, but fossil fuels have been used widely due to its property of high energy storage density and the mature technology available for refuelling along with time taken for the same, even though a potential replacement with help of batteries and electrical motor which completely eliminate the above mentioned drawbacks of internal combustion engine[1]. Batteries have low energy storage density and duration of time for charging is few hours compared to refuelling of fossil fuels which takes up to a maximum of twenty minutes, limiting the application of battery powered vehicle for short range distances of 400 km or less and unfavourable for distance above 400 km, especially in remote area without a proper electric charging infrastructure.

From the Figure 1.1, it can be observed that fossil fuels have higher energy density compared to batteries. To overcome the mentioned drawbacks and have a sustainable transport system with the advantages of internal combustion engine regarding energy density of fuel along with refuelling time and of battery electric vehicles which have zero tailpipe emissions, hydrogen fuel cell powered vehicles cater to all the required needs for clean energy transportation. The exhaust/tail pipe emission from the hydrogen fuel cell is just water vapour as the electrical energy obtained from fuel cell is with conversion of hydrogen fuel, which only emits water vapor as the bi-product of the reaction. If the fuel used for propulsion in fuel cell is obtained from green hydrogen production methods, then the emissions in the overall chain of fuel from production to energy conversion is free of carbon emissions[2]. In the following sections, advantages and disadvantages of hydrogen fuel over conventional fuels used for propulsion will be discussed.

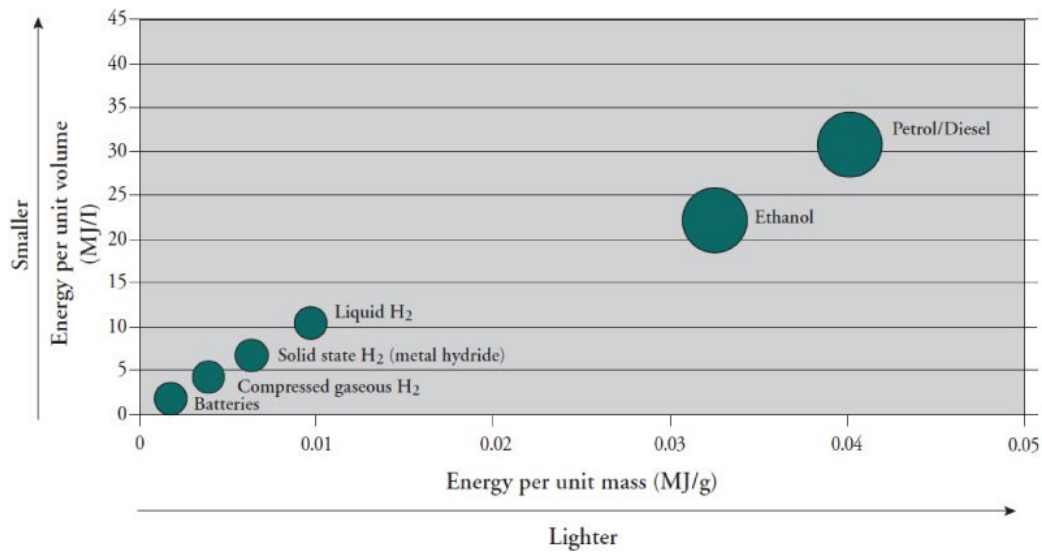


Figure 1.1: Comparison of Energy densities of fuel [3]

1.1.1 Fuel Cells

Fuel cell is a component where the hydrogen fuel is converted into electricity with help of electro-chemical reaction and the process how electricity is generated could be viewed in figure 1.2. From Figure 1.2, it can be observed that hydrogen gas (H₂) flows into the fuel cell at anode, only proton is allowed to pass through the membrane and electrons will pass through an electric circuit with a load, thereby a flow of electric current. On the cathode side, air flows in and a reduction reaction takes place which forms water as the bi-product.

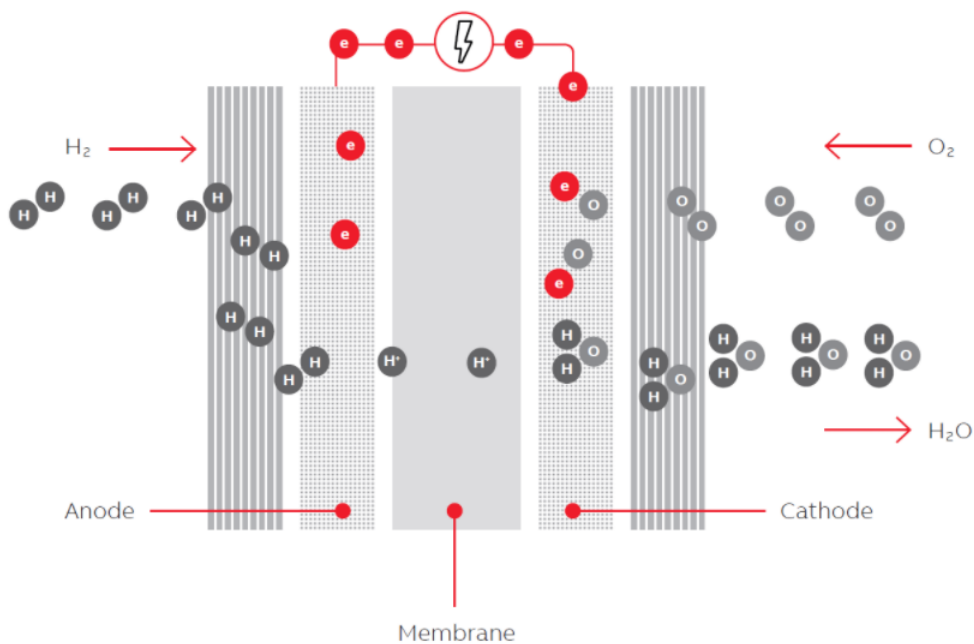
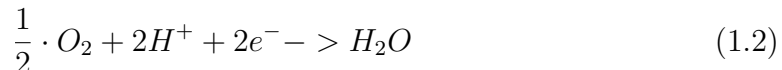


Figure 1.2: Fuel cell [4]

Reaction at anode: **Oxidation reaction:** Hydrogen molecule is broken down into protons and electrons



Reaction at cathode: **Reduction reaction:** Hydrogen protons flow through the membrane and the flow of electrons through an external circuit. Hydrogen reacts with oxygen at the cathode to form water and heat as products of chemical reaction.



Water (H₂O) in the form of vapor is let out through exhaust as temperature of fuel cell operation is high. The generated electricity is either used for propulsion or energy storage in batteries for later utilization. This is the fundamental principle behind application of a fuel cell and main focus of our thesis is hydrogen fuel storage. Fuel cells can generate electricity at 60 % efficiency [11], it's a very promising alternative to power vehicles.

1.1.2 Hydrogen storage

Similar to a fossil fuel tank in an conventional vehicle, fuel cell driven vehicle requires a storage tank to store hydrogen fuel. The fuel stored in the tank for a given volume capacity, partly influences the driving range of truck. One way to increase the driving range would be to achieve higher fill density of fuel in order to drive for longer duration to cover the distance to the destination with fewer stops for refuelling and time duration for refuelling is few minutes whereas for charging of batteries is in a few hours and the driving range of battery electric vehicles is limited by weight and cost of the battery. Hydrogen gas needs to be stored as a compressed gas at pressure of 350 bar to 700 bar which is a requirement to obtain high storage density of fuel in storage tank up to 40 kg/m^3 , with temperature ranging from -40 C to 85 C. According to Elberry Am et al., hydrogen gas when compressed to be stored in a tank, it deviates from the laws, prediction where hydrogen occupies a larger space[5]. This deviation is overcome with the correction factor named compressibility factor influences the mass of hydrogen stored. Compressibility factor is a function of temperature and pressure, where for a constant pressure of hydrogen fluid, the compressibility factor increases with decrease in fluid temperature. Hydrogen gas has a low density value of 0.0873 kg/m^3 at a temperature of 25 C and 1 bar pressure. Compression energy required to store compressed hydrogen is high when compared to helium and methane due to its low value of density. Also, storage tanks for hydrogen in automotive application has limitation on volume and mass of tank, more on this topic will be explained in the upcoming Section 2.5.

In a regular conventional passenger vehicle driven by gasoline fuel, according to U.S Department of Energy, a passenger vehicle in highway conditions would experience energy losses at the IC engine partly due to combustion, exhaust heat etc up to 69 % , leaving only 31 % of the energy conversion from fuel being used to power the wheels [6]. Compared to Fuel cell driven vehicles which as stated above, could generate electricity at 60 % efficiency in general and that efficiency could vary based

on power demand from the truck, but in general fuel cell have been stated to have a higher energy conversion efficiency than IC engines. In storage applications this implies a higher amount of fuel needing to be used in IC engines compared to fuel cells in order to generate the same amount of energy.

Later in this report, a more extensive and further factors that should be taken in consideration will be discussed.

1.1.3 Hydrogen as an alternative fuel

Using hydrogen as a fuel for transportation which can be a replacement to conventional fossil fuels could be produced by mainly three different means shown in Figure 1.3.

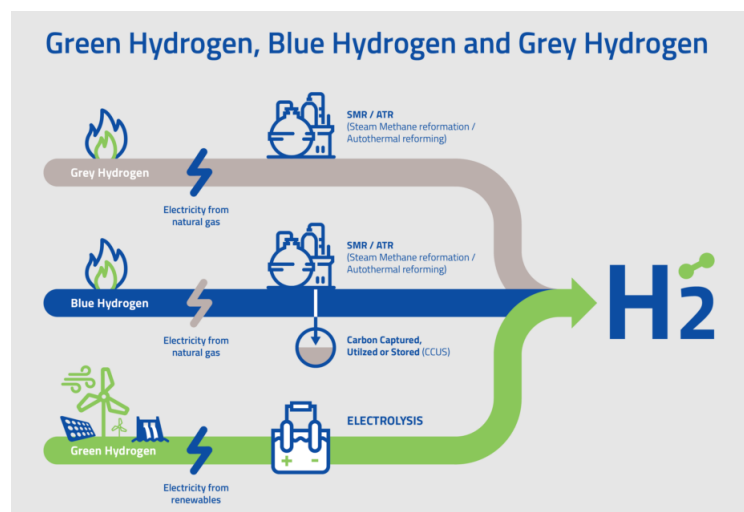


Figure 1.3: Green, blue, grey hydrogen [7]

Grey hydrogen production process produces hydrogen by a process called "Steam Methane reformation" which in grey hydrogen production process is powered by electricity generated from natural gases such as methane or coal [2], where as a blue hydrogen production process method has similar strategies except around 80 % of the carbon emissions arising from the production, is stored underground, decreasing the environmental impact. Using hydrogen that has been produced with renewable energy sourced electricity such as wind and solar, with almost no carbon emissions through electrolysis is called green hydrogen which should be considered as one of the main advantage for fuel in fuel cells.

Other advantages of hydrogen fuel are listed below:

- Significantly lower refuelling time for hydrogen compared to electric vehicle charging.
- Fuel cell energy conversion efficiency which translates to amount of usable energy after conversion including losses is better than conventional IC engine efficiency.
- It's a clean energy source, meaning that it has minimal or almost zero impact on the environment when green hydrogen is used as a fuel.

When compared to fossil fuels and its harmful by-products of combustion such as carbon dioxide and nitrogen oxides, the key benefit of using green hydrogen is none harmful emissions. However there are still few challenges in dealing with hydrogen and some of the disadvantages with hydrogen for current market could be viewed below:

- Difficulties with storing hydrogen since temperature and pressure has to be controlled.
- Fluid density at 1 bar pressure and 273 K temperature of diesel is 0.85 kg/L and that of hydrogen is 0.089 g/L [9]. There is a large difference in value of fluid densities, hence pressurised compressed storage of hydrogen is necessary to increase fluid density.
- Thermal insulation demand to avoid heat ingress into the storage from surrounding environment when hydrogen fluid is stored in liquid phase at cryogenic temperature of below 120 K.
- Embrittlement of storage tank due to hydrogen adsorption, which results in reduction of tank material strength and durability.
- Hazardous, as hydrogen is both flammable and explosive when stored as compressed fluid. Hydrogen has a flammability range of 4-75% concentration in air and ignition energy of 0.018 MJ [10].

1.2 Aim

To model a thermodynamic system for cryogenic-compressed hydrogen storage tanks in different truck operation scenarios. The evaluation will be performed to study the characteristics of the hydrogen state properties, based on the hydrogen mass flow, temperature and pressure of the tank as a function of power requirement from the fuel cell to provide electricity to the system. The simulation will be carried out with the following questions as an input/case under study:

- Quantification of boil off losses (% of fuel).
- Quantification of average usable tank capacity in long-haul truck application in kilograms of hydrogen.
- Sensitivity analysis of heat ingress impact on dormancy time.
- Sensitivity analysis of tank temperature on tank capacity.
- Define max parking time at different SOC until full fill still can be achieved.

The outcome of the project will be the evaluation of the results obtained, and a fundamental step towards further work in the field of cryo-compressed hydrogen storage for automotive applications.

1.3 Delimitations

The scope of this thesis is the study of thermodynamics of hydrogen storage tank, and the tank structure or design in terms of automotive applications will not be included. The operation of fuel cell and input to the fuel cell based on power demand will not be considered during the modelling of hydrogen storage tank. The main

focus would be the thermodynamic state properties of cryo-compressed hydrogen over time, and anything related to the design aspects of the storage tank will be the limitation.

1.4 Specification of issue under investigation

The study mainly focuses on hydrogen storage with respect to fill density, dormancy time, hydrogen consumption towards energy conversion, and the change in state properties over time, as the pressure and temperature inside the storage tank would change during truck operation. Modelling of a thermodynamic system which will track the state properties of hydrogen in storage over time, will help to answer the questions/objectives mentioned. Understanding the fundamentals of thermodynamics and how the hydrogen state properties change over time would be the main focus to answer the questions.

2

Theory

As a part of this thesis, a literature study on cryo-compressed hydrogen and thermodynamic properties of hydrogen, to have an understanding of hydrogen as a fluid and the physics behind how the hydrogen behaves under various temperature and pressure.

2.1 Thermodynamic model

A thermodynamic model is used to observe the state properties of a working fluid which is a function of temperature and pressure. Based on this thermodynamic model, fluid properties such as specific heat, entropy and enthalpy of the system/fluid is calculated using the state equations. With the help of GT-SUITE [12], computation of solution to the state equations is not complex as the simulation software takes care of all the calculation of state properties based on boundary conditions to each of the components in a system. Thermodynamic model has a range of operational temperature and pressure in which the solution of state equations are valid. GT-SUITE has several in-built thermodynamic fluid properties and there is a template option to have our own fluid properties in a given temperature range.

2.2 Thermodynamic property of Hydrogen

Hydrogen is the lightest substance in nature, which has a density value of $0.08 \text{ kg} \cdot \text{m}^{-3}$ at a temperature of 300 K and 1 bar pressure. At atmospheric pressure of 1 bar and temperature lower than boiling point of hydrogen 20.28 K, hydrogen exists in a liquid phase having a higher density value of $70.8 \text{ kg} \cdot \text{m}^{-3}$ [13]. Hydrogen exists as two spin isomers, para-hydrogen and ortho-hydrogen. Para-hydrogen has symmetric nuclear rotation and anti-symmetric nuclear spin whereas ortho-hydrogen has anti-symmetric nuclear rotation and symmetric nuclear spin [14].

