FACULDADE DE ENGENHARIA DA UNIVERSIDADE DO PORTO

Optimization of hydrogen liquefaction method under steady state circumstances

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Resumo

O hidrogénio é atualmente visto como um vetor chave para a descarbonização da economia e redução da dependência de combustíveis fósseis. Esta tese investiga a liquefação do hidrogénio para armazenamento e transporte, um conceito amplamente estudado e aplicado com sucesso ao gás natural (GNL). No entanto, a liquefação do hidrogénio permanece dispendiosa e energeticamente ineficiente, necessitando de melhorias nesses parâmetros. As soluções potenciais incluem a otimização dos parâmetros operacionais e a reutilização do calor rejeitado pelo sistema.

Para simular a liquefação do hidrogénio, são necessários múltiplos balanços térmicos simultâneos, e o MATLAB é uma ferramenta poderosa para esse propósito. Permite realizar esses cálculos e inclui ferramentas de otimização capazes de melhorar o desempenho do sistema.

O estudo divide-se em três partes:

1. **Interação dos Componentes e Simulação do Sistema:** A primeira parte envolve funções para os vários componentes do sistema interagirem dentro de uma função principal que representa o ciclo inteiro.
2. **Modelo de Otimização:** A segunda parte é o modelo de otimização, que procura reduzir o consumo de energia no ciclo ajustando a taxa de fluxo do refrigerante (hélio) no sistema.
3. **Análise de Sensibilidade:** A última parte é o modelo de análise de sensibilidade, que representa graficamente a variação de uma variável escolhida e seu impacto nos parâmetros chave, como o consumo de energia ou o calor rejeitado.

As principais conclusões revelam que o aumento das eficiências isentrópicas nas turbinas e compressores leva a processos de arrefecimento mais eficientes, como evidenciado pela diminuição dos valores de UA dos permutadores de calor. No entanto, esse ganho de eficiência também resulta em temperaturas de saída mais baixas nas turbinas, potencialmente reduzindo a capacidade total de rejeição de calor. Além disso, verificou-se que pressões mais altas melhoram a condutividade térmica e a densidade do hélio, melhorando as capacidades de transferência de calor. Apesar disso, o aumento esperado na rejeição de calor não foi consistentemente observado, provavelmente devido a limitações no fluxo de massa da água de arrefecimento.

O estudo também examina a integração do calor rejeitado dos processos de liquefação do hidrogénio em redes de aquecimento urbano (DHNs), demonstrando um potencial significativo para aumentar a eficiência energética e reduzir as emissões de CO_2. Esta abordagem utiliza eficazmente o calor residual, proporcionando um método sustentável para satisfazer as necessidades de aquecimento. Além disso, a pesquisa identifica várias oportunidades de otimização, incluindo um melhor controlo das taxas de fluxo de massa e configurações de pressão para maximizar a eficiência dos permutadores de calor e do processo de liquefação como um todo.

No geral, esta tese avança o entendimento dos ciclos de liquefação do hidrogénio e sua integração com sistemas energéticos sustentáveis, oferecendo insights valiosos para a otimização desses processos e destacando áreas potenciais para exploração e melhoria futuras.

Abstract

Hydrogen is currently viewed as a key vector for decarbonizing the economy and reducing dependence on fossil fuels. This thesis investigates hydrogen liquefaction for storage and transport, a concept widely studied and successfully applied to natural gas (LNG). However, hydrogen liquefaction remains costly and energetically inefficient, necessitating improvements in these parameters. Potential solutions include optimizing operating parameters and reutilizing rejected heat from the system.

To simulate hydrogen liquefaction, multiple simultaneous thermal balances are required, and MATLAB is a powerful tool for this purpose. It allows for these calculations and includes optimization tools capable of enhancing system performance.

The study is divided into three parts:

1. **Component Interaction and System Simulation:** The first part involves functions for the various system components interacting within a main function that represents the entire cycle.
2. **Optimization Model:** The second part is the optimization model, which seeks to reduce energy consumption in the cycle by adjusting the refrigerant flow rate (helium) in the system.
3. **Sensitivity Analysis:** The final part is the sensitivity analysis model, which graphs the variation of a chosen variable and its impact on key parameters such as energy consumption or rejected heat.

Key findings reveal that increasing isentropic efficiencies in turbines and compressors leads to more efficient cooling processes, as evidenced by decreasing UA values of heat exchangers. However, this efficiency gain also results in lower exit temperatures at the turbines, potentially reducing the overall heat rejection capacity. Additionally, higher pressures were found to enhance the thermal conductivity and density of helium, thereby improving heat transfer capabilities. Despite this, the expected increase in heat rejection was not consistently observed, likely due to limitations in the cooling water mass flow.

The study also examines the integration of rejected heat from hydrogen liquefaction processes into district heating networks (DHNs), demonstrating significant potential for enhancing energy efficiency and reducing CO_2 emissions. This approach utilizes waste heat effectively, providing a sustainable method for meeting heating demands. Furthermore, the research identifies several optimization opportunities, including better control of mass flow rates and pressure settings to maximize the efficiency of heat exchangers and the overall liquefaction process.

Overall, this thesis advances the understanding of hydrogen liquefaction cycles and their integration with sustainable energy systems, offering valuable insights into the optimization of these processes and highlighting potential areas for future exploration and improvement.

Acknowledgements

All the work developed in the last few months required a somewhat high degree of concentration and time management. It was a challenging, rewarding, and exhausting experience that would not have been possible without the direct and indirect contribution of some people to whom I would like to express my gratitude.

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To the people who supported me, mainly my family and Sofia, in my transition from my previous degree to this one, who always believed in my abilities and work ethic.

To my family, the people that gave me the ability to change degree at 22 years of age, without limiting or blocking my path, and supported me throughout the 4 years that I did in Mechanical Engineering, including the thesis abroad.

I would like to dedicate this work to my grandparents, that even though they are no longer with us, I know they would be proud to see their grandson as an engineer.

Nuno Machado

“Per aspera ad astra”
Through hardships to the stars

- Seneca

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Abbreviations and Symbols

ATR	Autothermal Reforming
CAPEX	Capital Expenditure
C	Specific Heat Capacity
CHP	Combined Heat and Power
DHN	District Heating Network
EU	European Union
GDP	Gross Domestic Product
GSHP	Ground Source Heat Pump
HX	Heat Exchanger
LMTD	Log Mean Temperature Difference
NTU	Number of Transfer Units
PEM	Proton Exchange Membrane
POX	Partial Oxidation
POM	Partial Oxidation of Methane
PSA	Pressure Swing Adsorption
SEC	Specific Energy Consumption
SMR	Steam Methane Reforming
SOEC	Solid Oxide Electrolysis Cell
TES	Thermal Energy Storage
UA	Overall Heat Transfer Coefficient
COP	Coefficient of Performance
$\dot{m}$	Mass Flow Rate
$\dot{Q}$	Heat Transfer Rate
$\dot{W}$	Work Done
ΔT	Temperature Difference
ε	Effectiveness of Heat Exchanger
η_i	Isentropic Efficiency of Component
h_{ent}	Enthalpy at Entrance
h_{ext}	Enthalpy at Exit
h_{ext_i}	Enthalpy at Exit (Isentropic Transformation)
h_n	Enthalpy at Point n
T_n	Temperature at Point n

Chapter 1

Introduction

1.1 Background and Motivation

Energy is one of the most important resources in humanity. It is directly related to GDP and the living standards of a country. The energy demands of a country increase with the increase in quality of life, wealth, and population. In the 20th century, energy consumption and economic developments were tied to fossil fuels. This led to two major problems. Firstly, many countries are not fossil fuel producers, making them vulnerable to market fluctuations and dependent on others in the area of energy safety. Secondly, these fuels are not only finite but also highly pollutant, leading to global warming and climate change, which are highly detrimental to the planet (5).

One of the ways that the problem was addressed was through the implementation of renewable energies. These utilize naturally acquired resources (such as air, water, and sunlight) to produce the electrical power required by societies to function, accounting for 30% of the electricity production in 2022 (6). For other energy uses like transportation, heating, and industry, there are other methods beyond electrification.

One of the leading areas in the world in the renewable market is Europe (7). The continent's lack of strategic resources, primarily oil and natural gas, has resulted in dependence on foreign neighboring countries from North Africa, the Middle East, and Russia. To counteract this energy (and consequently economic) dependence, Europe has heavily invested in this new sector. This investment aims not only for "greener" production but also to decentralize the production of electricity, making the European (mainly the EU's) economy less volatile to outside events. This need for energy security became particularly evident in 2022 with the Russian Federation's invasion of Ukraine. The resulting market destabilization and sanctions on Russian gas led to record-high inflation and significantly increased electricity prices (8), affecting other goods as a natural consequence.

Recently, hydrogen has been seen as one of the main vectors for decarbonizing the economy. It serves as a direct substitute for natural gas and gasoline, to be used in the transport, heating, and industrial sectors, among others. The EU has placed great importance on hydrogen as one of the ways to achieve its goal of reducing dependence on other countries through the REPowerEU plan (9). This plan covers three main areas: saving energy, clean energy production, and diversifying energy production. The EU has set a goal of producing 10 million tonnes of renewable hydrogen by 2030, investing in production, infrastructure, and research.

Hydrogen is indeed one of the best avenues for this purpose, with its main characteristics being (10):

- The highest Low Heating Value on a mass basis of all known fuels;
- Virtually unlimited supply;
- The possibility of its production being integrated with renewable energies, making it 100% free of carbon emissions.

The possible integration on a large scale of hydrogen into the market, including in its liquefied form, can revolutionize the energy market. However, its major hurdles now are its energy consumption to liquefy and its storage (due to its temperature of -253ºC) (1). Therefore, it is vital to find ways to increase the efficiency of this process to make large-scale production and liquefaction a common practice.

1.2 Objectives

The main objectives of this dissertation were:

- To study the influence of certain thermodynamic factors (pressure of refrigerant and temperature) on the efficiency of the liquefaction process;
- To study the heat rejected by the system when liquefying hydrogen;
- Create a reliable program in MATLAB that can accurately model a large-scale plant;
- To find optimal flow rates for the refrigerant in different conditions;
- To create a program that is intuitive enough to be used in future studies;

1.3 Structure

This work is divided into 5 chapters:

- **Introduction**: Containing the background and motivation for the research, as well as the structure of the work;

- **State of the art**: An approach to the theoretical component, covering the most important subjects of this dissertation: Hydrogen as a resource, its production and liquefaction, as well as its associated challenges;
- **Materials and Methods**: A detailed description of the methodology of the project, with the model and parameters being explained;
- **Results and discussion**: Presentation of the results obtained through simulation and subsequent discussion about them.
- **Conclusions and future works**: The findings lead to meaningful conclusions, and proposing additional research is recommended to build upon, expand, and provide more comprehensive support for the work conducted in the dissertation.

Chapter 2

State of the art

2.1 Introduction to Hydrogen and its liquefaction

Hydrogen is the lightest and most common element in the universe, having on total three forms. Its most common form is protium(^{1}H) with a proton and electron, the other two are isotopes, deuterium (^{2}H) and titrium (^{3}H), these are commonly used in nuclear fusion. It's a non-toxic, colourless and odourless gas with a high energy density (the highest of all know substances), on a mass basis, approximately 3 times the value of gasoline (11).

In the table 2.1, it is presented some of the most relevant properties of hydrogen (1):

Table 2.1: Properties of hydrogen.

Properties	Value
Lower Heating Value (MJ/kg)	118.8
Viscosity at 25ºC (cP)	0.000892
Critical Temperature (ºC)	-240
Critical Pressure (MPa)	1.3
Density of gaseous hydrogen at 0ºC (kg/m^3)	0.08987
Density of liquid hydrogen at -253ºC (kg/m^3)	70.85
Density of solid hydrogen at -259ºC (kg/m^3)	858
Heat Capacity of gaseous hydrogen at 0ºC (kJ/kg.ºC)	14.3
Heat Capacity of liquid hydrogen at -253ºC (kJ/kg.ºC)	8.1
Heat Capacity of solid hydrogen at -259ºC (kJ/kg.ºC)	2.63
Heat of vaporization at -253ºC (kJ/kg)	447
Latent heat of vaporization (kJ/kg)	461
Thermal conductivity (20ºC, 1 atm) (W/m.K)	0.1825

One of the most relevant properties of the diatomic hydrogen is the existence of the ortho and para-hydrogen, these two forms differ in the direction of the proton spin, if its parallel (ortho-hydrogen) or anti-parallel (para-hydrogen). On a exclusively chemical level, both forms are equal, but thermally, optically and magnetically there are certain differences, the concentration of isomers varies with temperature, the lower the temperature, the bigger the percentage of para-hydrogen, it

evens out at 25% para and 75% ortho-hydrogen at approximately 150 K (11), like shown on figure 2.1. The conversion of otrho to para is exothermic, releasing 703 kJ/kg, due to the ortho form being a form with more energy and as a consequence being more unstable.

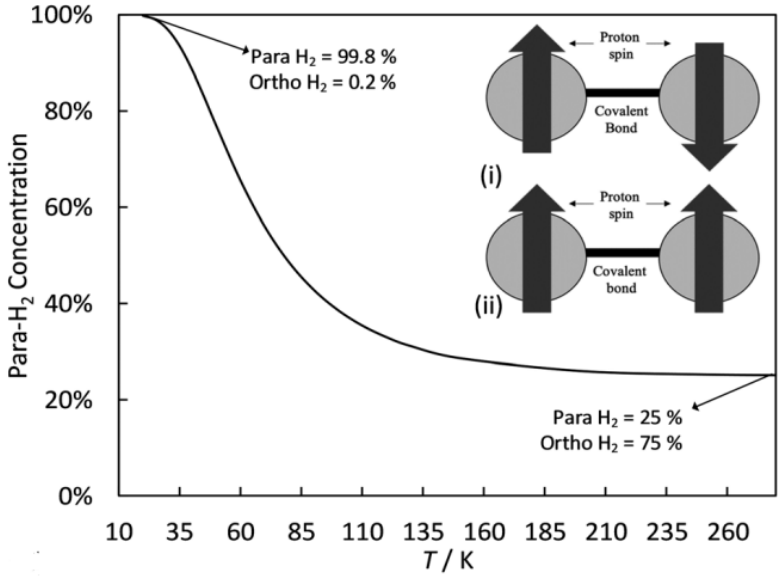


Figure 2.1: Para- and ortho-hydrogen isomers and content of para- as function of the temperature, obtained from (1)

There are three main areas of application of hydrogen currently(2) (12):

- Fuel for rocket ships;
- Upgrade of hydrocarbons in refineries (hydrotreating and hydrocracking);
- Chemical processes such as ammonia and methanol production.

One of the great advantages of hydrogen as previously mentioned, is the possibility to integrate its production with renewable energies, making it a clean energy carrier, through electrolysis, but in fact there are several ways of producing hydrogen, ranging from using hydrocarbons as fuel, to using biomass and solar energy, in the table below the equations of the main forms of hydrogen production will be presented, the technologies themselves will be explained further in the next chapter (2).

Table 2.2: Equations for Hydrogen Production Methods

Method	Equation
Steam Methane Reforming (SMR)	$CH_4 + H_2O \rightarrow CO + 3H_2$
Partial Oxidation of Methane (POM)	$CH_4 + \frac{1}{2}O_2 \rightarrow CO + 2H_2$
Autothermal Reforming (ATR)	$CH_4 + \frac{1}{2}O_2 + 2H_2O \rightarrow CO_2 + 4H_2$
Water Electrolysis	$2H_2O \rightarrow 2H_2 + O_2$
Biomass Gasification	$C_nH_m + nH_2O \rightarrow nCO + \left(\frac{m}{2} + n\right)H_2$
Photoelectrochemical Hydrogen Production	$2H_2O + \text{light energy} \rightarrow 2H_2 + O_2$

The liquefaction process is still an energy expensive process and improvements to its efficiency are vital to make it more popular, but it unlocks a great means of transportation of fuels through large distances, transport and storage of hydrogen as a liquid is its best form, it has a bigger energy density (mass basis)(12), its safer and less expensive when compared to other technologies of transport, from pipelines with compressed hydrogen or even transportation through truck, especially when reaching great distances (1).

2.2 Hydrogen production technologies

2.2.1 Steam Methane Reforming (SMR)

Currently the most common method of producing hydrogen, it uses natural gas (CH_4) at high temperatures (1000 K-1400 K) in mixture with water vapour, generating carbon monoxide (CO) and hydrogen. It's and endothermic reaction, therefor it needs an external energy input in order to happen. Usually operated at 20 atm, after production the hydrogen is purified using the pressure swing adsorption (PSA) (13) method. The ratio of efficiency of conversion (output of hydrogen/input if energy) is between 75 % to 80 % (2).

The main factors that influence the rate of production is, due to Le Châtelier's principle, temperature, pressure and also the catalyst, being the most common Nickel (Ni) due to its low price.

2.2.2 Partial Oxidation of Methane (POM)

The major difference from this method to the previous one is the source of oxygen, while in the SMR it was water, in this one it's oxygen. It happens at a high temperature, not needing catalysts and it's an exothermic reaction, unlike SMR. It has a worse efficiency than SMR and also needs different equipment, like a partial oxidation reactor (2). Normally present thermal efficiencies of 60-75%. (14).

To achieve the complete conversion, there is normally an excess of oxygen introduced in the reactor to ensure a bigger conversion of the methane, that operates at 3-10 MPa. When there isn't a catalyst, this process is executed at higher temperatures to avoid the formation of soot and increase thermal efficiency. If a catalyst is wanted, normally it's used either nickel or rhodium (15), allowing to operate at lower temperatures and pressure.

The end product is syngas (16), which can be converted into other products, to separate the hydrogen from the syngas there are three main methods (17) (18):

- **Pressure Swing Method** - An adsorbent material (activated carbon for example) selectively captures one component from a gas mixture (hydrogen in this case) under high pressure and releases it under low pressure, enabling purification or separation ;
- **Membrane Separation** - Its based on partial pressure differences through membranes, it's an easy operation, with high energy efficiency and easy scale up;
- **Absorption Purification** - Gas purification process involving the removal of acidic gases like carbon dioxide and hydrogen sulfide from gas streams through their selective absorption into a liquid solvent containing amine compounds .

The main advantage of this system are the smaller installations, both in weight and volume, required to process and produce the hydrogen (19).

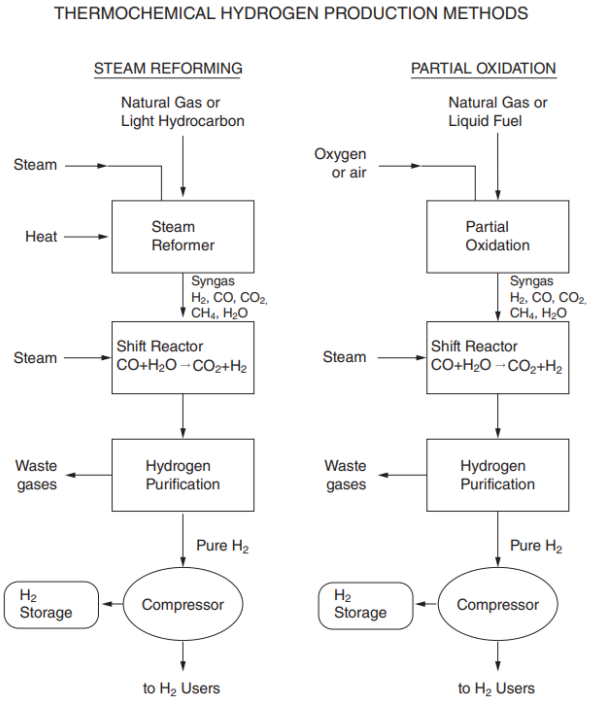


Figure 2.2: Comparative Schematic of SMR and POM, obtained from (2)

2.2.3 Autothermal Reforming (ATR)

It's a combination of steam reforming (endothermic) and partial oxidation (POX) (exothermal). A balance is needed as a smaller amount of oxygen will lead to a bigger amount of hydrogen but a smaller energy output. In an ideal situation, the level of oxygen would be the correct in a way to achieve a energetically neutral reaction, in which the exothermic reaction feeds the endothermic. As it stands, the POX reactions serves as an energetic fuel for the hydrogen formation without greatly harming the production itself (20) . One of the drawbacks of this is the requirement of great amounts of oxygen and compression capacity (21).

It's common the formation of coke in this technology, and some of the catalysts even promote the deposit formation.

Nowadays, research indicates new ways of production with this technology, including with oxygenated organic compounds , reducing the coke formation and increasing hydrogen yields (20).