The purpose of mentioning the spin isomers of hydrogen is that the conversion between the two spin isomers is dependent on temperature [14] and the conversion of para-hydrogen to ortho-hydrogen is a heat absorbing process which results in lowered temperature of the system [15]. Hydrogen fluid at cryogenic temperature (below 120 K) is available in the predefined GT-SUITE library of fluids, however a need of fluid composition/object which includes para to ortho hydrogen conversion and its cooling effects on the system is necessary. GT SUITE makes use of REFPROP [16] data for their refrigerant fluids and with the help from GT-Support, it was confirmed

that para to ortho hydrogen conversion effects is not included in the refrigerant hydrogen fluid. In the upcoming section, the explanation to how a fluid object can be created in GT-SUITE will be explained for the hydrogen spin isomers.

2.3 Hydrogen fluid object in GT-SUITE

To formulate a fluid object in GT-SUITE, there exists suitable templates with attributes of the fluid such as heating value, reference temperature range, fluid phase at STP, viscosity, thermal conductivity, etc[17]. The required inputs are calculated from CoolProp [18], which is an open source database for fluids. The fluid properties such as specific heat(C_p) is calculated for the temperature range which is represented in Equation 2.1.

$$\frac{C_p(T)}{R} = a_1 \cdot \frac{1}{T^2} + a_2 \cdot \frac{1}{T} + a_3 + a_4 \cdot T + a_5 \cdot T^2 + a_6 \cdot T^3 + a_7 \cdot T^4 \quad (2.1)$$

The seven coefficients are constant values, with input of temperature and universal gas constant R, specific heat is calculated. Specific heat is calculated for the entire range of temperature for para hydrogen, ortho hydrogen and normal hydrogen which corresponds to a mixture of 25 % ortho and 75 % para [19]. Further, the coefficients are calculated as the specific heat and temperature value is known, it is a simple computation of set of equations with unknown and know values. The plot of specific heat vs temperature is represented below.

The solution to the unknown coefficients from Equation 2.2 is as follows :

$$A = x \cdot b \rightarrow x = A \setminus b \quad (2.2)$$

Unknown coefficients are

$$x = (a_1, a_2, a_3, a_4, a_5, a_6, a_7)^T \quad (2.3)$$

Specific Heat

$$A = \left(\frac{C_{p1}}{R}, \frac{C_{p2}}{R}, \dots, \frac{C_{pn}}{R} \right)^T \quad (2.4)$$

Temperature range

$$b = \begin{pmatrix} \frac{1}{T_1^2} & \frac{1}{T_1} & 1 & T_1 & T_1^2 & T_1^3 & T_1^4 \\ \frac{1}{T_2^2} & \frac{1}{T_2} & 1 & T_2 & T_2^2 & T_2^3 & T_2^4 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{1}{T_n^2} & \frac{1}{T_n} & 1 & T_n & T_n^2 & T_n^3 & T_n^4 \end{pmatrix} \quad (2.5)$$

To compare the results obtained from the above calculation to a literature study conducted by Leachman et al[20], following plot in figure 2.1 is an illustration from the publication, where the specific heat of hydrogen isomers is a function of temperature.

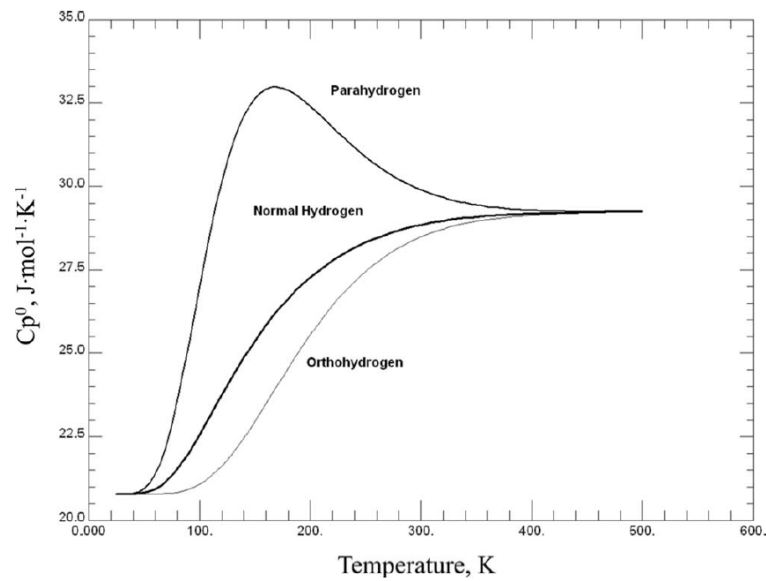


Figure 2.1: Specific heat capacity vs Temperature for para, ortho and normal hydrogen [20]

By making an estimation of the specific heat value for a temperature range and using these estimated values to solve the Equation 2.1, the seven unknown coefficients are calculated.

A plot of specific heat versus temperature for the two set of coefficients obtained from the two methods mentioned above and it is shown in Figure 2.2 that values of specific heat from estimation and CoolProp is very close.

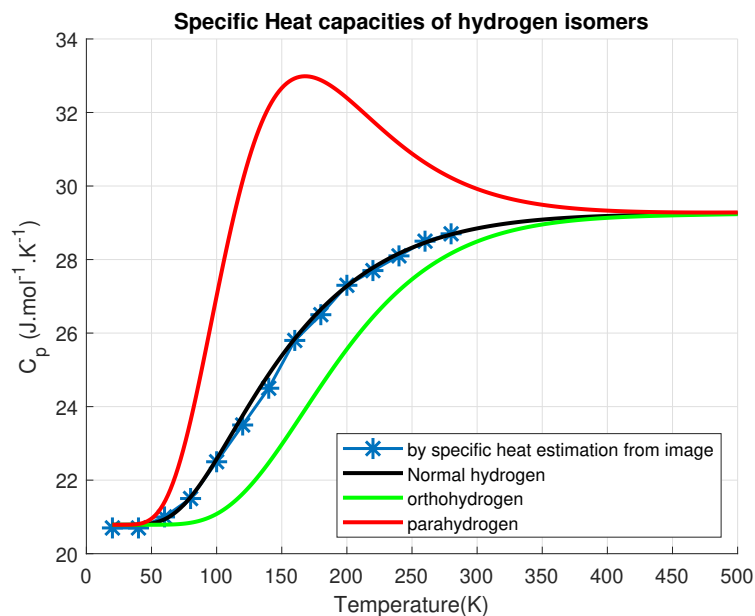


Figure 2.2: Specific heat vs Temperature

The fluid object hence obtained from the computation in Eqn 2.2 to Eqn 2.5 represents para, ortho and normal hydrogen.

2.4 Hydrogen storage regime

Hydrogen storage exists in three different operating regimes of temperature and pressure. First one is liquid hydrogen (LH_2), where the temperature of hydrogen is below the boiling point, fluid is in liquid state, with high density of fluid with low storage pressure. Compressed Gaseous hydrogen (CGH_2) is beyond -40 C temperature and the density of fluid is high with higher storage pressure. Cryo-compressed hydrogen CcH_2 , which is in between the two regimes, which can achieve higher density than LH_2 with increased storage pressure. The figure 2.3 below is a representation of the different operating regimes of hydrogen storage as mentioned by Klass et al(2012) [21].

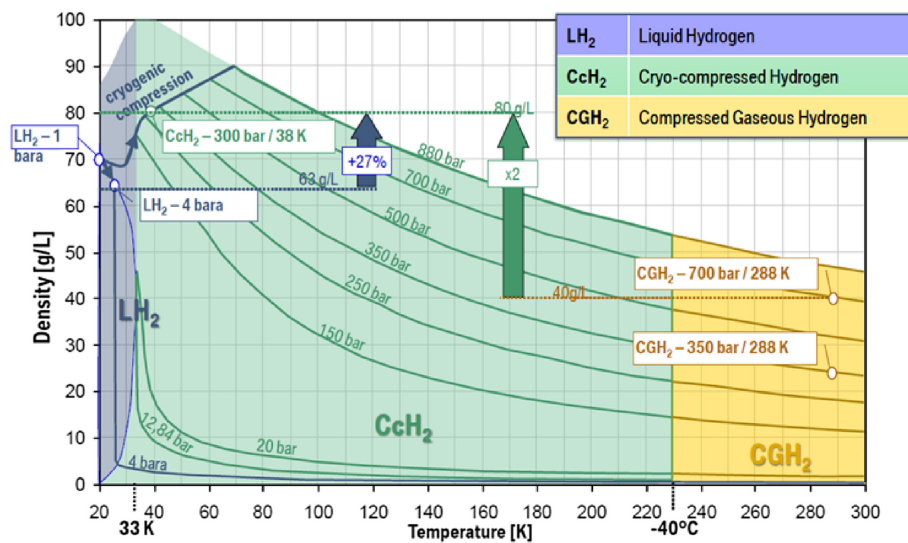


Figure 2.3: Density as a function of Temperature and pressure [21]

2.5 Hydrogen storage

Hydrogen fluid can be stored in following methods of storage [22]:

- Compressed gas in pressurised tanks
- Cryo-compressed hydrogen at cryogenic temperature
- Liquid hydrogen
- Metal hydrides

For automotive application where volume and weight of tank is crucial, hydrogen is mostly stored as compressed gas or cryo-compressed hydrogen. A storage tank for cryo-compressed hydrogen should be able to withstand high design pressure which is a resulting factor of achieving high fill density, good thermal insulation to limit the heat ingress into the tank and leak proof to avoid any hazards of hydrogen. The limitation of hydrogen storage tank is the thickness of inner and outer volume walls which affect the volumetric capacity, weight of the tank as this restricts the total load carrying capacity.

Based on using hydrogen as a fuel in automotive application, there are currently four types of storage tanks, which are as follows [23]:

- Type I - metal vessel, stated to be mostly used in stationary purposes, due to heavy weight.
- Type II - metal vessel with loop liner wrapped, unsuitable for automotive application as the hydrogen storage density is low, and due to hydrogen embrittlement.
- Type III - wrapped composite cylinder with a metal liner that serves as hydrogen permeation barrier. Improved weight performance with 25-75% mass gain over type I & II, making them ideal for automotive applications. Ability to withstand pressure up to 450 bar with good reliability.
- Type IV - cylinder made of composite material with high density polyethylene as liner. Ability to withstand high design pressure with carbon fiber composite up to 1000 bar.

Below in figure 2.4 an illustration of how material in the outer shell is added to increase strength could be observed

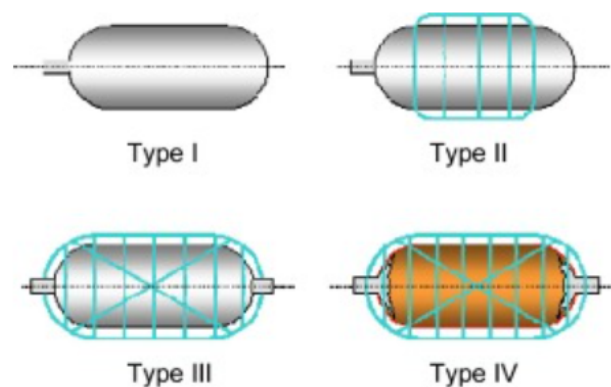


Figure 2.4: Pressure vessel types for compressed hydrogen storage [23].

Type III storage tank is commonly used for cryo-compressed hydrogen storage as the operating pressure range is of 250-350 bar [24] and below the maximum design pressure that is stated for type III. Figure 2.5 is an illustration of Type III tank, the vacuum enclosure and multi-layer insulation (MLI) is part of thermal insulation. Various components necessary for a storage system performance shown in Figure 2.5 and explained below :

- Heat exchanger - To add external heat to hydrogen fluid in the event of fluid entering liquid phase or insufficient pressure for extraction from storage tank towards fuel cell.
- Refuelling line used to fill hydrogen
- Multi layer insulation in vacuum space to limit heat transfer across tank wall layers.
- Over-wrapped pressure liner to act as a barrier for hydrogen permeation.

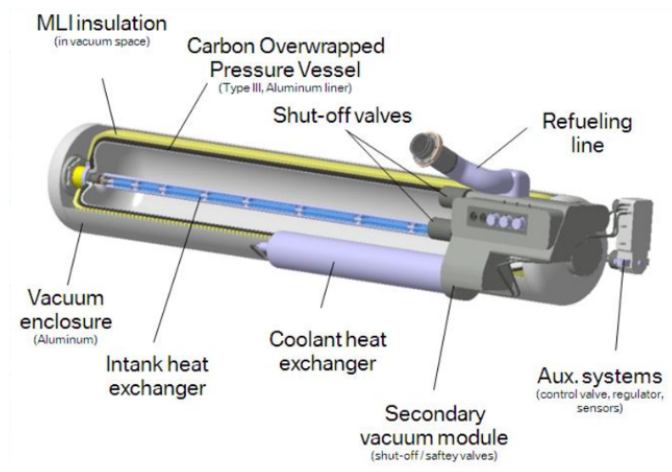


Figure 2.5: Type III tank [25]

2.5.1 CcH_2 versus CGH_2

Compressed gaseous hydrogen means that hydrogen is stored at near ambient temperature (around 298 K), compared to cryo-compressed hydrogen that is stored at temperatures below 230 K which could be observed in figure 2.3. With the knowledge that hydrogen at 1 bar pressure and temperature at 80 K hydrogen is 3.73 times denser compared to hydrogen at 298 K and at 1 bar pressure [26]. This will in storage applications, for cryo-compressed hydrogen mean, an increased mass capacity which corresponds to amount of H_2 / unit volume [27], in other words an increased density as a resulting fact of storing more amount of hydrogen with a fixed volume and reducing gravimetric capacity meaning less required weight of the storage tank to store given amount of hydrogen [27].

Highest density of stored hydrogen is achieved at low temperature and high pressure, but gaseous hydrogen when stored at near ambient temperatures above 273 K, increased storage pressure is necessary to achieve higher density to fulfil long range driving beyond 400 kilometers. Storage applications for CGH_2 requires a pressurized tank between 350-700 bar [28] relative to storage for cryo-compressed hydrogen which requires tank pressurized to less or equal to approximately 350 bar. Increased pressure in the tank will lead to an increased requirement of high strength and durability of tank material as mentioned in section 2.5, carbon fibre may be used, to increase the ability to withstand higher design pressure and reduce weight. CcH_2 will then lead to a possibility of decreasing the amount of carbon fibre being used as the design pressure of tank is lowered to 350 bar resulting in reduced usage of high strength tank material and resulting in lowered cost, since carbon fibre comes at a high cost.

2.6 Fill density of storage tank

For a fuel storage system, one of the the most important factor is density of fuel/fluid stored in the tank, as mass of fuel will influence the driving distance/range and this is a key factor for transport industry.

From chapter 2.4, it is understood that CcH_2 can achieve higher density when compared to LH_2 and CGH_2 . According to Blanco et al(2018), fill density of storage tank is a function of temperature, which mean fill density is directly proportional to the temperature of tank and to obtain high fill density, colder vessel end state for refuelling is desirable. Fill density also depends on fuel delivery temperature, and fuel pump performance, where fuel temperature and pump pressure will need to operate in the hydrogen storage regime.