2.2.4 Water electrolysis

An electric current is passed through water (H_2O), and the water molecules are split into hydrogen (H_2) and oxygen (O_2). It has three different types of methods, electrolyte alkaline, proton exchange membrane (PEM) and solid oxide electrolysis cells (SOEC) and even though the chemical reaction is the same in all cases, the way they do it is different, summing up each:

- **Electrolyte Alkaline** - Composed of electrodes, microporous separator and an aqueous alkaline electrolyte (Potassium Hydroxide or Sodium Hydroxide). The liquid is not entirely consumed in the reaction therefore it must be replenished over its use. Water is introduced in the cathode, being converted into hydrogen and hydroxide, while the hydroxide goes to the anode to form oxygen, the hydrogen stays in the solution, being afterwards separated from the liquid;
- **Proton Exchange Member** - Uses materials like Pt black, ruthenium and rhodium for catalysts and Nafion membrane for separation, which includes gas separation. The water is introduced in the anode being split into protons and oxygen, the protons go through the membrane into the cathode, transforming into hydrogen. In the end, it's also separated from the liquid;
- **Solid Oxide Electrolysis Cells** - They replace the electrical energy required to split the atoms with thermal energy, avoiding power losses that exist in the previous technologies. Operation wise it's similar to the alkaline.

The three technologies have all endothermic reactions, the table below presents the major advantages and disadvantages of each technology (22).

Table 2.3: Main Advantages and Disadvantages of each electrolysis technology

	Electrolyte Alkaline	PEM	SOEC
Advantages	Cheapest technology	More efficient than alkaline	Most efficient
Disadvantages	Corrosion, Less efficient	No issues of SOEC, More expensive than Alkaline	Thermal cycling, Chrome migration

Even though it's a great technology to produce hydrogen without any carbon emissions, it has several drawbacks, it consumes a great amount of electricity and since there is no standardized way of measuring the efficiencies of the several electrolyzer producers, getting an accurate efficiency measurement is difficult (19).

2.2.5 Biomass Gasification

Its based on the gasification (3) of biomass and coal, this will result in producer gas (a mixture of hydrogen, methane, carbon monoxide, carbon dioxide and nitrogen), this process isn't very efficient due to the present of water vapour. Normally the reaction occurs in either a fixed bed or fluidized bed reactor (3), if water vapour or oxygen are added in the gasification process, the output will be called syngas, with a better H_2:CO ratio. To achieve high hydrogen yields it then passes a Water-Gas Shift (WGS) (23) process, afterwards there is a separation process in order to produce pure hydrogen.

This process has some drawbacks, firstly, the gasification process creates a lot of tar, to circumvent this a second reactor is added normally, but this makes the process too expensive for small scale plants. The second drawback is that this is a resource intensive process, to acquire the mass necessary to produce large amounts of biomass to be gasified is needed a great logistical network and support.

This process normally has an efficiency of 35-50% (14).

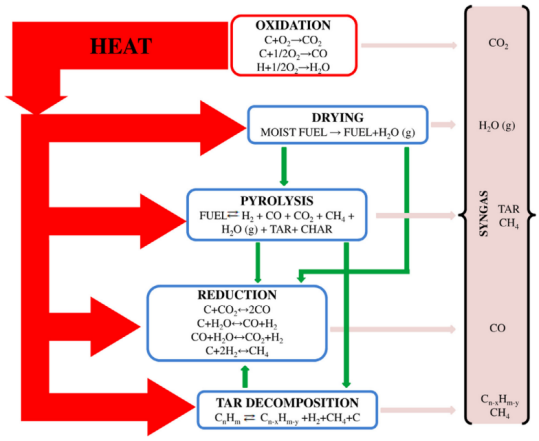


Figure 2.3: Schematic of Biomass gasification, obtained from (3)

2.3 Hydrogen liquefaction technologies

2.3.1 Linde-Hampson Cycle

It's the simplest of the cycles. Hydrogen gas in ambient conditions is compressed and cooled through heat exchangers, in the end, it passes through a throttling valve. The system requires the Joule-Thomson effect for liquefaction to happen, in which the pressure drop causes a quick temperature decrease (explained through the ideal gas law) causing condensation (24), thus this cycle can also be aptly name Joule-Thomson expansion cycle. The effect only happens at high pressures, and part of the gas will be transformed into liquid, the part that stayed gas will return and be used for the cooling process.

It's needed that hydrogen is cooled to at least -73ºC (200 K) at 1 atm. Liquid nitrogen is used to cool down the hydrogen, pressure adjustment is important for efficient cooling (1).

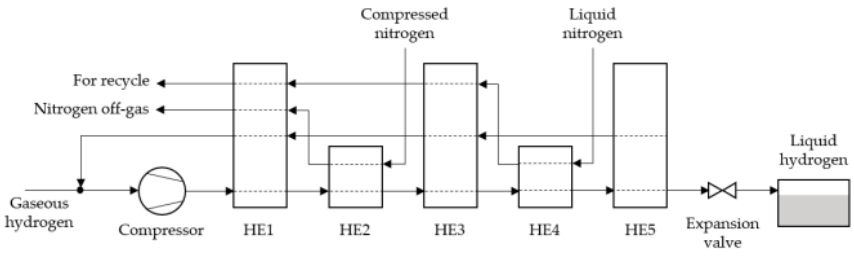


Figure 2.4: Schematic of Linde Cycle, obtained from (1)

2.3.2 Claude Cycle

An adaption of the previous cycle, it substitutes the Joule-Thomson valve with an expansion engine. This engine opens the possibility of a lower temperature after the isenthalpic expansion and

since it's the system's main refrigeration source, liquid nitrogen is not needed. Presented below in figure 2.1 is the diagram of the system (1).

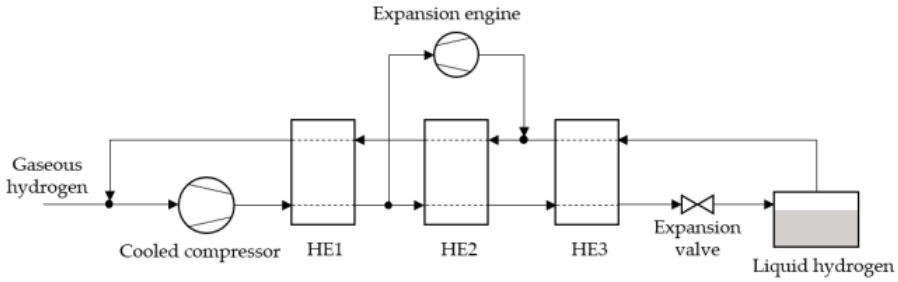


Figure 2.5: Schematic of Claude Cycle, obtained from (1)

The gaseous hydrogen is compressed and cooled through a heat exchanger, afterwards part of the gas goes to the expansion engine and used to cool the other one that goes to the heat exchanger, to be more efficient in a energetic and exergetic level it is used a precooler.

2.3.3 Magnetic Refrigeration

It uses a magnetic field to repeatedly magnetize and demagnetized the magnetic material, this creates a magnetocaloric effect. This is a phenomenon in that the temperature of the working material changes according to the reversible change in magnetic fields.

It adopts the principles of the reversed Carnot cycle and has 4 steps:

- **Adiabatic magnetization** - When an external magnetic field is applied and increased, in a thermally insulated environment, there's a decrease in entropy and heat capacity due to the alignment of the magnetic atom dipoles;
- **Isothermal magnetization** - heat is removed by another fluid and the magnetic field is maintained to avoid heat absorption by the dipoles;
- **Adiabatic demagnetization** - Magnetic field decreases in adiabatic conditions, cooling the material.
- **Isothermal demagnetization** - The magnetic field is kept constant to keep the temperature stable and has thermal contact with the hydrogen.

This cycle has a Carnot efficiency of 50%, bigger than a vapour compression system (38%) (1).

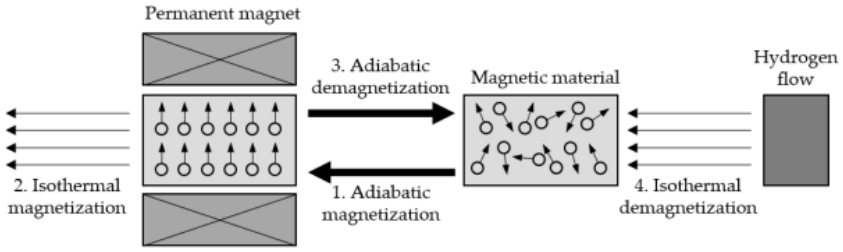


Figure 2.6: Schematic of Magnetic Refrigeration Cycle, obtained from (1)

2.3.4 Brayton Refrigeration

Helium or neon are used as refrigerants, the working fluid is compressed to high pressure and then expanded isentropically in an expanded to achieve the desired temperature. This fluid then cools down hydrogen until condensation, which was precooled using liquid nitrogen. In a standard Brayton cycle , the working fluid temperature at the exit of the turbine is lower than -253 ºC, one of the measures that is used to increase efficiency is to use 2 turbines in double stage expansion (series) or in parallel (11). This is the cycle that is going to be used in this work.

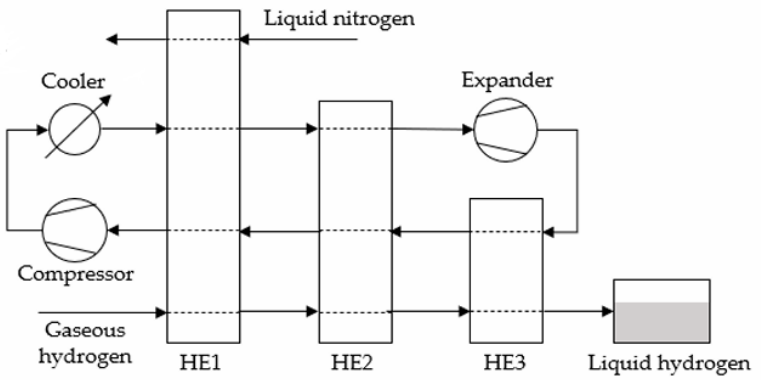


Figure 2.7: Schematic of Brayton Cycle with precooling, obtained from (1)

2.4 Challenges

2.4.1 Storage

No pipeline or storage tank is perfectly insulated, naturally there'll be heat leakage, making hydrogen evaporate, commonly called boil-off, this gas should be immediately released, an accumulation of gas will increase the pressure and will lead to safety problems, including a possible explosion. Some producers instead of releasing the boil-off hydrogen into the atmosphere, choose to recycle it.