2.7 Thermal insulation

Temperature operating range for CcH_2 is in the range of 33 K to 230 K and to maintain this temperature range, thermal insulation is essential between the inner and outer volume of the storage tank. One solution for thermal insulation is having a vacuum with multi layer reflective material to limit heat ingress into tank. The performance/extent of thermal insulation will depend on the materials used in vacuum layer, and the limiting factor is cost of materials and thickness of vacuum layer. With increase in thickness of vacuum layer, inner volume capacity for fluid in storage tank is reduced [19]. This leads to a decreased volume capacity and mass storage of fuel affecting the driving range of truck, which is unfavourable for automotive application with long range driving distance over 400 km.

2.8 Boil-off losses

Hydrogen stored in cryo-compressed storage regime has a temperature operating range of 33 K to 230 K. When the hydrogen storage is idle/dormant, meaning there is no filling or extraction of hydrogen, there is an increase in temperature of fluid inside the tank due to heat ingress from the surrounding ambient environment through tank insulation wall. This phenomena occurs when the truck is stationary and even with thermal insulation, there is heat ingress into the tank as the extent of thermal insulation is limited by cost of materials. With increase in temperature of fluid inside storage tank, pressure of the fluid builds up beyond a maximum allowable pressure limit, which is a safety hazard of compressed hydrogen. The pressure build up inside storage tank has to be relieved back to the safe operational limits with loss of hydrogen when a valve is opened to pressure relief. This loss of hydrogen to maintain pressure is known as boil-off losses of hydrogen. This process is mainly occurs in hydrogen storage regime of cryo-compressed hydrogen and liquid hydrogen where the temperature is cryogenic.

2.9 Hydrogen safety hazards

Awareness of compressed hydrogen safety hazard is vital and mandatory to avoid accidents due to negligence or human errors. Some of the hazards of hydrogen as mentioned by Schmidtchen(2002) [29] are as follows :

- Hydrogen is flammable
- Hydrogen is a small molecule with low viscosity and high leak rate.
- Rapid diffusion of hydrogen
- Hydrogen embrittlement which causes cracking.
- Hydrogen gas is undetectable by human senses, i.e, hydrogen flame is almost invisible, and hydrogen gas has almost no smell. Hence, hydrogen gas detectors must be installed when working with hydrogen storage.
- Hazardous, as hydrogen is both flammable and explosive when stored as compressed fluid. Hydrogen has a flammability range of 4-75% concentration in air and ignition energy of 0.018 MJ [10].

3

Modelling

For thermal and flow computation of a system in 0-D or 1-D, GT SUITE is a productive tool which can be used to model different components of a system as objects and the attributes of individual components can be described in object properties. These properties for the individual blocks/objects for example pressure, temperature, volume, material properties will be obtained from a literature review of current on-going research on cryo-compressed hydrogen storage. GT SUITE solves the primary solution variables based on the time step used for simulation and required plots/reports maybe selected as an output from simulation. Various objects/components of a system are chosen such that the boundary condition of each one can be specified and the state properties are calculated either at the boundary or volume based on whether the state property is a scalar or vector quantity.

The simulation model in the study consists of the following sub-systems which will comprise a hydrogen storage system :

- Refuelling
- Hydrogen storage tank
- Boil-off/venting
- Hydrogen consumption

Figure 3.1 below is a schematic representation of the simulation model.

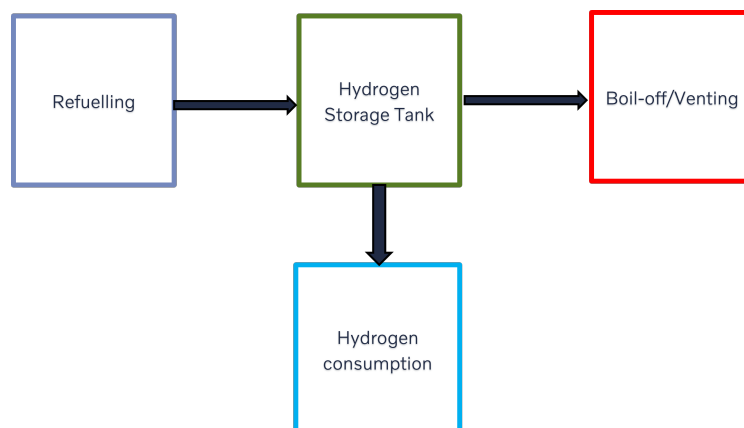


Figure 3.1: Schematic representation of hydrogen storage

The four sub-systems each have their own function during truck operation. Refuelling sub-system is the filling of hydrogen in the storage tank, boil-off system

is essential for maintaining the pressure inside the tank within the safe operating limits which is based on the maximum design pressure of the tank and extraction/-consumption of hydrogen towards fuel cell for energy conversion. In the following sections, the sub-systems are explained further.

3.1 Refuelling

Filling of hydrogen storage tank is entirely different to that of a conventional fuel filling of petrol/diesel, where the fuel flow is controlled based on the fill level and venturi effect, whereas for hydrogen filling, it is a function of temperature and pressure of the tank, where the mass flow is controlled to achieve a target pressure for a given temperature in the storage tank based on a closed feedback control loop. For a given volume of storage tank, based on fill density of hydrogen, mass of hydrogen stored in the tank varies which affects the driving range of the truck.

The inputs/boundary conditions to the refuelling system are as follows:

- Ambient temperature
- Fluid temperature
- Tank initial pressure
- Target Pressure
- Pressure rise rate
- Fluid composition/Fuel
- Maximum fluid flow rate

The above mentioned inputs are necessary as per SAE J2601-Fueling Protocols for Light Duty Gaseous Hydrogen Surface Vehicles, which is a standard protocol to fill hydrogen into a tank [30]. Refuelling/filling of hydrogen operation is pressure controlled, which means that beyond a pressure in storage tank, the refuelling is stopped.

Referring to the below Figure 3.2, the filling of hydrogen starts from with inputs - temperature of fuel, fluid composition and mass flow rate of hydrogen. The pressure inside storage tank starts to build up due to mass flow of fuel into a confined volume. Pressure inside storage tank is measured at each time step and the condition for filling of hydrogen is based on the pressure limit of storage tank. The process/flow chart from Figure 3.2 is a schematic representation of control logic for refuelling system.

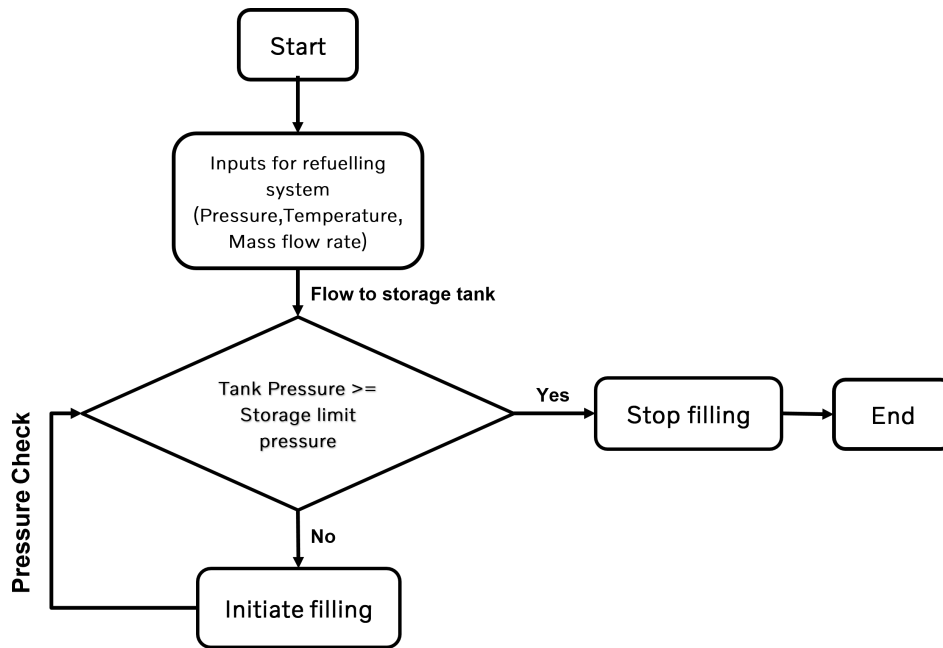


Figure 3.2: Process of Refuelling system

3.2 Hydrogen storage tank

A cylindrical volume object with multiple wall layers for thermal insulation, aluminium overlap layer is made up of composite materials. The dimensions of storage tank depends on volume capacity and surface area. These two factors affect the amount of hydrogen stored in tank and performance of thermal insulation respectively. Performance a storage tank would depend on thermal insulation to limit heat ingress from environment, also geometric dimensions of the tank is of importance as heat transfer is a function of surface area.

Factors that influence mass of hydrogen stored in tank are as follows:

- Pressure and temperature of fluid entering storage tank
- Initial temperature and pressure of storage tank

Since cryo-compressed hydrogen storage is at cryogenic temperatures, storage tanks should be well insulated with multi layer thermal insulation to limit the heat ingress leading to pressure build up inside storage tank.

3.3 Boil-off system

When the truck is stationary and there is no consumption of hydrogen from storage tank towards fuel cell, then the storage tank is in dormant state. In this dormant state, there is a possibility for heat to transfer across the walls of storage tank layers, even in the presence of thermal insulation and raise the temperature of stored hydrogen fluid. Beyond a certain point of pressure build up, it will be a safety hazard issue and to resolve it, pressure relief/venting is required to bring back the pressure inside storage tank to operating conditions.

The maximum margin of safety for pressure is 50 bar above the maximum allowable pressure and the pressure drop after venting could be varied. From Figure 3.3, the process/logic for the pressure relief system is represented in a flow chart. The opening and closing of vent valve is based on pressure check at the storage tank.

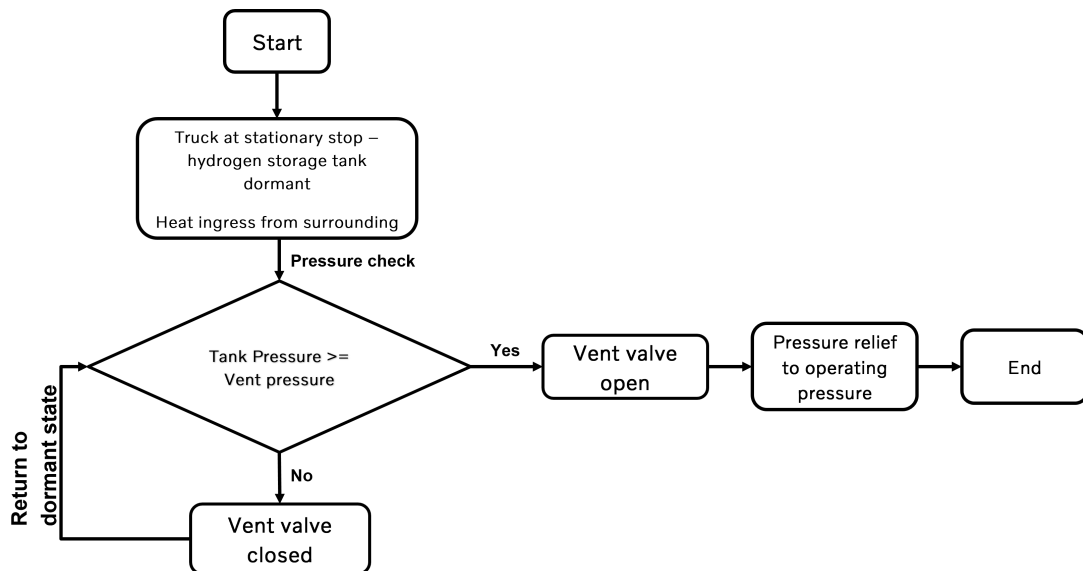


Figure 3.3: Process of pressure relief

3.4 Hydrogen consumption

Hydrogen consumption/extraction is where hydrogen is consumed from storage tank to fuel cell. Amount of hydrogen that is consumed is a function of power requirement from the fuel cell and truck operation such as driving, parking and loading. How consumption affects state properties in the tank would therefore vary based on different truck operations. During consumption of hydrogen from storage tank, there is a drop in pressure and temperature due to the mass flow of hydrogen across the boundary of storage tank. When modelling hydrogen consumption, it is time based and must incorporate the truck operation based on legislation for maximum duration of driving, stationary stop for break/lunch, overnight stop and weekend stop. The time based truck operation is explained in upcoming section duty cycles along with time duration for each of the truck operation.

4

Simulation

In this chapter, considering all the requirements from theory and modelling, the simulation environment is setup and all the inputs/boundary conditions to individual objects are represented. The simulation for each sub-system as mentioned in Chapter:3 is run in an order and not all at once so as to reduce/limit any computational error from solver in GT-SUITE. The fluid composition to be used for the simulation has to be unique in GT-SUITE, which is a drawback as the fluid composition of isomers of hydrogen as discussed in section 2.3 para-ortho conversion can not be included. This is because the fluid composition properties for each of the isomer varies and only one of the fluid composition can be used. Hence, to have stability and homogeneity in the simulation, hydrogen fluid object from GT-SUITE library of fluids is adopted.

4.1 Case setup

In GT-SUITE, there is a possibility to assign different values to individual parameters to observe the influence of each parameter on the result and this function called case setup. This function gives an opportunity to investigate how different initial conditions of storage tank will affect the results. An option called "previous case setup" is an advantage, where it will allow simulations to be run continuously where results from one simulation is given as an input to the next simulation and this will be helpful to observe how storage tank evolves over multiple simulations/cycles.

4.2 Parameter variation

Based on literature and how much the components is allowed for parameter variation in GT-Suite, state properties would be evaluated, more specific different cases of temperature, pressure and volume would be used as an input to the hydrogen storage tank. In boundary conditions for refuelling, temperature of fuel delivery will be varied as well, based on data for which refuelling stations could deliver hydrogen at. A parameter/input variation to observe the trend in change of results obtained, will help to understand the system through results by comparing different initial conditions and validating these results to the findings from literature review.

4.3 Refuelling

For refuelling/filling of hydrogen in cryo-compressed storage regime, currently there is no existing standard protocol for filling. A filling protocol does exist for compressed gaseous hydrogen as per SAE J2601-Fueling Protocols for Light Duty Gaseous Hydrogen Surface Vehicles [30], but this protocol has a higher end state target pressure than the required design pressure for cryo-compressed hydrogen storage, which cannot be used for our simulation. An alternative way to adopt conditions for filling of hydrogen is to use the target filling rate as mentioned by Cryomotive [33]. This would allow us to follow a protocol for filling rate which would impact the pressure rise rate, temperature and filling duration of hydrogen and this would be one of the best methods to adopt now, until a filling protocol based on temperature and pressure is available. In the Figure 4.1 shown below, components or objects used in the simulation model can be viewed.