This happens due to several reasons:

- **Ortho to Para conversion** - A natural process that occurs, resulting in heat generation, causing the evaporation of liquid hydrogen, consequently leading to a higher pressure inside the tank, therefore is recommended to convert all the ortho- to para-hydrogen before storage and transport.
- **Heat Leakage** - Hydrogen is stored at a very low temperature (-253ºC), even with a robust and effective insulation, heat from the ambient will enter the system. This makes the efficiency of thermal management of crucial importance to minimize this kind of problems. One of the steps is decreasing the surface-to-volume ratio, adopting diferent forms for the tanks, either spherical or cylindrical. Improving the insulating material quality is also relevant, having a double wall with vacuum in between is also a good way to decrease these kinds of losses;
- **Thermal Stratification** - The gas formed from evaporation creates a convection current inside the tank, increasing the pressure. This creates a liquid-vapour interface;
- **Sloshing** - Movement of liquid resulting from transport will worsen the boil-off by transferring heat in the form of dissipated kinetic energy and increasing the surface area between the liquid and vapour phases.
- **Flashing** - When a high pressure liquid is transferred to a low pressure environment part of it evaporates, leading to a certain amount of losses.

Finding a material to be a good insulator is hard, it need to contain a certain amount of properties such as resistance to hydrogen embrittlement and permeation, certain values of mechanical strength, thermal robustness, fire and heat resistance (1)(11).

2.4.2 Safety

It's a dangerous liquid due to its low temperature and direct contact lead to severe burns, frostbite and hypothermia, if it's air exposure, it could lead to asphyxiation, the condensed air drips from the pipes could be dangerous and result in cold burns.

Hydrogen leakage is extremely dangerous as it can lead to an accumulation and a subsequent explosion, if the leak is small it could ignite spontaneously in reaction with the air. The vaporized hydrogen is different from gaseous hydrogen, it is denser than air so it accumulates in a low level, and it could lead to a rapid phase transition if in contact with a hot liquid (1).

2.4.3 Transport

Transporting liquid hydrogen at atmospheric pressure leads to less losses than at higher pressures, but as a consequence it's less dense, a lesser amount is in fact transported. As mentioned previously, the insulation of pipelines is vital. During transfer is important to be careful with the

flammability of hydrogen and in distribution center with factors like overpressure, overfilling and overheating. In the system there should be equipment to detect hydrogen leaks.

Purging in the circuit is important for flammability reasons, normally helium is used in the process due its lower boiling temperature (1).

2.5 District Heating Network (DHN)

2.5.1 Introduction to the concept

The heat absorbed by the process needs to be discharged, normally it is into the environment, making this heat useless thermodynamically, nowadays one of the great priorities of research and development of plants is a greater efficiency, one of the ways that is seen as a possible increase is through the integration in Distric Heating Networks. District heating is a concept that is based on the transportation of heat from the source to costumers. This is an incredibly flexible service, since it can be integrated with a lot of different technologies, from renewable sources to the rejected heat from other processes such as production of electricity and liquefaction of hydrogen, being a good way to reduce CO_2 emissions (25).

Nowadays it is widely accepted that the technology reached its fourth generation, with a constant evolution towards lower distribution temperatures, the different generations consist of(26):

- **1st Generation DH** - The oldest of the technologies, almost 100 years old, consisted mainly in using steam through concrete piping, steam traps and compensators.
- **2nd Generation DH** - Instead of steam now pressurized hot water was used, above 100ºC, with concrete ducts still being used, incorporated with heavy valves and heat exchangers.
- **3rd Generation DH** - This generation managed to reach lower distribution temperatures, often below the 100ºC mark. These systems already include insulated pipes build underground as well as heat exchangers and other materials.
- **4th Generation DH** - While there is not a chosen definition for this new generation, the lower distribution temperature, aiming for 50 to 60ºC and the integration of various heat sources are the key components.

This direct substitution of production of heat for hot water or space heating allows like previously mentioned, a reduction on fossil fuel emissions but also increases the safety due to removing the necessity of transporting fuel in a city, it also reduces maintenance costs to the users of the DHN, due losing the need to have a heat supply, whether it was a boiler, an electric resistance or another source (27).

The normal flow of the water in a DHN consists in a forwards flow until the desired destination, and a return after usage until the heat production unit again (28) . There are three main categories of DHN:

- High temperature operating at above 90ºC.
- Medium temperature operating between 60 and 90ºC.
- Low temperature operating below 60ºC.

2.5.2 Integration from various heat sources

As previously mentioned, the integration from other heat sources, from solar thermal energy, industrial waste heat or other renewable sources is one of the focuses of the new generation of this technology.

One of the most interesting avenues of integration is the one through industrial processes, this is heat that normally would be wasted, and in large scale industry, it can reach easily the temperatures and quantities of heat needed to satisfy a large portion of the requirements, but a normal requirement is a certain level of proximity to the consumer base.

One of the ways for its integration that it is currently being studied is with solar collector panels, specially with solar heat storage. It is seen as a promising avenue to decentralize DH production, and it would be implemented through a large scale array of solar collectors, or small-scale house integration. One of the main issues with this technology is the low energy density, requiring large spaces for it to produce significant amounts of heat, but it is still seen as a good complementary option.

Geothermal District heating is one of the points of focus of this generation due to two main factors, the first is the fact that this power source is unending and has worldwide availability, the second one is the almost non existent environmental impacts. There are some setbacks associated, high CAPEX (Capital expenditure), possibility of earthquakes and the drawback of a small gradual decrease in heat provided over decades of usage (26).

2.5.3 Storage

It can be categorized into inter-seasonal and short-term storage. While inter-seasonal storage is still developing, short-term storage utilizes established technology. The distinction between the two is not clear-cut; large-scale short-term storage systems in extensive networks can sometimes serve inter-seasonal purposes in smaller setups. Additionally, buildings in District Heating (DH) systems can act as thermal energy storage (TES) due to their thermal inertia, potentially moderating short-term load variations similarly to hot water tanks but at a lower cost.

Short-term TES is primarily used to shift energy demand away from peak hours, provide rapid heating or cooling to meet sudden load changes, and enhance electric power output from Combined Heat and Power (CHP) plants by allowing increased electricity production when heat extraction is reduced. Inter-seasonal TES typically aims to store solar heat for winter or to serve as a thermal source for Ground Source Heat Pumps (GSHP).

TES technologies include sensible heat storage, latent heat storage, and chemical storage. Sensible heat storage is well-developed and widely implemented, while latent heat and chemical storage offer higher energy densities and reduced heat loss but are still in the experimental stages (26).

2.5.4 Challenges

One of their main obstacles is their need to be able to provide heat the whole year, specially during winter months. Losses in quality of supply, leaks and malfunctions in the system may lead to shortages or insufficient supply. This makes the most important objective for this technology an increase in its reliability and availability. (28)

One of the other problems is the loss of heat thru ought the system, managing the reach values as high as 32%, even if generally it is half of that. The fact that a good DHN requires meticulous planning and design to be effective and the least expensive possible is vital for its usage (26).

Chapter 3

Methodology

3.1 Simulation Method

The modelling was made using MATLAB, optimizing for the reduction of the SEC in the plant, through the adjustment of the mass flow. The layout of this cycle, a larger scale Brayton cycle, was based on the article published by Valenti and Macchi (4), the schematic being presented below:

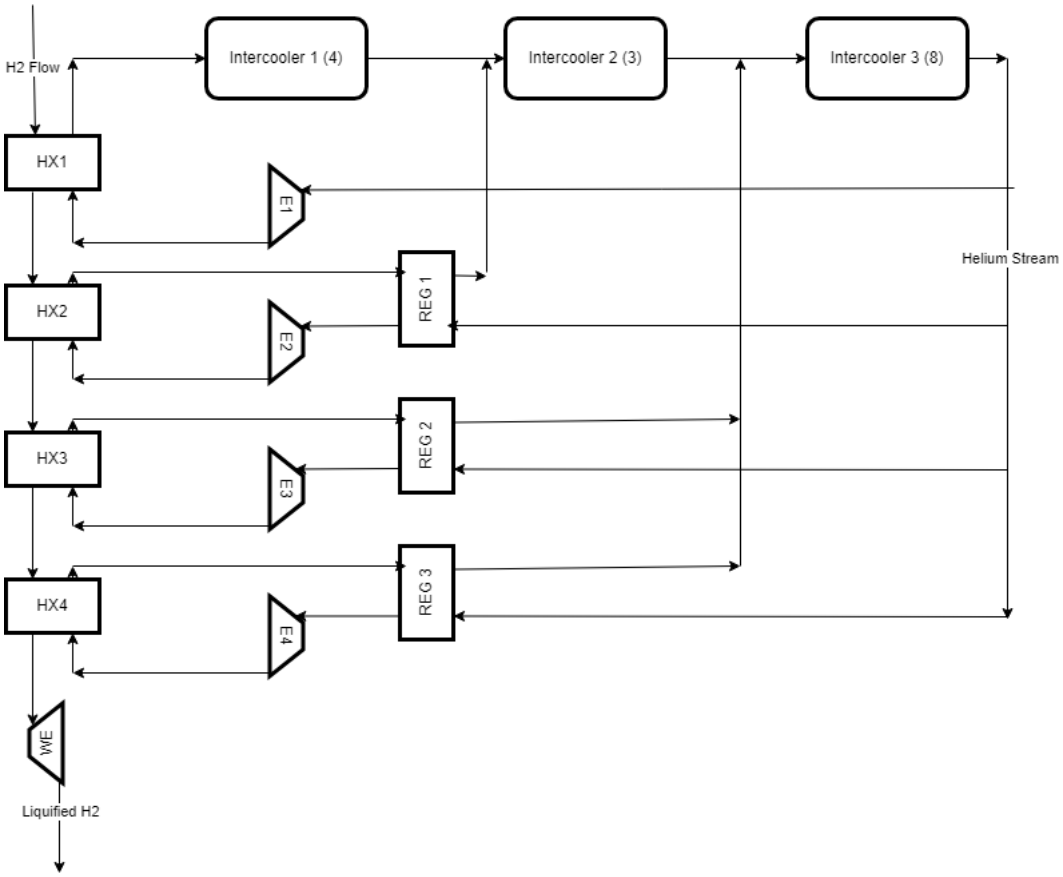


Figure 3.1: Cycle layout, inspired from (4)

The intercoolers are section in which the helium is compressed until a defined pressure intertwined with heat exchangers, acting as coolers, in the model validation the fluid used was air, while in optimization simulations water was used as the coolant, a more detailed example of the intercooler is presented below, it is important to mention that the number between the brackets for each intercooler represents the number of stages it has, the image below is a description of Intercooler 2, which has 3 compressors and 3 heat exchagers:

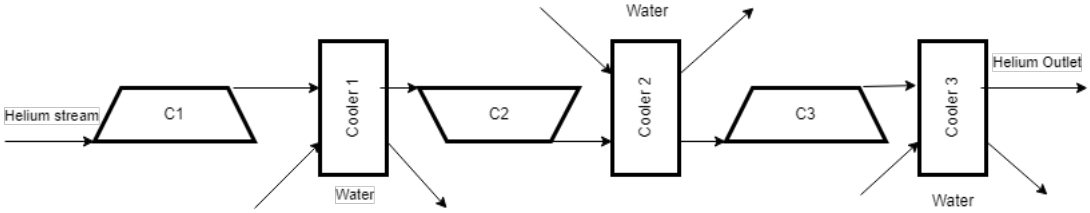


Figure 3.2: Intercooler schematic, inspired from (4)

There are three main sections of this cycle: The heat exchangers that will reduce the temperature of the supercritical hydrogen, the Helium regenerators coupled with the turbines, that allow the helium to reach a low enough temperature to cool the hydrogen, and finally the three intercoolers, that will allow to pressurize the helium and expel the heat generated in the process.