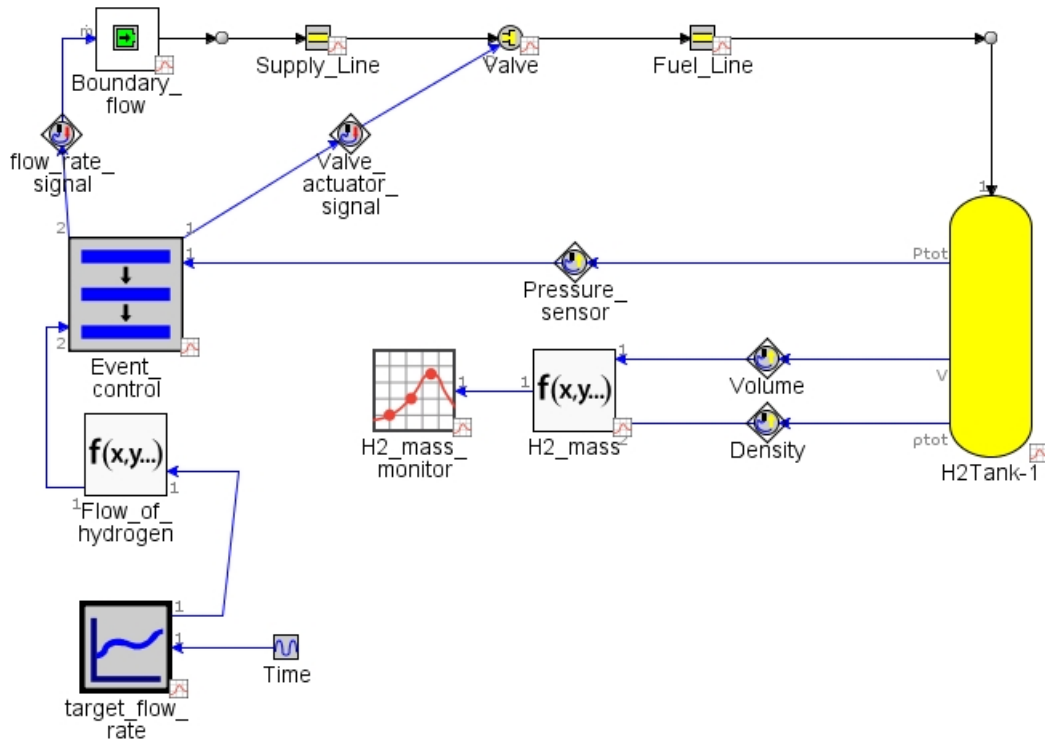


Figure 4.1: Refuelling system

Inputs/boundary conditions for components/objects in refuelling sub-system are :

- Boundary flow - Mass flow(kg/s), temperature of fuel(K) and hydrogen fluid composition from GT SUITE library of fluids.
- Event control - control logic for filling of hydrogen, when pressure limit is reached, refuelling is stopped by actuating the valve to close
- Target flow - input of required mass flow of hydrogen

- Storage tank - Volume, surface area, initial state properties-pressure and temperature

The value of target mass flow, temperature of fuel and pressure control for hydrogen filling is obtained from Cryomotive[33]. The volume of tank mentioned is a calculated number which could possibly carry 40 kg of hydrogen in a single tank for a given fill density of tank to be $66\text{kg}/\text{m}^3$. The boundary condition for storage tank could vary as it is a function of truck operation, where temperature and pressure could depend on hydrogen extraction and dormant state of hydrogen tank. Hence a case study/sensitivity analysis for the parameters affecting the fill density of storage tank is carried out in the simulations. which could be observed in table 4.1

Target mass flow	500-900 kg/h
Temperature of fuel	35-50 K
Fluid composition	Hydrogen
Refueling pressure control	400 bar
Volume of tank	600 L

Table 4.1: Boundary condition for filling of hydrogen

Briefly explained, the model operates with pressure check of tank at each time step, and filling of hydrogen event takes place until the storage pressure limit is reached. The control logic for filling of hydrogen and actuator for the valve to open/close is through the Event_control object.

4.4 Hydrogen storage tank & boil-off losses

For hydrogen storage tank, the important aspect in terms of simulation is thermal insulation/heat ingress from surrounding environment. This factor/parameter is key for hydrogen loss free stationary time which means the time duration until which hydrogen fluid in storage tank requires pressure relief due to pressure build from heat ingress and increased temperature inside the tank. Thermal insulation demand can be varied widely based on the balance/optimization between cost of thermal insulation and amount of hydrogen lost due to boil off. Also, the information on what materials are used for thermal insulation and different combination of multi layer insulation would lead to a lot of options available for thermal insulation demand. Instead, to overcome this ambiguous situation, a sensitivity analysis for thermal insulation demand could be very useful as the insulation demand is quantifiable and this data can be used to procure the right insulation required from the supplier.

To conduct the sensitivity analysis, thermal properties of tank wall layers is set as adiabatic condition, where there is no heat transfer between tank wall layers with surrounding environment and fluid stored inside tank. Instead a constant value of heat is added to the fluid which would be very similar to heat ingress as a function of thermal insulation performance. This is possible in GT-SUITE for a flow volume object and it can be set as a parameter in the case setup to observe the effects of varying heat ingress. Surface area of storage tank corresponds to that of a

4. Simulation

cylinder object which is the default setting in GT-SUITE and would not require any assumption or a parameter variation, instead it would only depend on the volume of storage tank.

In Figure 4.2 below, hydrogen storage tank is highlighted and the initial/boundary conditions of storage tank would vary as per truck operation, as explained in previous section.

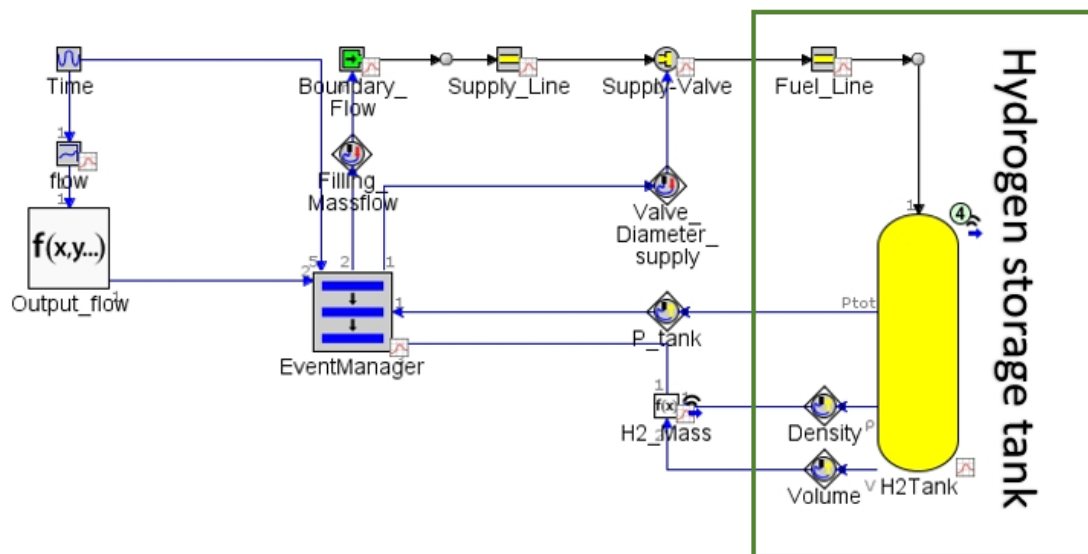


Figure 4.2: Storage system

As mentioned above about the heat ingress into storage tank, this process will increase temperature and pressure build up of the fluid stored. Above a certain pressure limit, excess pressure beyond the maximum allowable pressure limit should be relieved or vented. It is a safety hazard for pressure venting of hydrogen, especially in a confined space/parking of truck. The pressure venting process is carried out with the help of rupture discs where the hydrogen fluid flows through them to regulate pressure within storage tank. In simulations, the pressure venting is according to a control logic where the valve is opened to let hydrogen fluid flow and observe the changes of state properties inside storage tank. An illustration of the model could be observed in figure 4.3 below

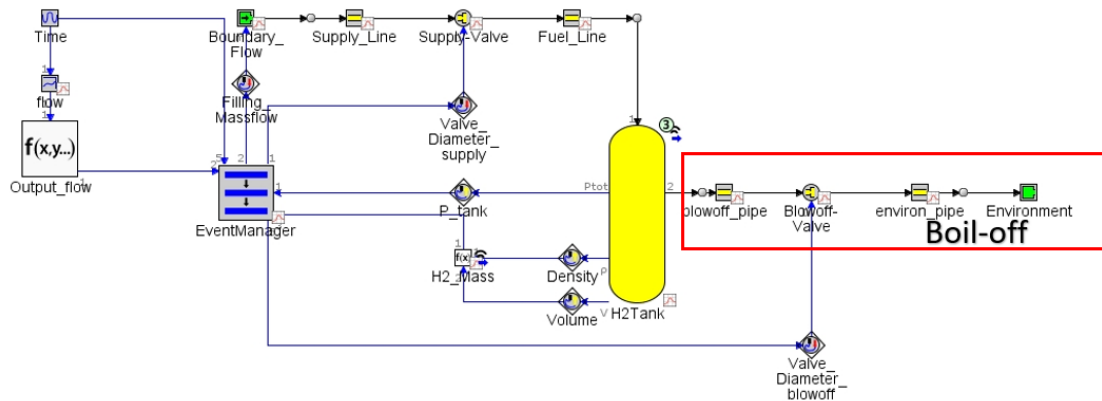


Figure 4.3: Boil-off system

For controlling boil-off, pressure of storage tank would be an input to the control system, for when to open the valve and relieve the tank to a certain pressure. When the control conditions are satisfied and the tank pressure has decreased until the safe operating pressure, the valve would then close until the pressure has reached maximum allowed pressure again and the above process is repeated.

4.5 Hydrogen Consumption

Hydrogen consumption in the simulation model is time based so that it consumes hydrogen from storage tank during truck operation and when the truck is stationary with fuel cell shut-off, hydrogen consumption is shut off. When the truck is in a driving state, fuel cell is consuming hydrogen and a certain mass flow is input for hydrogen consumption. Value of Hydrogen consumption used in our simulation is adopted from a testing of fuel cell truck by retailer Coop in Switzerland, where a 34 ton truck had a hydrogen consumption of 8kg/100km [32]. Now considering the maximum legal speed limit for trucks on motorway to be 90 km/h, the truck would cover roughly 400 kilometers in 4.5 hours which corresponds to a consumption of 32kg of hydrogen for the journey. Utilizing this consumption rate in our simulation, simulation results for hydrogen storage cycle was obtained. Below in figure 4.4 an illustration of the model could be observed

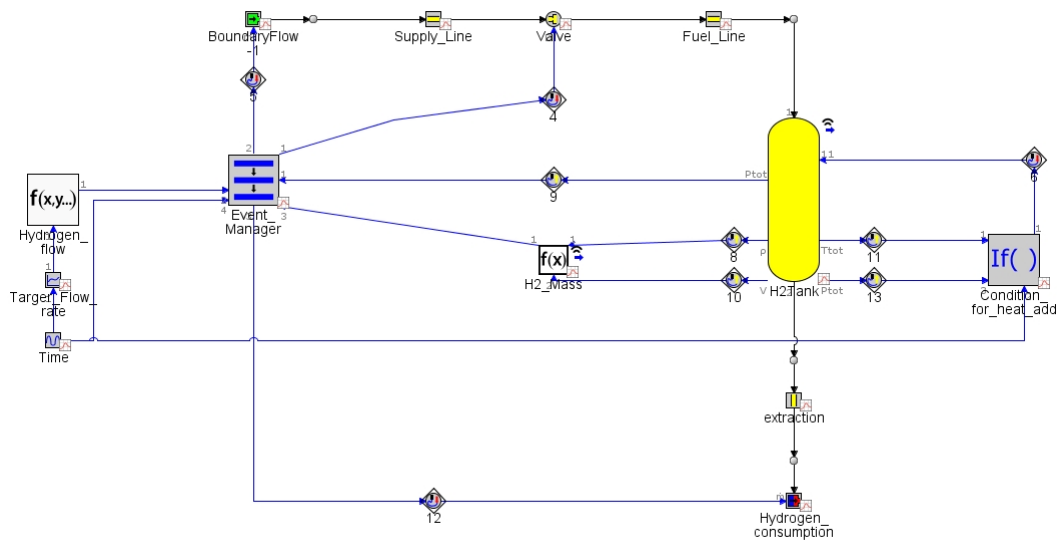


Figure 4.4: Hydrogen Consumption

Depending on truck operation and state of fill in hydrogen storage, state properties in storage tank is influenced by truck operations such as dormancy, loading and driving. Truck operation will influence the fill density as a function of pressure and temperature of storage tank. According to Blanco et al (2019), fill density increases with daily driving distance since the tank will cool down during hydrogen consumption[19]. When refuelling of hydrogen post consumption event, storage tank initial temperature will be colder leading to a higher fill density. In Figure 4.4, a representation of simulation model for hydrogen consumption. During hydrogen consumption, pressure drops in the storage tank as a function of mass flow out of the tank with drop in temperature, a self cooling process[33]. When the temperature and pressure of hydrogen in storage tank drops below the critical point, hydrogen enters liquid phase, which makes it difficult for extraction. Hence, to maintain a minimum pressure required for consumption towards fuel cell from storage tank, hydrogen fuel is heated and a constant pressure is maintained for consumption. The source of heat for maintaining the pressure is not under study but the range of heat required could in a few kilowatts. State properties of hydrogen storage tank evolve over time due to truck operation, this will be discussed with results.

4.5.1 Duty cycles

Simulations are carried out in GT-SUITE with different duty cycles i.e truck operation as a function of hydrogen consumption, in order to simulate real conditions of scenarios that a truck would be exposed to. Duty cycles that are evaluated in the model are based on EU regulation that allows truck drivers to operate maximum 9 h/day [34]. During these 9 hours different event takes place such as driving, loading, refuelling, lunch/snack stop and overnight stop. An illustration of how different events are distributed in one day cycle/weekly cycle could be observed in figure 4.5a below.

Stationary time corresponds to a parked truck with fuel cell shut off and no inflow or outflow of hydrogen mass at storage tank. During the stationary period, tank properties evolving could be observed based on heat ingress from the environment. Consumption corresponds to fuel cell operational and extraction of hydrogen from storage tank. Refuelling/filling of hydrogen takes up a small portion of time during truck operation and this is advantageous over battery charging taking up more time before truck can be on the road again.

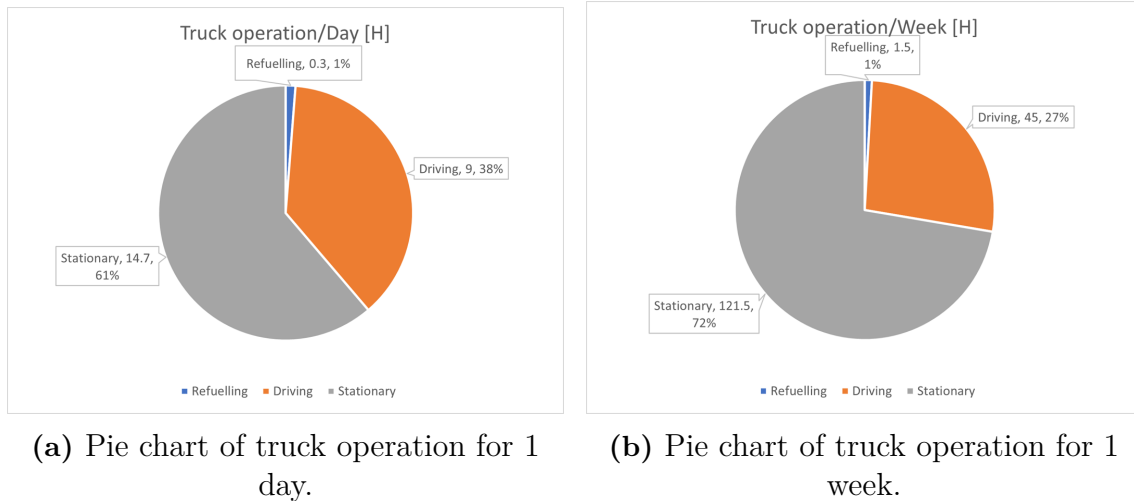


Figure 4.5: Illustration of Truck operation duty cycles

The distribution of time for truck operation is represented in the Figure 4.5, where a duty cycle for a given day with overnight stop and a week long cycle including five working days and two stationary weekend days. Truck operation is represented in hours for a given day/week.