The thermodynamical properties were obtained through the CoolProp (32) function, in which for two specified parameters, for example Pressure and Temperature, are used to obtain a certain thermodynamic property. In section 3.3, the code and each script will be, even if briefly, explained. The full code will be presented in the appendix A.

3.2 Model Assumptions

- **Steady state conditions** - The system is assumed to be in a stable and unchanging state during the analysis;
- **Ideal gas behaviour** - The gas is assumed to follow the ideal gas law, with negligible inter molecular forces and volume occupied by the gas molecules;
- **No pressure drop or heat losses in piping and equipment** - The operating parameters of the system, such as pressure, remain constant throughout the analysis;
- **Constant UA** - The UA of each heat exchanging equipment was calculated and assumed to be constant throughout the entire simulation.
- **Equipment behaviour** - It was assumed that all heat exchanging units were adiabatic with the exterior and that the piping offered no thermal resistance and the same isentropic efficiency for the compressors and expanders.

3.3 Thermodynamic analysis

In the following subsections a detailed analysis of the thermodynamic balance of the several components of the system.

3.3.1 Compression

The objective of a compressor is admitting the low pressure fluid, pressurizing it and delivering it to a high pressure area. Normally, the capability of compressing a certain flow (on a mass basis) of fluid is presented by the following equation (33):

$$\dot{W}_C = \dot{m}_r(h_{ext} - h_{ent}) \qquad [W] \tag{3.1}$$

Since most of the points are being optimized and do not have specified values,h_{ext} is an unknown value and needed to be calculated taking into account that the compressor has an isentropic efficiency $(\eta_i) < 1$, the formula to obtain is:

$$h_{ext} = h_{ent} + \frac{(h_{ext_i} - h_{ent})}{\eta_i} \qquad [J/kg] \tag{3.2}$$

3.3.2 Heat Exchanger

They operate on a permanent regime and allow the heat transfer between two fluids at different temperatures without contact (from the hotter to the colder fluid). Normally they are considered adiabatic with the exterior and operate at constant pressure (33).

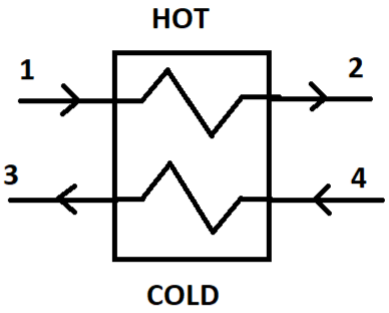


Figure 3.3: A schematic of a counter current heat exchanger

In this work, the heat exchangers used are counter current, in three different areas:

- In the liquefaction of hydrogen, with hydrogen and helium being the used fluids.
- In the helium cycle as a regenerator, cooling the fluid before entering the turbine.
- In the helium intercoolers, between water and helium, allowing a staged compression.

Based on the schematic presented above we can use two main methods to ascertain the parameters and outlet temperatures of and heat exchanger, depending on what is desired:

3.3.2.1 LMTD Method

This is a particularly useful method for obtaining the characteristics of a heat exchanger, such as the UA, the equations are presented below:

$$\dot{Q} = UA \times LMTD \qquad [W] \tag{3.3}$$

With Logarithmic Mean Temperature Difference (LMTD) being calculated as:

$$LMTD = \frac{(T_1 - T_3) - (T_2 - T_4)}{ln(\frac{T_1 - T_3}{T_2 - T_4})} \qquad [K] \tag{3.4}$$

And the heat balance applied to the streams:

$$\dot{Q} = \dot{m}_{cold} \times (h_3 - h_4) \qquad [W] \tag{3.5}$$

$$\dot{Q} = \dot{m}_{hot} \times (h_2 - h_1) \qquad [W] \tag{3.6}$$

Instead of using $C_p \times \Delta T$ for calculating the heat exchange between the inlet and outlet of the heat exchanger, enthalpy values were chosen for their greater accuracy.

3.3.2.2 ε-NTU Method

This method is good for obtaining the outlet temperatures the first step is calculating the maximum transferable heat in the system, calculated through:

$$\dot{Q}_{max} = C_{min} \times \Delta T_{max} \qquad [W] \tag{3.7}$$

The variable C represents the heat capacity, calculated through the multiplication of the mass flow with the specific heat capacity, and the ΔT_{max} represents the maximum possible heat difference in the system, being that of the temperature difference between the inlets.

With C_{min} being the minimum between the heat capacities of both the streams, this way the can calculate the heat transfer as a fraction of the maximum heat possible, this fraction is called effectiveness:

$$\dot{Q} = \varepsilon \times \dot{Q}_{max} \qquad [W] \tag{3.8}$$

The effectiveness, in the case of the cross flow heat exchanger has two specific formulas depending on the value of c, this is a ratio between the C_{min} and C_{max}, if the value is 1:

$$\varepsilon = \frac{NTU}{1 + NTU} \tag{3.9}$$

If c is below 1:

$$\varepsilon = \frac{1 - e^{-NTU(1-c)}}{1 - c \times e^{-NTU(1-c)}} \tag{3.10}$$

The Number of Transfer Units, commonly abbreviated to NTU, is an adimensional value that is usually used to evaluate the capacity of heat transfer, calculated as a ratio of the UA and C_{min}.

3.3.3 Turbine

A turbine is a rotary mechanical device that extracts energy from a flowing fluid, such as gas or steam, and converts it into rotational motion. In the context of the liquefaction process, turbines are often used to expand the high-pressure fluid, reducing its pressure and temperature. Turbines operate based on the principle of converting the kinetic energy of the fluid into rotational motion through the action of turbine blades. Applying the First Law of Thermodynamics (33):

$$\dot{W}_T = \dot{m}(h_{ext} - h_{ent}) \qquad [W] \tag{3.11}$$

For the turbine, like the compressor the same situation happens, the equation is similar to equation 3.2, presented below:

$$h_{ext} = h_{ent} + \eta_i(h_{ext_i} - h_{ent}) \qquad [J/kg] \tag{3.12}$$

3.3.4 System performance

3.3.4.1 Liquefaction efficiency (Specific Energy Consumption)

Liquefaction efficiency is a critical measure of how efficiently the system converts gaseous feedstock, such as hydrogen, into its liquefied form, the goal is to minimize energy consumption while achieving the desired liquefaction outcome, reducing operational costs and minimizing environmental impact.(34).

$$\text{SEC} = \frac{\dot{W}}{\dot{m}_{H_2}} \qquad [W/kg] \tag{3.13}$$

3.3.4.2 Rejected Heat

The rejected heat by the system is the heat that is absorbed by the water (or other possible fluid) in the cooler, allowing a possible re-use of the heat produced in this cycle, from the compression stages and the direct absorption from hydrogen, it is the sum of the heat exchanged in all the coolers in the system, the equation is presented below:

$$\dot{Q}_{rej} = \sum_{i=15}^{1} \dot{Q}_{cooler_i} \qquad [W] \tag{3.14}$$

3.3.4.3 Coefficient of Performance (COP)

The COP can be defined as a way to evaluate the efficiency of a system, in this case it is measured by its capacity to cool the hydrogen divided by the total work required to do it, the higher the value, the better, normal values are below of 0.20 according to (34).

$$COP = \frac{\dot{Q}_{cooling}}{\dot{W}} \tag{3.15}$$

3.4 Hydrogen liquefaction modelling

This model is composed of several different functions that work together into a main one (cycle.m) with five different input variables: Inlet Temperature of Hydrogen (in Kelvin), Inlet Pressure (in Pa), Storage Pressure of Hydrogen (in Pa), Mass Flows of the system (in kg/s) and isentropic efficiency (from 0 to 1). In table 3.1, the inputs, outputs and parameters of all the functions in this program will be presented. It is important to take into account that what is broadly defined as an input in the table, which is, any variable that can be changed, in reality in the system some of these inputs will become parameters of the system, for example

- The isentropic efficiency is always the same, it does not vary in each iteration.
- The pressure remains unchanged since there are no losses, once defined it remains unaltered.

And among the rest of the code, the same can be applied to other variables in the system.

Table 3.1: Inputs, Parameters and Outputs of all functions in the program

Function	Input	Parameters	Outputs
Paracontent	Temperature (K)		Para content
H2Props	Temperature of H2 (K), Pressure of H2 (Pa), Para content		Enthalpy (J/kg), Entropy (J/kg.K)
WetExpander	Inlet Temperature (K), Inlet and Outlet Pressure (Pa), Para content, H2 mass flow (kg/s), isentropic efficiency		Produced Work (W), Outlet Temperature (K)
CalculateUA	Inlet and Outlet Temperatures fluid 1 and fluid 2 (K), Pressures of fluid 1 and 2 (Pa), Para content, Fluid 1 and 2 mass flows (kg/s), type of HX		UA (W/K)
HX	Inlet Temperatures of Fluid 1 and 2 (K), Pressures of Fluid 1 and 2 (Pa), Para content, Mass flows of Fluid 1 and 2 (kg/s), UA (W/K), type of HX		Heat Exchanged (W), Outlet Temperatures (K), corrected mass flow of helium (kg/s)
Expander	Inlet Temperature (K), Inlet and Outlet Pressure (Pa), Helium mass flow (kg/s), isentropic efficiency		Produced Work (W), Outlet Temperature (K)
Compressor	Inlet Temperature (K), Inlet and Outlet Pressures (Pa), Helium mass flow (kg/s), isentropic efficiency		Required Work (W), Outlet Temperature (K)
Cycle	Inlet Temperature of H2 (K), Storage pressure of H2 (Pa), He mass flow (kg/s)	H2 mass flow (kg/s), Inlet pressure of H2 (Pa), isentropic efficiency	SEC (W/kg), Rejected Heat (W), corrected helium mass flow (kg/s)
mdotfinder	Inlet Temperature of H2 (K), Inlet pressure of H2 (Pa), Storage pressure of H2 (Pa), H2 and He mass flows (kg/s), isentropic efficiency		Minimum SEC (W/kg), Optimal Helium Mass Flow (kg/s), Rejected Heat (W)

This function will be the one that will be optimized or be studied depending on the desire (mdotfinder for optimization or plotvariable.m for parametric study), the flow diagram is presented below and the program will be explained in further detail in this section.