4.5.2 Hydrogen storage cycle - Supplier data

Cryomotive is one the leading companies working on a solution for hydrogen storage system [33], and with their information and data made available to us by Volvo, validation of the thermodynamic model for hydrogen storage in our study with simulation results would be possible. Adopting a duty cycle as seen in Figure 4.6, simulation results from the thermodynamic model and the evolution of state properties during truck operation can be evaluated. The duration of truck driving and stationary stops is in accordance with the EU regulation for truck drivers as discussed in Section 4.5.1.

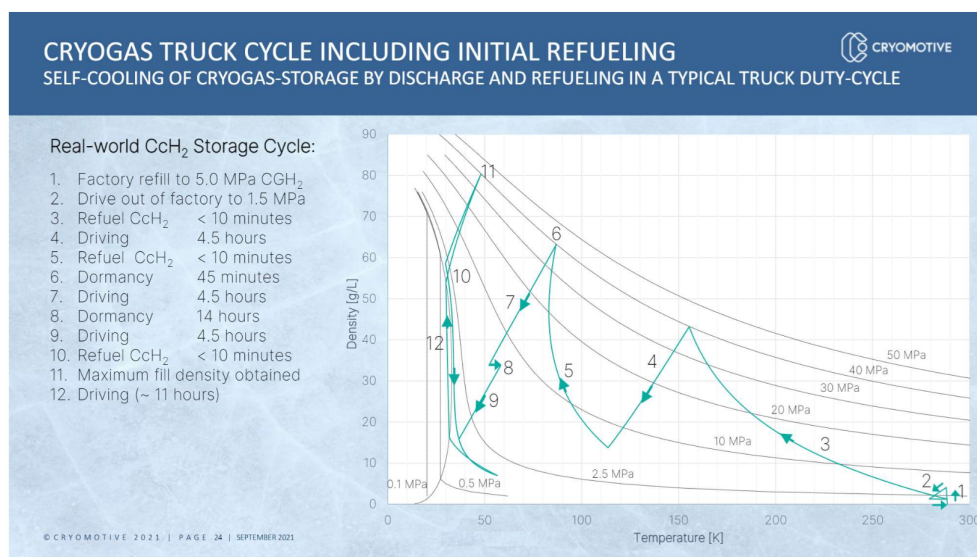


Figure 4.6: Plot obtained from Cryomotive [33]

4.6 Adaptation of GT SUITE for simulation of hydrogen storage in our study

When setting up a simulation environment in GT-SUITE for hydrogen storage application, following adaptations or settings was necessary.

- Use of Redlich-Kwong equation in the GT-SUITE solver state equation to incorporate Joule-Thomson effect for hydrogen.
- Decreasing GT-SUITE solver tolerance limits to reduce the computational error for state properties. This decrease in tolerance limit results in prolonged simulation duration, which was handled by running the simulation on the GT-SUITE distributed cluster.
- Initialising refrigerant hydrogen fluid as fluid composition from predefined library of fluids present in GT-SUITE. The refrigerant hydrogen has fluid properties and transport properties up to temperatures as low as 1 K.
- Implementing hydrogen consumption based on truck operation duty cycle, where truck driving and stationary stop is distinguished along with refuelling when the storage tank has reached low state of fill of hydrogen.
- Ability to carry out case studies for refuelling and boil-off losses, where state properties of tank are setup as parameter which can be varied. The results obtained from varying parameters will help us to understand the function of state properties of storage tank on the end state of simulating truck operations.
- Simulation with previous case initialised, where successive truck operation simulation can be carried out.
- External heat addition to fuel when it enters liquid phase during extraction/consumption to maintain a constant pressure towards fuel cell.
- Assumption of homogeneous initial conditions of GT-SUITE objects to reduce the non-convergence solver steps during computation.

5

Results & discussion

In this chapter, results from simulation are presented and discussed. The validation of thermodynamic model is with the help of results obtained. Case studies are conducted to observe the influence of tank initial state properties on fill density, dormancy/stationary condition.

5.1 Refuelling

For refuelling of hydrogen, the fill density depends on initial storage tank conditions, fuel temperature and following case study will illustrate the results obtained from simulation.

5.1.1 Case study for initial tank conditions

Simulation run for different initial tank conditions to observe the fill density, refuelling time and temperature at the end of fill. The input parameters and the results are presented in the table 5.1. Initial conditions of storage tank is the parameter and density, mass of hydrogen, refuelling duration is the results, all put together in a table. Conditions from filling station for refuelling of hydrogen is listed in Table 4.1.

Table 5.1: Input parameters and results

	Case 1	Case 2	Case 3
Initial tank pressure (bar)	20	70	15
Initial tank temperature (K)	288	112	58
Density (kg/m ³)	59.56	65.6	72
Mass of hydrogen (kg)	28.93	31.87	34.96
Temperature at the end of fill (K)	96.7	81.2	66.5
Refueling duration (s)	560	527	593

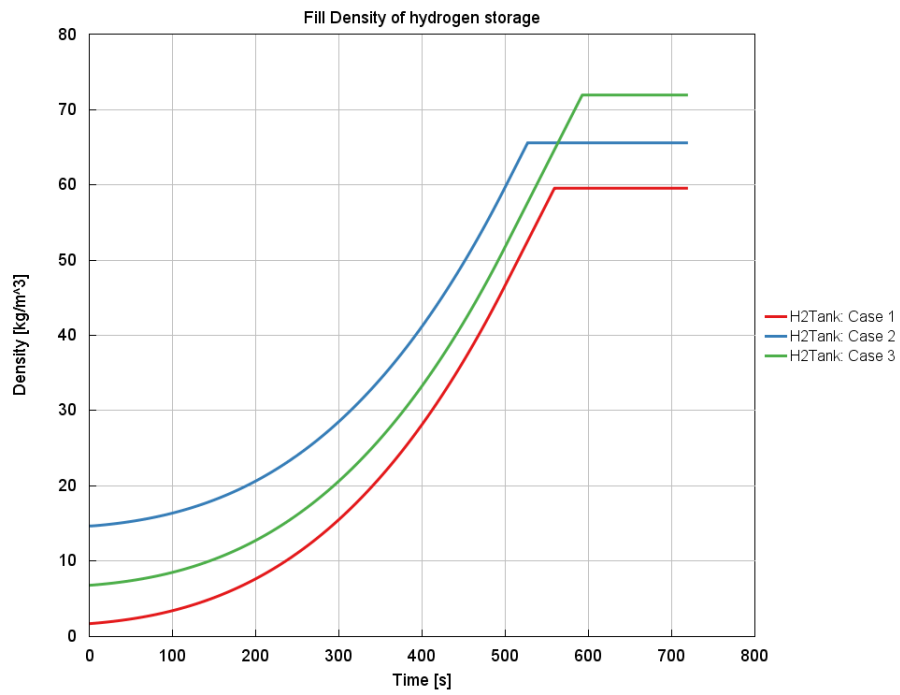


Figure 5.1: Fill density of hydrogen storage

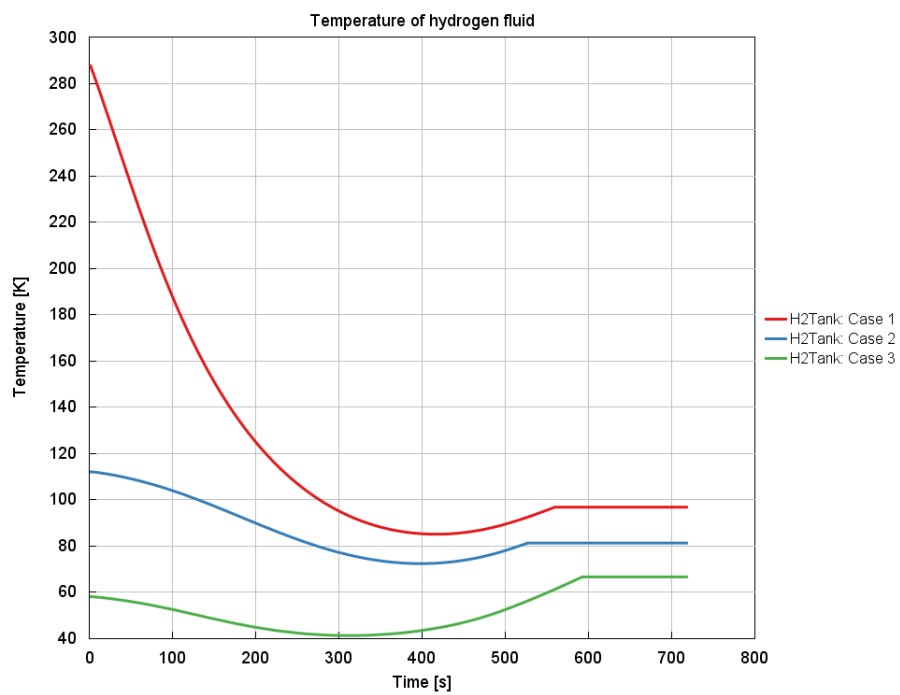


Figure 5.2: Temperature of hydrogen fluid in storage tank

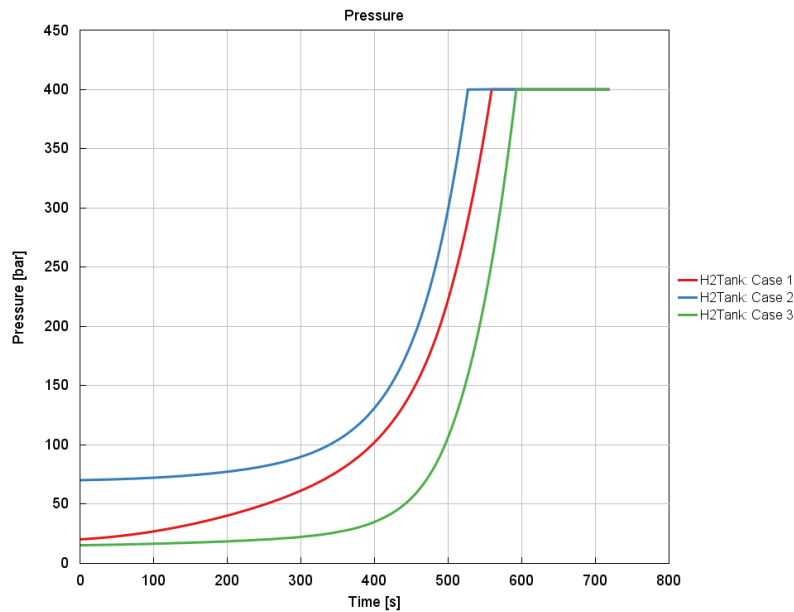


Figure 5.3: Pressure of hydrogen fluid

From Figure 5.1, it can be observed how fill density varies with initial tank conditions. The highest fill density is obtained for the lowest initial tank temperature. This can be explained as the pressure build up during filling of hydrogen due to the mass inflow of hydrogen and increased initial tank temperature and pressure leads to shorter refuelling time as the criteria/control for refuelling is pressure based and the rate of pressure build up is dependent on initial tank conditions. Due to this effect, fill density depends on initial tank temperature and pressure, therefore to obtain higher fill densities, colder vessel condition is favourable.

The unavailability of a filling protocol for cryo-compressed hydrogen and with the adoption of target mass flow rate as the input for filling, results obtained at the end of filling may vary but the trend/pattern of results based on initial tank conditions for fill density and filling time could be observed. The results obtained is henceforth validated with the data from CRYOMOTIVE[33] for fill density. Results of case 2 is validated, whereas for case 1 and case 3, fill density value deviates. For case 1, it is a warm vessel and in case 3, hydrogen fluid does not enter liquid phase as the temperature does not drop below the boiling point of hydrogen, this can be observed from Figure 5.2. The mentioned issue and deviation from results can be solved with the help of a filling protocol which will operate based on tank pressure and temperature to modify fuel temperature and pressure for a warm or cold vessel.

From the temperature plot in Figure 5.2, the drop in temperature of hydrogen fluid is due to the cooling from expansion of hydrogen fuel into a large volume. However, this cooling effect is due to Joule-Thomson effect, where the fluid cools down upon expansion and beyond inversion temperature which is a function of fluid pressure, the fluid starts to heat up upon expansion[35]. The cooling or heating of the expanding gas depends on Joule-Thomson coefficient and the switching point between heating and cooling is called inversion point.

5.1.2 Case study for temperature and mass flow of fuel

Varying fuel temperature and mass flow of fuel during refuelling event. Initial condition of storage tank is at a temperature of 112 K and pressure of 70 bar. The mass flow of fuel is increased by a factor of two from case 5 onward, this is to observe how filling curve/mass flow of hydrogen would influence fill density, filling time and temperature of fluid at the end of refuelling event.

Table 5.2: Input parameters and results

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8
Fuel flow rate multiplier	x1	x1	x1	x1	x2	x2	x2	x2
Fuel temperature	35 K	40 K	45 K	50 K	35 K	40 K	45 K	50 K
Fill Density (kg/m^3)	65.56	63.06	60.61	58.32	65.55	63.07	60.61	58.32
Refuelling time (s)	544	530	520	509	405	396.6	388	380
Temperature at the end of fill (K)	81.2	87.48	93.82	100.1	81.23	87.48	93.8	100

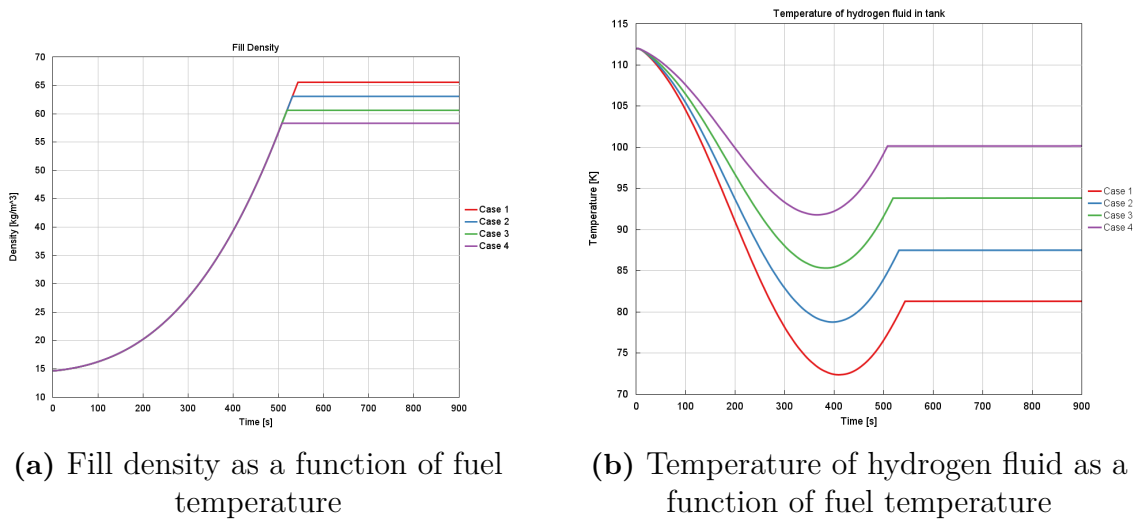


Figure 5.4: Fuel temperature of hydrogen influence on storage properties

From Figure 5.4a, it can be observed that fill density for case 1 to case 4 varies which is due to changes in fuel temperature. Case 1 has the least fuel temperature and attains highest fill density whereas case 4 achieves lower fill density when compared to case 1 with only change in fuel temperature and same initial tank conditions. This observation of change in fill density can be explained with the help of a temperature plot in Figure 5.4b, where the temperature of hydrogen fluid at the end of filling varies. Density is a function of temperature and pressure as mentioned in Section 2.4, and fuel delivery temperature is one of the factors affecting the temperature at the end of filling.

Now, when the mass flow of hydrogen is increased by a factor of two, following results are obtained.

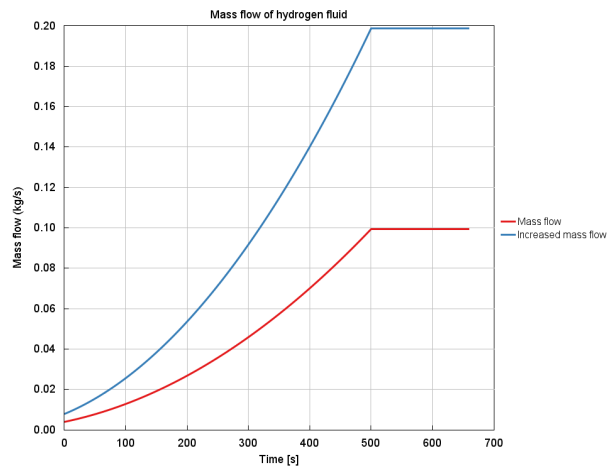


Figure 5.5: Mass flow of hydrogen during refuelling

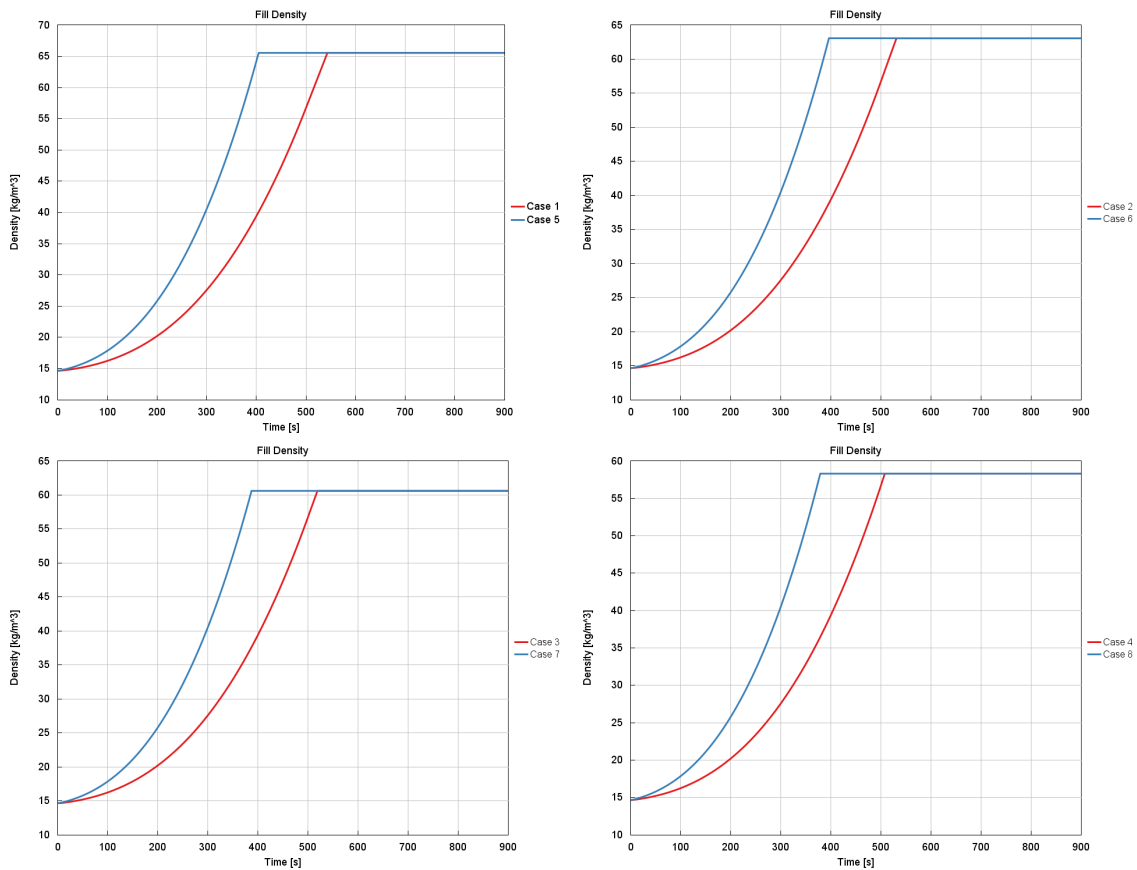


Figure 5.6: Fill density as a function of varying fuel temperature and massflow

From Figure 5.6, comparing case 1 and case 5, where the only change between the two is an increase in mass flow rate, fill density is unchanged as it is influenced by initial storage tank conditions and fuel temperature. This is also true for temperature at the end of refuelling event. From this case study, one of the observable changes is the duration of refuelling and the results can be viewed in Table 5.2.

5.2 Boil-off losses

To study the amount of hydrogen lost due to boil-off losses, case study based on initial conditions of tank before refuelling and sensitivity analysis of heat ingress during stationary/dormancy time is carried out. Also, the margin of safety for pressure after venting could be altered to observe the amount of hydrogen lost and number of pressure venting events during dormancy. The maximum duration of stationary park/dormancy time considered for simulation run is 63 hours which resembles for a scenario where the truck is parked from Friday evening till Monday morning, to resume truck driving/operation.

5.2.1 Varying initial conditions of tank

Considering different initial conditions of storage tank before refuelling, as adopted in Chapter 5.1.1. Results are represented in form of table and plots. Tank pressure at the end of refuelling is 400 bar and safety of margin for pressure relief is 50 bar. Post pressure relief, storage tank pressure is dropped back to 400 bar.

	Case 1	Case 2	Case 3
Initial tank temperature (K)	288	112	58
Initial tank pressure (bar)	20	70	15
Density of hydrogen (kg/m ³)	59.56	65.58	71.95
Mass of Hydrogen (kg)	28.94	31.87	34.96
Heat ingress (W)	10	10	10
Time until first pressure relief (h)	60.3	52.3	45.43
Number of pressure relief events	1	1	1
Amount of Hydrogen lost (kg)	0.95	0.91	0.84
% of Hydrogen fuel lost	3.2	2.85	2.4
Hydrogen loss rate (g/(W·h))	1.5	1.44	1.33

Table 5.3: Input parameters and results for boil off when initial tank conditions are varied

Key results to observe is the time taken until the first pressure relief which corresponds to minimum dormancy time before pressure relief and amount of hydrogen lost. The least time for pressure relief is observed for tank with maximum fill density as pressure increase due to heat ingress is a function of mass of hydrogen and Case-3 has the highest mass of hydrogen in storage.

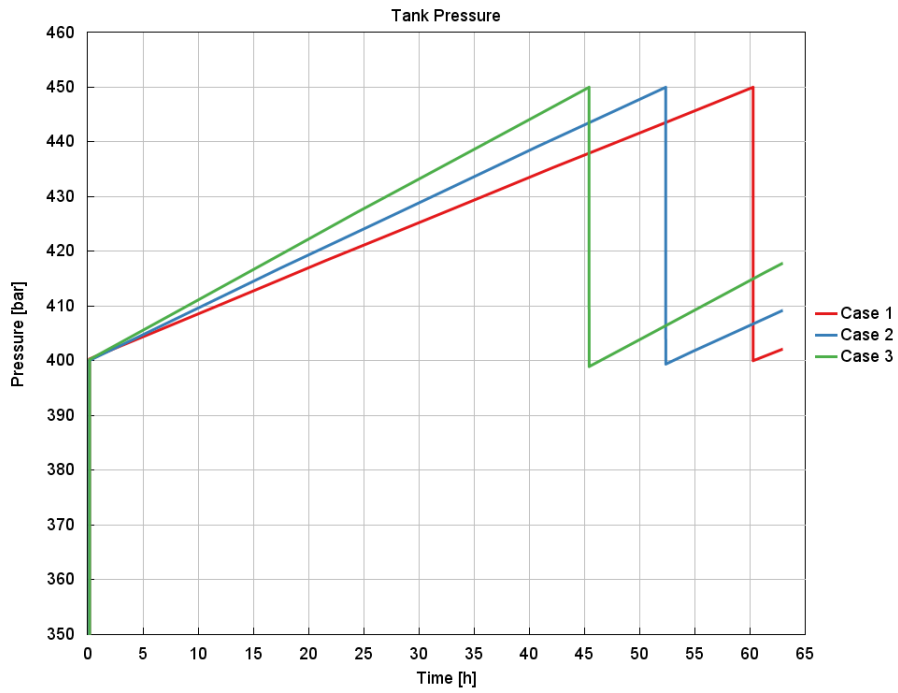


Figure 5.7: Tank pressure and pressure relief

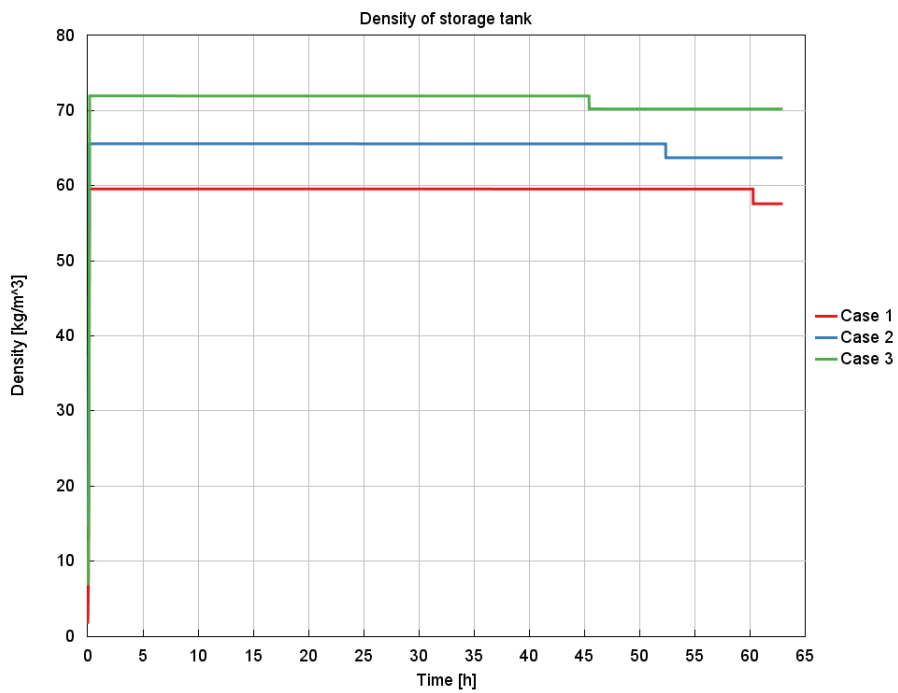


Figure 5.8: Density of hydrogen

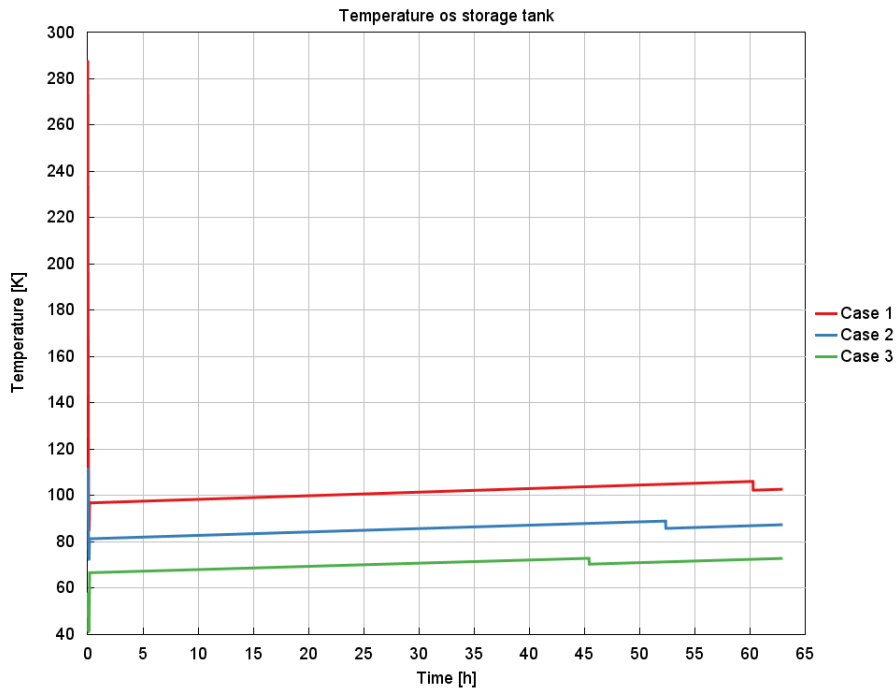


Figure 5.9: Increase in tank temperature due to heat ingress

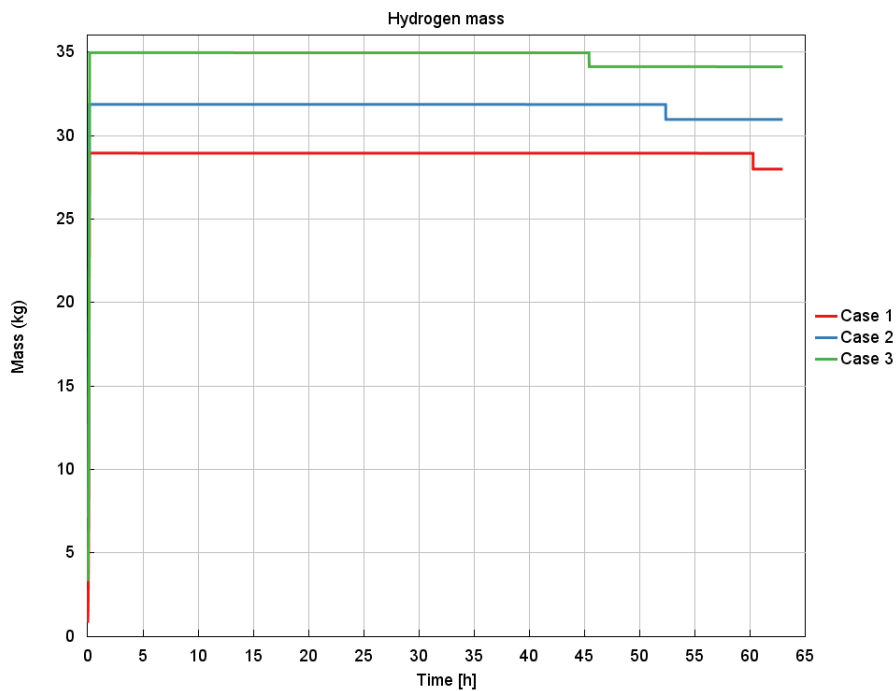


Figure 5.10: Mass of hydrogen

From Figure 5.7 and Figure 5.8, the rise in pressure due to heat ingress and pressure relief event can be observed where pressure drops back to 400 bar post venting event and highest fill density case has the least dormancy time. Rise in temperature is represented in Figure 5.9, and mass of hydrogen in Figure 5.10.