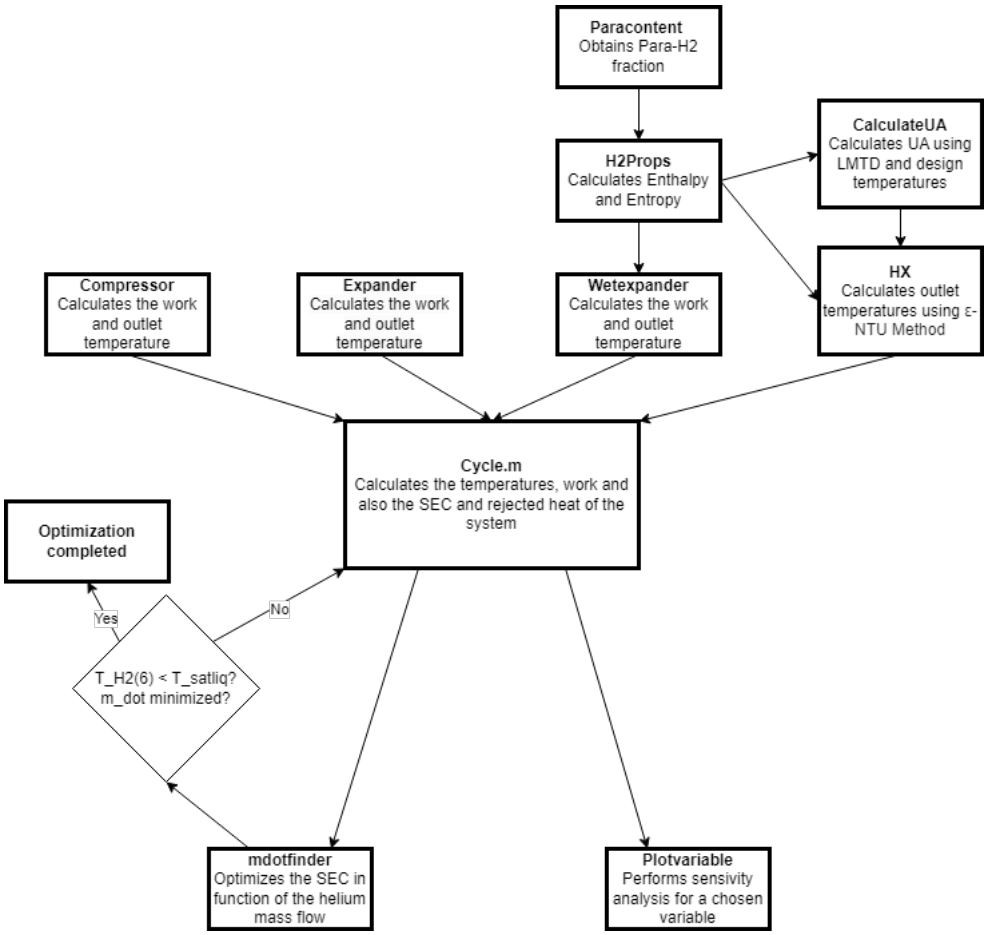


Figure 3.4: Flowchart of the program

The programs starts by calculating the para-hydrogen content in function of the temperature in Paracontent.m. The values obtained from this will be used in H2props.m, that calculate through interpolation the respective value for the enthalpy in function of the para H_2 content, temperature and pressure, based on literature (35).

Afterwards, there are the functions to calculate the work produced (expander.m and wetexpander.m) and the work required (compressor.m) by the respective flows. the main different between the expander and wet expander is the working fluid and the base function for the properties, to improve code simplicity, both codes are identical, having the same thermodynamical basis, but for the expander.m which uses helium, it was used CoolProp and for wetexpander.m it was used H2props.m. For the compressor.m, the process was identical as the expander.m only changing the equations for the appropriate ones, like shown in chapter 3.3.

The next two functions presented are the CalculateUA.m and HX.m, perhaps the more complex regarding thermodynamics and implementation, after a thorough research of the literature, it was

decided to calculate the UA through the LMTD method and the outlet temperatures with ε-NTU method. This is due to, according to Çengel (36), the LMTD method is very accurate to estimate the properties of the HX, knowing the entrance and exit temperatures, the ones used were from literature (4). While the LMTD method is good to calculate the UA, the best method to calculate the outlet temperatures of an HX is the previously mentioned ε-NTU method, both of these methods were explained in further detail in the previous section (3.3). This applies to all heat exchangers in the system, H_2-He HX, Regenerators or Coolers.

There are two points in the cycle where there is a mixture of streams, therefore a function was created to calculate, through simple heat and mass balance the output temperature of the fluid after mixing.

Cycle.m is the main script of the program, like previously mentioned, it is divided into several parts:

- Initialization - This section initializes the variables regarding the Pressures, Temperatures and Mass flows in the system and the characteristics of the fluid used in the coolers, in this particular case, being air.
- Temperatures - This section specifies the temperatures in the cycle, initial guesses and specific values.
- Pressures - This section specifies the working pressures in the several points of the cycle.
- Mass balance - This section serves to specify to points of divergence and convergence of the mass flows in the cycle.
- Cycle - The main body of the script, it calculates the the temperatures in every point in the cycle from the initial guesses, in a loop, and when paired with the next two parts, it allows to either find the optimal points or study the sensitivity of the system.
- Parameters - Calculates the two main desired parameters, the SEC and the rejected heat by the coolers, and is optimized to reduce the SEC.

For optimization of the streams, the function mdotfinder.m was used, in which it searched for the minimum energy consumption in function of the mass flow, for different pressures of helium and isentropic efficiencies.

In the beginning of this section, the input variables for the system were mentioned, in the following table the range of values studied for each of the variables will be presented.

Table 3.2: Input values for simulation for isentropic efficiency variation

Temperature (K)	Inlet Pressure (MPa)	Storage Pressure (kPa)	Mass flows (kg/s)	Isentropic efficiency
300	6	150	10 for H_2	0.7-1

Table 3.3: Input values for simulation for Helium pressure sets

Temperature (K)	Inlet Pressure (MPa)	Storage Pressure (kPa)	Mass flows (kg/s)	Isentropic efficiency
300	6	150	10 for H_2	0.85

Table 3.4: Input values for Helium pressure sets

Set Point	P1 (kPa)	P2 (kPa)	P3(kPa)	P4(kPa)
1	150	300	550	2000
2	150	350	650	3000
3	150	400	750	4000
4	150	450	850	5000
5	150	500	950	6000

The second part of the work consisted in the study of the possibility of the usage of the rejected heat as useful heat to heat District Heating Network (DHN), knowing the temperature requirements of 333K for the water exiting the plant and 313K for the return, or the water that enter the heat exchanger in the intercooler. The solution was obtained through two different ways:

- Adjustment of the pressure in the Intercoolers.
- Adjustment of the water mass flow in each cooler.

Afterwards, the values were compared with the original ones to see if it is a viable solution.

Chapter 4

Model Validation and Sensitivity Analysis

4.1 Model Validation

Since the cycle was based on the work previously done by Valenti and Macchi (4) the values were expected to be similar, but not equal, this was due to:

- The H2props function, while a decent approach, it doesn't truly replicate the behaviour of hydrogen at low temperature, while in the Valenti and Macchi's work (from this point forwards it will be referred as "original work") , Aspen was used with the Benedict–Webb–Rubin–Starling equation of state (EOS) being the basis of the thermodynamical properties, making it a more accurate model.
- In the original work, there were different assumptions, mainly the loss of pressure through the equipments, increasing the SEC in comparison to this work, the isentropic efficencies also were different between the several components in the system, while in this one all have the same specific isentropic efficiency, the value chosen was 85%.
- For simplicity it was chosen a isentropic model to estimate the pressure ratio between the several compressors in the intercoolers, although much simpler, it doesn't truly replicate the pressure ratio in the system, leading to some differences in the values.

Two calculations were made, one with the mass flows presented in the original work, and optimizing with the parameters of the original work, and the relative error was calculated presented in a following table, in order to validate the model, it is necessary to take into account that even though the work was made with water as coolant, these simulations used air, to properly replicate all of the conditions of the original work, the results are presented in the table below:

Table 4.1: Method validation results

	Original Work	Optimization	Cycle with original work's mass flows
SEC (MW/kg)	18.14	17.44	19.8
Rejected Heat (MW)	226.92	201.65	219.7
Mass flow (kg/s)	132.96	120.26	132.96

Table 4.2: Relative error for the results

	Optimization	Cycle with original work's mass flows
SEC (MW/kg)	3.86%	9.15%
Rejected Heat (MW)	11.14%	3.97%
Mass flow (kg/s)	9.55%	–

The errors were relatively small, being able to consider this a reliable model to copy the behaviour of the original work. If the error was too big, there might have been a coding error, the CoolProp functions weren't properly working or incorrectly simulating the behaviour of hydrogen, in another possibility certain assumptions previously made regarding the model and its components were very inaccurate.

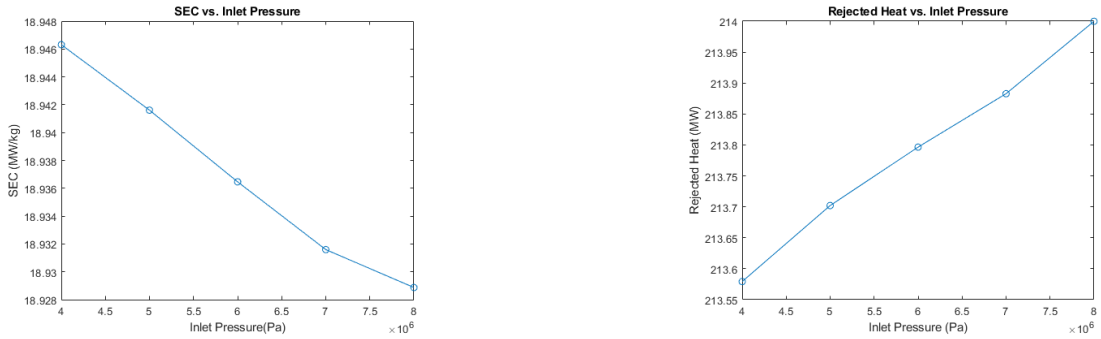
4.2 Parametric Study

To be able to validate the model is also essential to verify if it behaves as expected, if the values of the SEC and Rejected Heat change accordingly to the change made. All of the variables of the system will be studied and its behaviour evaluated. The values used and its resultes are presented below.

Table 4.3: Values used for Sensivity Analysis

	Inlet Temperature (K)	Inlet Pressure (MPa)	Storage Pressure (kPa)	Mass Flows	Isentropic Efficiency	SEC (MJ/kg)	Q_rej (MW)
Isentropic efficiency	300	6	150	10 for H2 140 for He	0.7 to 1	51.18 to 15.04	435.2 to 187.2
Inlet Temperature	250 to 350	6	150	10 for H2 140 for He	0.85	17.75 to 19.81	204.9 to 229.7
Inlet Pressure	300	4 to 8	150	10 for H2 140 for He	0.85	18.95 to 18.93	213.58 to 214
Storage Pressure	300	6	100 to 200	10 for H2 140 for He	0.85	18.9359 to 18.9376	213.8

4.2.1 Effect of the Inlet Pressure

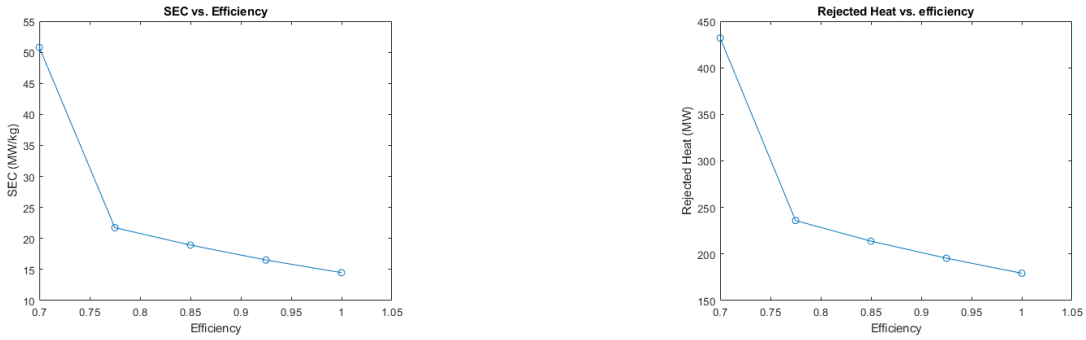


(a) (b)

Figure 4.1: Effect of the variation of the inlet pressure in the SEC (a) and rejected heat (b)

When studying the impact of the inlet pressure it is known that higher inlet pressures result in increased enthalpy levels due to the greater energy content of the gas, this causes a higher value of heat absorbed by the helium. Taking this into account, the system behaves as expected.

4.2.2 Effect of the Isentropic Efficiency

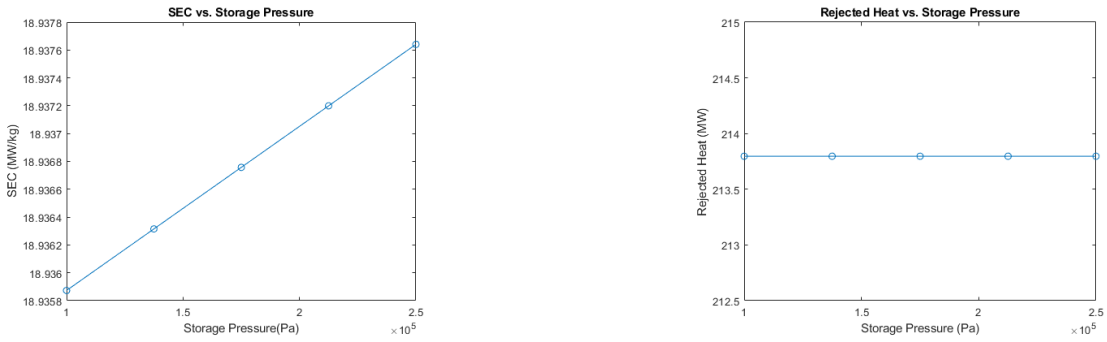


(a) (b)

Figure 4.2: Effect of the variation of the isentropic efficiency in the SEC (a) and rejected heat (b)

In regards to the isentropic efficiency, when its closer to 1 the system will require less energy to do the same cooling and the compression will be more efficient, transferring less heat to the working fluid, leading to lower SEC and Rejected heat with higher efficiencies. This way we can conclude that the system behaves as expected.

4.2.3 Effect of the Storage Pressure

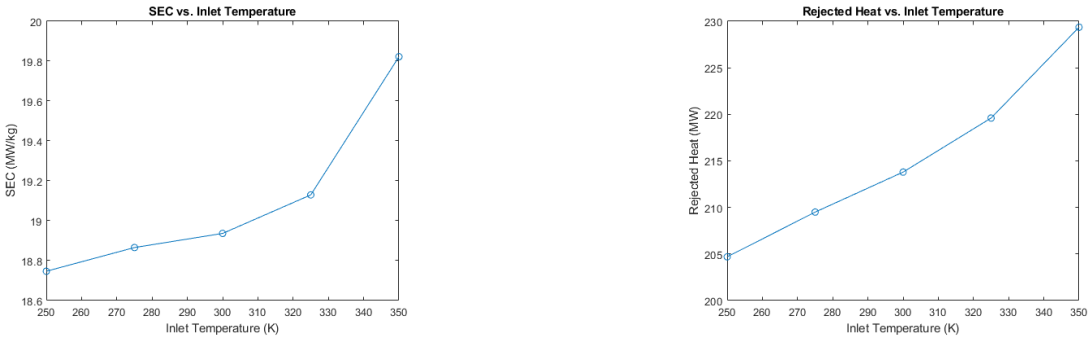


(a) (b)

Figure 4.3: Effect of the variation of the storage pressure in the SEC (a) and rejected heat (b)

The increase in storage pressure was expected to increase the SEC due to a lower pressure difference in the wet expander, reducing the work produced by it, while it was expected to affect very little the rejected heat. In the system the SEC behaved like expected while the rejected heat didn't change, this can be due to the value change being so low that it isn't noticeable in the graph.

4.2.4 Effect of the Inlet Temperature



(a) (b)

Figure 4.4: Effect of the variation of the inlet temperature in the SEC (a) and rejected heat (b)

It was expected that that both the SEC and rejected heat would increase with the increase of the temperature, this is due to the bigger absorption of heat by the refrigerant. In this way the system behaves as expected.

end

Chapter 5

Results and discussion

5.1 Study of the Enthalpy-Entropy Diagram (H-S)

In Annex B of this work a schematic of the cycle with all of the points indicated is presented for better clarity of the code and interpretation of the work. The H-S diagram is the first part in understanding the cycle, how it behaves and evaluate if it is thermodynamically correct, this being applied for the base case of the system, in the following sections the variation of the parameters will be studied.

5.1.1 Hydrogen

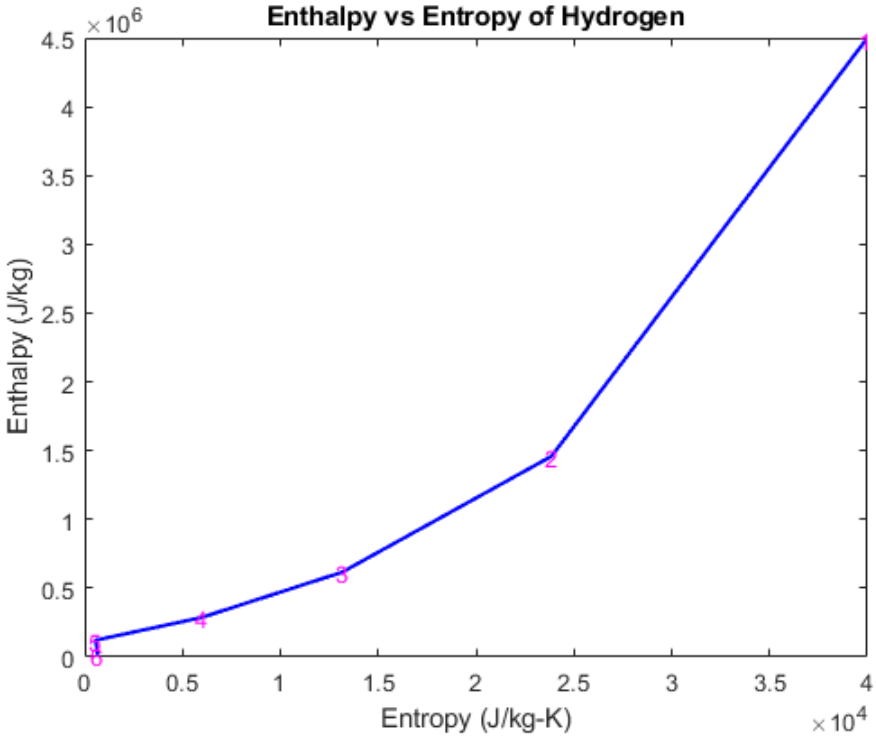


Figure 5.1: H-S diagram for Hydrogen

In the figure above, it is presented the H-S diagram of Hydrogen, under the original work's conditions, except for water as coolant for the intercoolers, it has 6 total points, from the inlet (point 1) to the liquefaction outlet (point 6), from the diagram it is possible to notice that the cooling is more intensive in the first heat exchanger, which will be discussed further ahead in the following chapters, from the point 5 to 6 it is its passage through the wet expander to transform into saturated liquid, while previously it was always in supercritical state.

5.1.2 Helium

In the figure below it is presented the H-S diagram of the Helium.