5.2.2 Sensitivity heat analysis

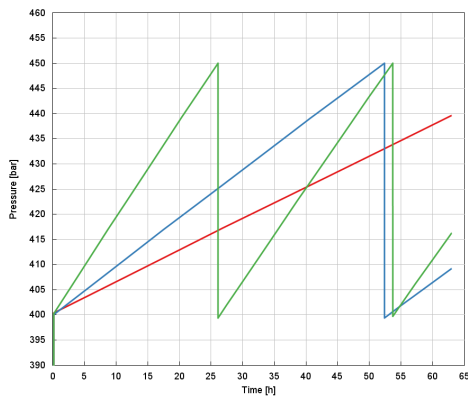
In this case study, varying the heat input/ingress for a given initial condition of storage tank to observe the effects on minimum dormancy time, number of pressure relief events and amount of hydrogen lost. The initial condition of storage tank is set as 70 bar pressure and 112 K temperature.

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6
Heat ingress (W)	6.5	10	20	25	30	50
Time until first pressure relief (h)	N.A	52.3	26.09	20.85	17.5	10.56
Number of pressure relief events	0	1	2	2	3	5
Amount of Hydrogen lost (kg)	0	0.91	1.83	1.83	2.77	4.7
% of Hydrogen fuel lost	0	2.85	5.74	5.74	8.7	14.75
Hydrogen loss rate (g/(W·h))	0	1.44	1.45	1.16	1.46	1.49

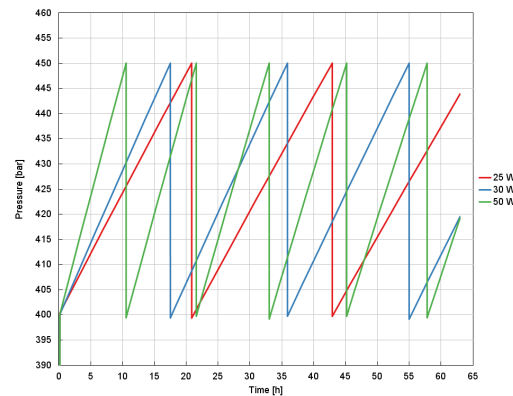
Table 5.4: Sensitivity analysis for thermal insulation demand for storage tank

With increase in heat ingress, it can be observed from Table 5.4 that minimum time duration for pressure relief decreases as increase in pressure to the maximum safety pressure is quicker. This can be seen in Figure 5.11 & Figure 5.12.

Number of pressure relief events is increasing with increase in value of heat ingress and amount of hydrogen lost is progressively increasing from one case to the next. The extent of rise in temperature is depending mainly on heat ingress and amount of hydrogen lost is directly proportional to number of pressure relief events. For Case 1 with 6.5 W heat input, the pressure build up does not reach the maximum pressure of 450 bar for pressure relief event to be active, hence at 6.5 W thermal insulation demand, there is no loss of hydrogen and pressure build up at the end of 63 hours dormancy reaches to a value of 440 bar.



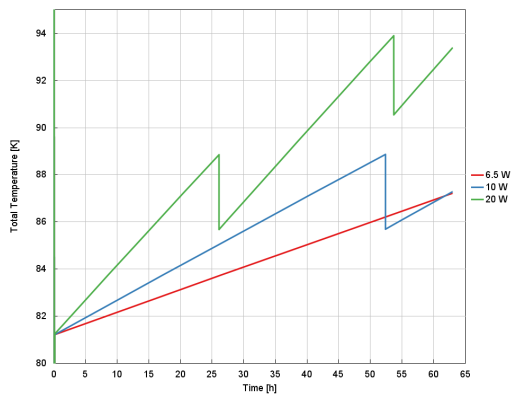
(a) Thermal insulation demand influencing tank pressure



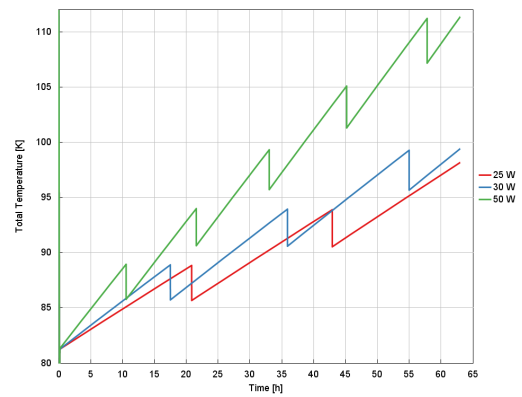
(b) Thermal insulation demand influencing tank pressure

Figure 5.11: Thermal insulation sensitivity analysis - Rise in tank pressure

5. Results & discussion

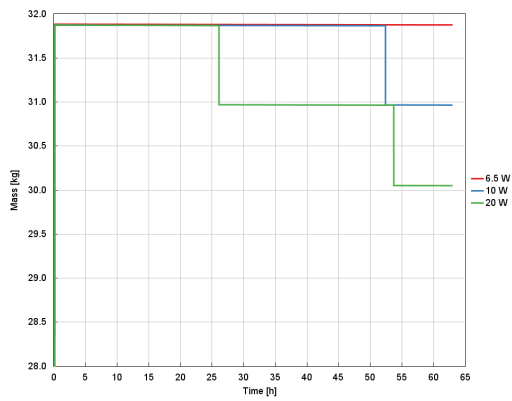


(a) Thermal insulation demand influencing tank temperature

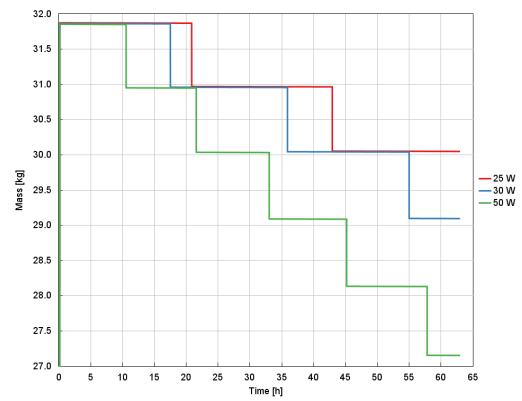


(b) Thermal insulation demand influencing tank temperature

Figure 5.12: Thermal insulation sensitivity analysis - Rise in tank temperature



(a) Thermal insulation demand influencing boil off loss



(b) Thermal insulation demand influencing boil off loss

Figure 5.13: Thermal insulation sensitivity analysis - Hydrogen boil off loss

5.2.3 Varying margin of pressure post venting/pressure relief event

In this case study, the value of pressure drop after pressure relief is varied to observe how number of pressure relief events and mass of hydrogen lost is affected. The initial condition of storage tank is 70 bar pressure and 112 K temperature with a constant value of 25 W as heat ingress from surrounding.

	Case 1	Case 2	Case 3
Pressure value post venting event (bar)	400	425	440
Time until first pressure relief (h)	20.85	20.85	20.85
Number of pressure relief events	2	4	10
Amount of Hydrogen lost (kg)	1.83	1.81	1.86
% of Hydrogen fuel lost	5.7	5.67	5.83

Table 5.5: Case study results

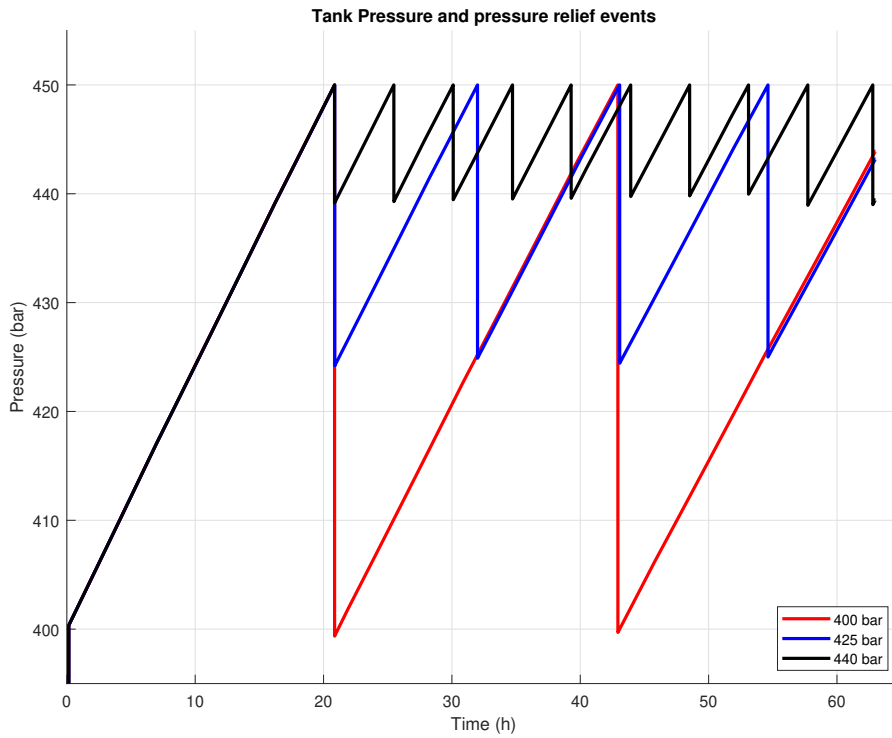


Figure 5.14: Pressure relief event as a function of margin of pressure post venting

From this case study, it can be observed that only the number of pressure relief events is changing but the amount of hydrogen lost due to boil-off does not change significantly. Hence, amount of hydrogen lost and minimum dormancy time before pressure relief would mainly depend on the initial conditions and heat ingress into storage tank.

5.3 Consumption

Consumption of hydrogen from storage tank towards fuel cell is a function of truck operation, hence simulation results vary with each scenario. To focus on thermodynamic modelling and observe state properties of storage tank, a simulation run based on a hydrogen storage cycle which includes refuelling and consumption of hydrogen from storage tank. With the help of hydrogen storage cycle data mentioned in Cryomotive[33], simulation for consumption of hydrogen is carried out, mainly focusing on the state properties of hydrogen storage along with additional external heat input required to maintain constant pressure during extraction. Truck operation scenarios and plots from simulation results are represented below.

5.3.1 Warm storage vessel refuel with driving

When initial conditions of storage tank is near ambient environment, with low residual mass in storage tank, refuelling operation is carried out followed by a truck driving event. Refuelling of hydrogen is same as mentioned in Chapter 5.1, whereas for consumption of hydrogen is in regard with data from Section 4.5. Input for consumption of hydrogen is to the Hydrogen consumption object as represented in Figure 4.4. Results and plots obtained for the simulation are as follows :

From the Figure 5.15, the drop in pressure and temperature of hydrogen storage is due to hydrogen consumption can be observed. Drop in temperature is due to the self cooling phenomena during extraction, decrease in pressure is due to hydrogen extraction across the boundary of storage tank. Pressure of storage tank during hydrogen consumption does not drop beyond 20 bar, hence external heat input to hydrogen fluid is not necessary to maintain constant pressure during consumption. Mass of stored hydrogen at the end of refuelling is 42.38 kilograms and after driving for 4.5 hours, residual mass of hydrogen is 10.56 kilograms. Residual mass of hydrogen is low for continuing an uninterrupted driving of 4.5 hours, hence filling of hydrogen at the beginning of next drive cycle is necessary.

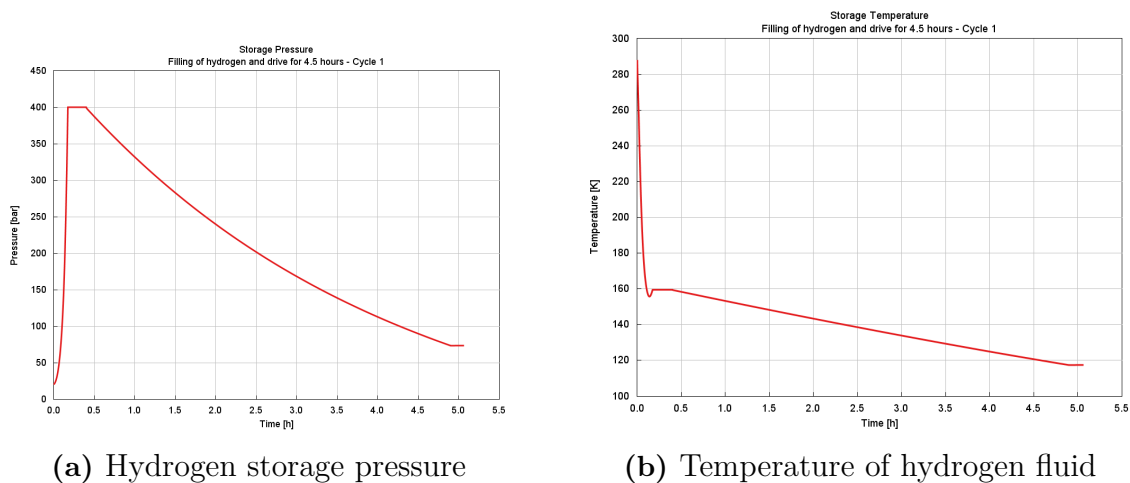


Figure 5.15: Storage cycle 1

5.3.2 Hydrogen storage refuel with driving and dormancy

Continuing from the end of previous driving/simulation cycle, residual mass of hydrogen is insufficient for 4.5 hours of uninterrupted driving, hence refuelling of hydrogen storage is carried out followed by driving and a overnight stop/stationary/dormancy for 14 hours is necessary as the truck driver should not drive for more than 9 hours on a given working day. Following results are obtained.

The drop in temperature due to self cooling during extraction and pressure drop due to hydrogen mass flow across storage boundary is similar to previous driving scenario except for the end state temperature and pressure value as the initial condition for refuelling is different compared to previous simulation, which leads to new values of temperature and mass of hydrogen stored post refuelling event. This is in accordance with obtaining higher fill density of storage tank as mentioned in Chapter 5.1. There is an increase in temperature and pressure due to heat ingress during dormancy. Pressure of storage tank during hydrogen consumption does not drop beyond 20 bar, hence external heat input to hydrogen fluid is not necessary to maintain constant pressure during consumption.

Mass of hydrogen stored is 68.6 kg, an increase from previous refill event and post truck driving event for 4.5 hours and dormancy for 14 hours, residual mass of hydrogen left in storage tank is 36.7 kg. Residual mass left in storage tank should be sufficient for an upcoming driving event of 4.5 hours, hence the cycle continues after 14 hours of dormancy.

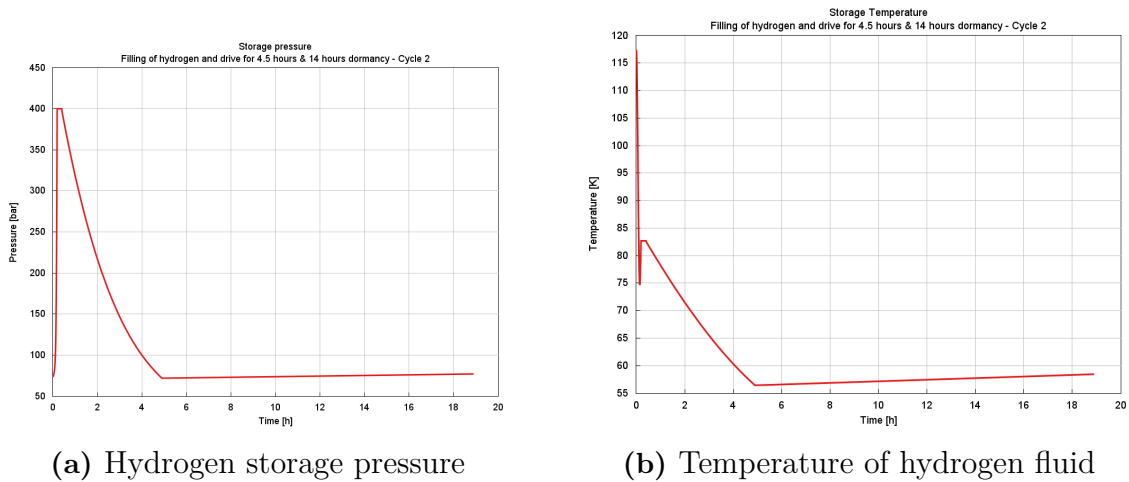


Figure 5.16: Storage cycle 2

5.3.3 Continued truck driving

Truck driving is continued after overnight stop, with sufficient mass of hydrogen in storage tank. Pressure and temperature continue to drop during hydrogen consumption. When the pressure in storage tank begins to drop below 20 bar, external heat input to hydrogen fluid is initiated to maintain constant pressure of 20 bar in storage tank necessary for hydrogen mass flow across tank boundary towards fuel cell. The amount of heat required is in the range of few kilowatts but the source of heat for this operation is not under the scope of thesis. The constant pressure maintained at 20 bar and rise in hydrogen fluid temperature due to heat added can be viewed in the results below. Residual mass of hydrogen left in storage tank at the end of driving is 4.5 kg, which will be insufficient for an upcoming driving event, hence, refuelling of hydrogen is initiated in the beginning of next cycle.

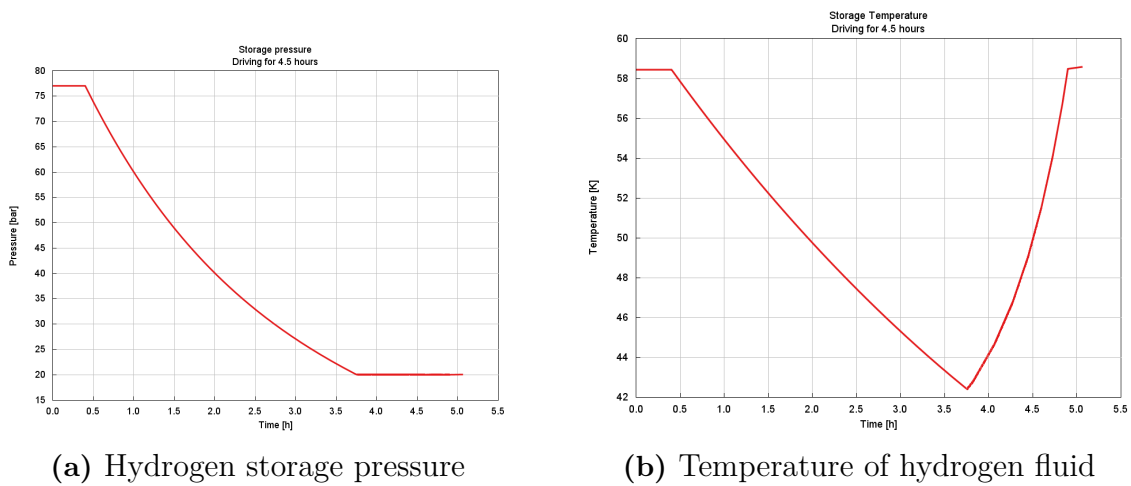
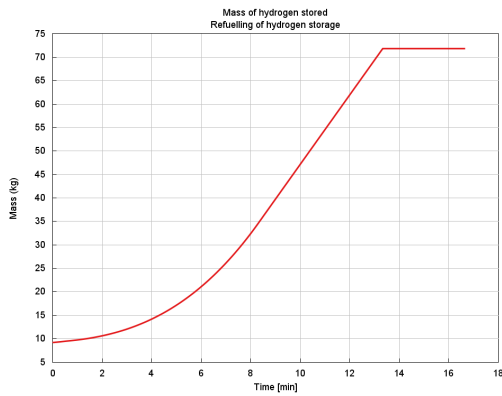


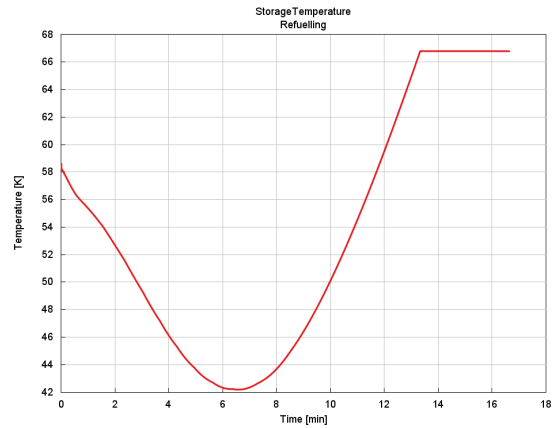
Figure 5.17: Storage cycle 3

5.3.4 Refuel of hydrogen storage

Filling of hydrogen storage to replenish the mass of hydrogen stored and continue driving. In this scenario for refuelling, the initial tank temperature and pressure is more favourable than the previous two refills of hydrogen as a higher fill density is obtained in this scenario with 71.8 kg of hydrogen stored. Plots for temperature and mass of hydrogen stored is attached below.



(a) Mass of stored hydrogen -
Storage cycle 4



(b) Temperature of hydrogen fluid

Figure 5.18: Storage cycle 4

5.3.5 Hydrogen storage cycle

Now, combining all the four hydrogen storage cycles mentioned in the previous sections with density as a function of temperature and pressure in a single plot. Pressure is plotted as iso-lines and temperature along X-axis to track how density varies during the operation of hydrogen storage. The following plot in Figure 5.19 will be beneficial to visualise how storage properties change/vary/influenced by truck operation.

From Figure 5.19, it can be observed that density of hydrogen increases with driving as the tank reaches cooler temperature and fill density is a function of temperature. External heat addition to maintain constant pressure of 20 bar and rise in temperature can be observed in cycle 3. The final storage cycle 4 which is refuelling deviates from what is intended, this can be resolved with the help of a refuelling protocol. Even in the absence of a filling protocol, a higher fill density is achieved from successive truck operation cycles.

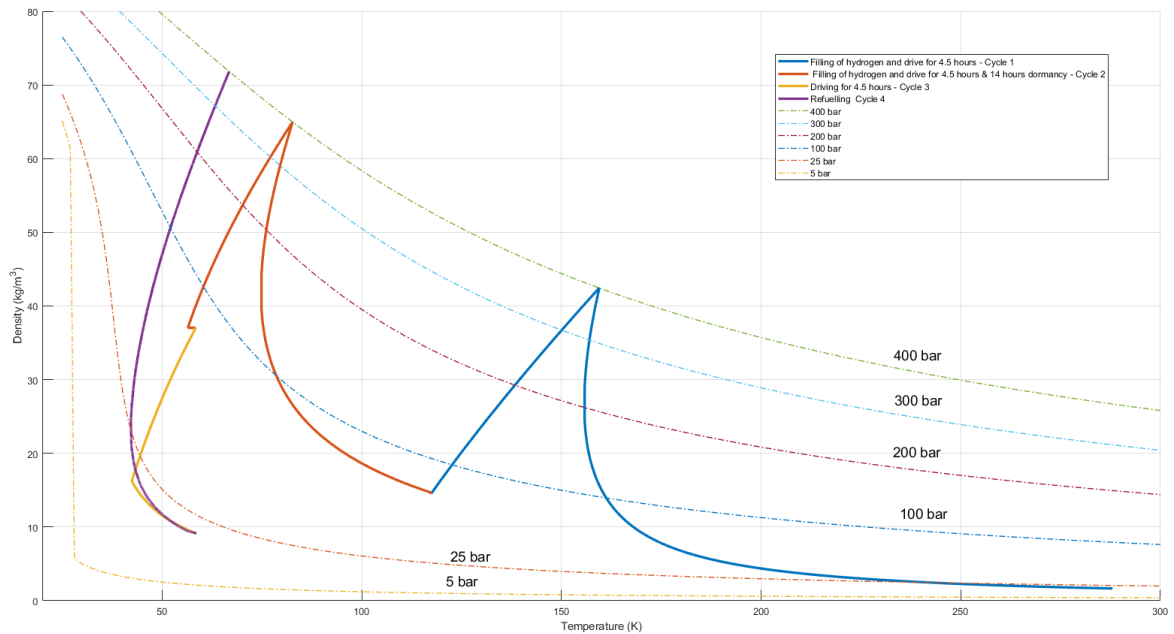


Figure 5.19: Hydrogen storage cycle

5.3.6 Thermodynamic model validation

To validate the thermodynamic model with results obtained from simulation and comparing the hydrogen storage cycle from Cryomotive as discussed in Section 4.5.2:

- Hydrogen storage cycle with respect to drop in pressure and temperature holds good, but with a protocol for hydrogen refuelling, filling of hydrogen during cycle 4 as mentioned in Figure 5.19, will push the hydrogen fluid to enter liquid phase, achieving higher fill density with the same end pressure of 400 bar.
- Data for consumption of hydrogen can vary depending on the application and power demand from the fuel cell, which could possibly change the slope/extent of drop in pressure/temperature, but the thermodynamic model will check for working condition such as mass of hydrogen available for extraction and the minimum pressure required for consumption of hydrogen towards fuel cell. This will allow for operating the hydrogen storage in the storage regime of CcH_2 .
- Results obtained for boil-off losses from simulation when compared with data from Cryomotive, the minimum holding/dormancy time and the hydrogen loss rate are within the limits, with possible improvements when Para-ortho hydrogen conversion is included.
- Regarding the software used for simulation GT-SUITE from Gamma Technologies, the output/results from simulation is stable, without any flow instabilities. Convergence for the solver used in computation is well within the tolerance limits. This is the outcome of a simulation model with known boundary conditions and initialisation of working fluid at each of the objects included in the simulation.

6

Conclusion

The objective of this thesis study has been to model a thermodynamic model for hydrogen storage tanks in GT SUITE, enabling the possibility to perform simulations for different truck operations. Results obtained from simulation would then help in observing evolution of storage tank properties based on truck operation over time. Final words of this thesis is mentioned in respective subsection stating how well the model performed and how results obtained could be used to characterize expected behaviour of a storage tank in a truck application when hydrogen fluid is in cryo-compressed hydrogen storage regime.

6.1 Thermodynamic Model

The thermodynamic model is fairly simplified, compared to what would be implemented in a real world storage system application. Main focus on storage tank and its state properties evolving over time gives an initial overview of the performance of storage tank. Initial tank conditions, thermal insulation demand, fuel temperature, mass flow rate of fuel set as parameters in each of the subsystems helped to understand their influence on results when varied. Setting up the simulation as a previous case initialisation made it easier to run multiple truck operation scenarios. Referring to the Section 5.3.6, the thermodynamic model is validated with results obtained from simulation against literature review and Cryomotive data [33].

The thermodynamic model could be made better/improved with the addition of para to ortho hydrogen conversion, resulting in cooling effects during dormancy/stationary stop, leading to an increased minimum holding time before pressure relief/boil-off losses. But, in most of the truck driving operation, hydrogen is consumed and at state of fill in storage tank less than or equal to 50%, the dormancy/minimum holding time is infinite without pressure build up beyond the safety margin pressure, hence resulting in zero boil-off losses.

6.2 Simulation results

Results obtained from simulation in various case studies helps us to have an understanding of performance of storage tank. Some of them are as follows :

- In case study for refuelling, it is observed that storage vessel with colder initial temperature can reach higher fill densities.

- Fuel temperature influences the fill density and temperature at the end of filling event.
- Minimum holding time before pressure relief during dormancy is inversely proportional to fill density, meaning higher fill density has lower holding time before boil-off losses.
- Thermal insulation demand is a key factor affecting boil-off losses. With poor thermal insulation demand, boil-off losses are high. The cost of thermal insulation is expensive with increase in material costs for insulation when performance of thermal insulation increases. Hence, thermal insulation demand is a trade off between the cost of materials for insulation and amount of hydrogen lost due to boil-off losses, which is also a function of truck operation application.
- During refuelling and consumption of hydrogen, from hydrogen storage cycle in Figure 5.19, it can be concluded that the hydrogen fluid is present in the CcH_2 storage regime and operating conditions with cooling effect and drop in pressure during consumption.

6.3 Ethics and sustainability aspect of thesis study

Since the beginning of the study, majority of the work done in the process involves study of scientific articles related to hydrogen fluid and its storage applications along with discussions on various occasions with Examiner and Supervisor both at Chalmers and Volvo Group, hence regarding the sustainability aspect of the study, there is a low impact on the environment during the process. The outcome of the study and its application in the automotive industry in upcoming years will have a significant positive impact on the environment with reduced carbon emissions and particulate matter.

6.4 Value of the thesis study

The outcome of the study will provide information about the state properties of hydrogen when stored in cryo-compressed regime. The evolution of state properties of storage tank during truck operation would help in understanding the functioning of the system through simulation results and provides information regarding operational parameters to engineers to develop a product such that this principle can be implemented into truck application. The thermodynamic model has been formulated in a way where the parameters such as temperature and pressure can be altered to observe the change in results obtained. This provides a feature where the model can be used to understand how the system operates at different conditions.

6.5 Recommendations and future work

As this thesis work has carried out mostly for modeling a system that should simulate storage applications of hydrogen, such as refuelling, pressure relief of storage tank at maximum design pressure and extraction of hydrogen from the tank for consumption. Based on the time limitation of this thesis, certain parameters that in reality would be affecting state properties and overall storage performance such as the Para-Ortho hydrogen spin isomer conversion that takes place as a function of temperature and pressure could be included with the help of equations governing the heat absorbed during the conversion. This inclusion of P-O conversion could result in increased dormancy time during stationary stop.

Next would be to implement a thermal insulation in the tank layer, which would be helpful for results with material properties instead of value for thermal insulation demand. This could also help us to understand the heat transfer between the fluid and tank walls with a convection coefficient rate. Weight of the tank could be calculated as the dimensions and material properties of storage tank is known.

Implementation of a refuelling protocol will result in obtaining standard refuelling rate with pre-determined end state temperature and density. An upgrade to the model in the field of hydrogen consumption data which is derived from real world driving conditions would lead to an improvement in results obtained and would also help calculate the loss of hydrogen due to boil-off and average usable tank capacity of hydrogen during truck operation. Sensitivity analysis for heat ingress and tank temperature was successfully carried out, and with the addition of hydrogen consumption data, we can obtain answers to the remaining question mentioned in Section 1.2.

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