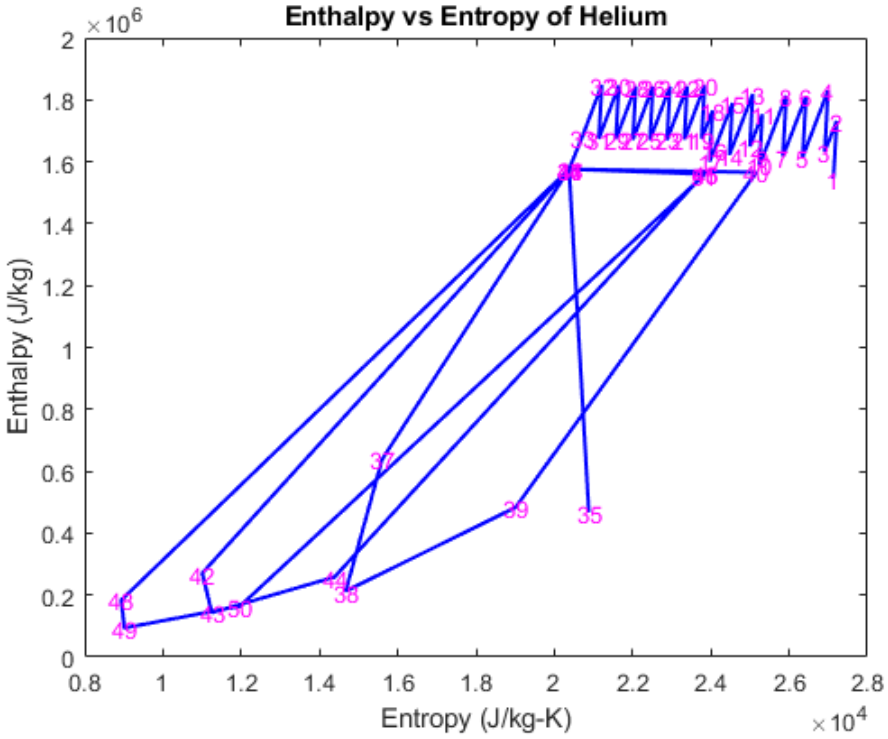


Figure 5.2: H-S diagram for Helium

It was also obtained under the same inputs and conditions, this diagram is more complicated than the hydrogen on, so for easier comprehension, its analysis will be divided:

- The top of the diagram from point 1 to 33, with a great concentration of values in a "zig-zag" pattern, is the intercoolers, in which the helium was progressively compressed, mixed with other flows and cooled down.
- The middle with points 34 and 36, 40-41, 45-47 and 51, with a great concentration of numbers represent the points near the regenerators with different levels of entropy according to its pressure.
- The bottom part, point 37-39, 42-44, 48-50 and 35, where the helium is at low temperatures is related to the outlet from the cold part of the regenerator, which will be further cooled through the turbine, then heat in the heat exchanger with the hydrogen and return to the middle section through the hot part of the regenerator. An example of this evolution would be 47 to 48 (cooled in regenerator) , 48 to 49 (cooled through turbine), 49 to 50, (heated in heat exchanger), and 50 to 51 (heated in regenerator).

It is important to point that point 35 and 1 are connected even if in the diagram there is not a line connecting them.

5.2 Variation of the Helium Pressures

One of the first points of optimization of this work was varying the the pressure in the helium according to previously defined set points and study the effects of it on several parameters and components of the cycle.

5.2.1 Mass Flow Rates

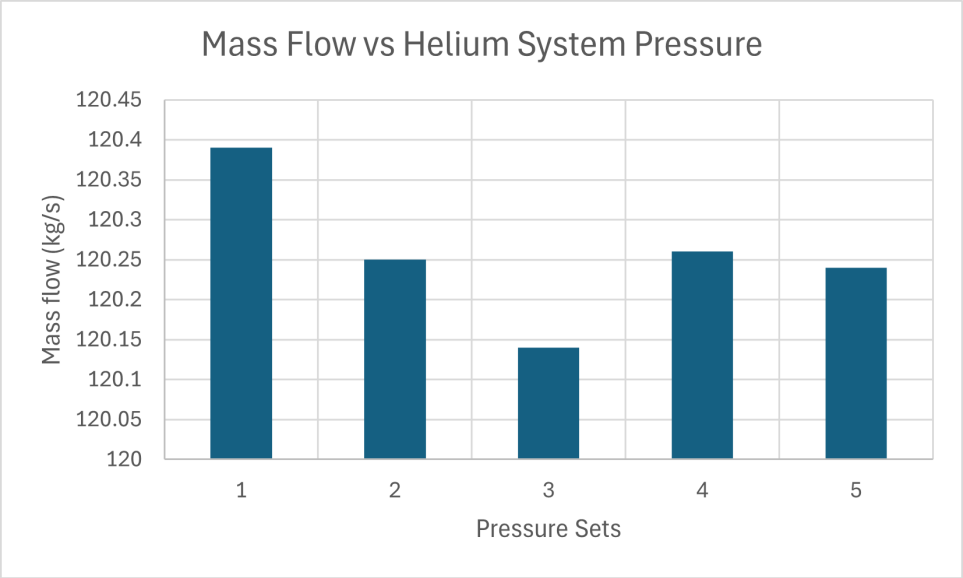


Figure 5.3: Variation of Mass Flow rate of helium in function of the helium pressure sets

In the figure above is presented the variation of the mass flow optimization in function of the previously defined helium pressures, from analyzing the graphic it is possible to see that the helium mass flow does not have a specific shape or pattern, with the minimum value being at set point 3.

The variation of value is really small, between 120.15 kg/s to 120.4 kg/s, it allows to see that for a variation in pressure in the helium system, even thought the pressure increases throughout the system set points, the variation in enthalpy is not large enough to cause a significant change in the mass flows of the system.

5.2.2 UA

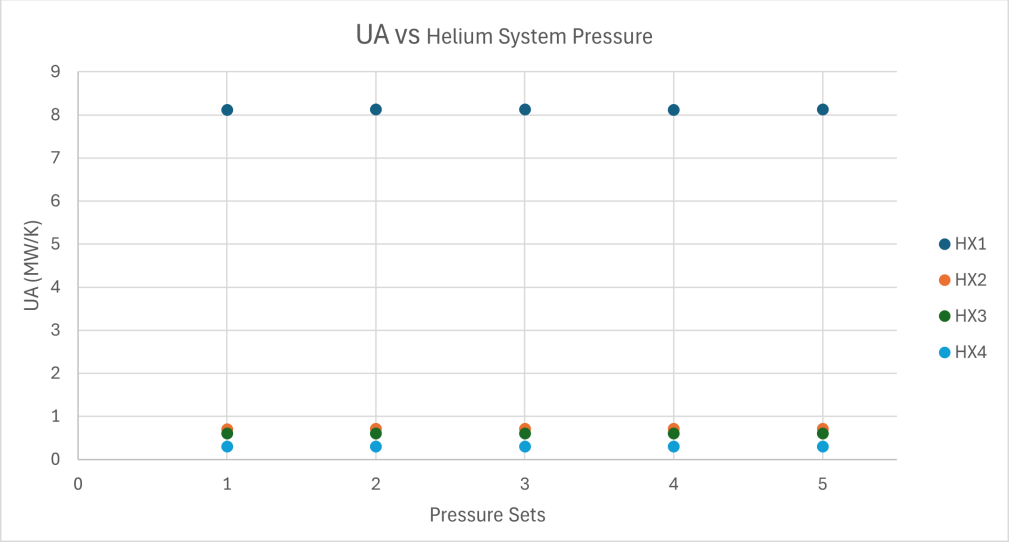


Figure 5.4: Variation of the heat exchanger's UA in function of the helium pressure sets

In Figure 5.4, the variation of the UA (overall heat transfer coefficient) of the heat exchangers in the system is shown according to different helium pressure sets.

Normally, it would be expected to see a progressive increase in the value of UA. This expectation arises because higher pressure generally leads to higher thermal conductivity and density, enhancing the capability for heat transfer.

The behavior of each heat exchanger will now be analyzed separately to determine if it follows the expected trend:

- **HX1**: The UA value stays approximately constant, varying overall 0.02 MW/K across all set points.
- **HX2**: This heat exchanger increases slightly the value for UA from set point 1 to set point 2, which is its maximum, valued at 0.714 MW/K, and afterwards it stabilizes.
- **HX3**: The UA values behave similarly to HX2, with the highest value being 0.607 MW/K.
- **HX4**: The values increase throught the pressure changes in the various set points from a mininum of 0.298 MW/K at set point 1 to 0.304 MW/K at set point 5.

The inconsistent behavior across the heat exchangers can be attributed to flow allocation adjustments. The system was programmed to readjust mass flows to minimize the SEC. Consequently, the mass flow will have a unpredictable value, affecting the UA values.

5.2.3 COP

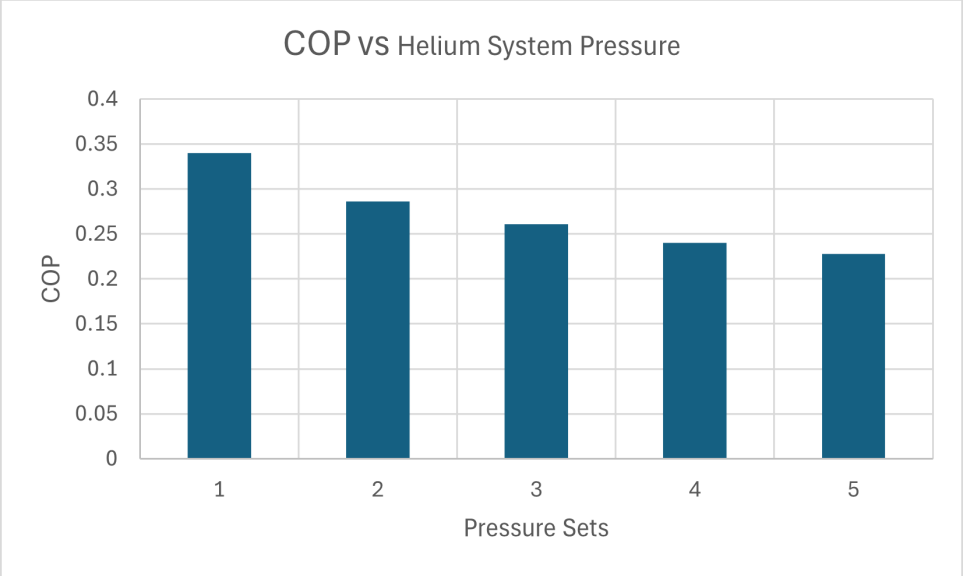


Figure 5.5: Variation of the Coefficient of Performance of the cycle in function of the helium pressure sets

In the figure 5.5 presented above, it can be observed the variation of the COP in function of the helium system pressure.

Before analysis, the expectation would be an increase of the COP as the pressure is increased, due to a bigger efficiency in the heat exchanger efficiency and work produced by the wet expander ate the end of the hydrogen flow.

After observation of the graphic it can be ascertained that the COP is decreasing as the pressures in the system increase. The mass flows as seen in section 5.2.1, barely have impact due to being practically constant. One of the reasons might be the proportion of compressors to turbines in the system, there are 15 compressors to 3 turbines. Another reason might be the fact that by changing pressures, the pressure ratio also changes, and it has impact in how the compressors work in each intercooler, leading to a difference of 0.34 to 0.228 from biggest to lowest value.

5.3 Variation of the Isentropic efficiency

The other point of optimization was varying the isentropic efficiency of the turbines and compressors between 0.7 to 1, and study its effects on the cycle.

5.3.1 Mass Flow Rates

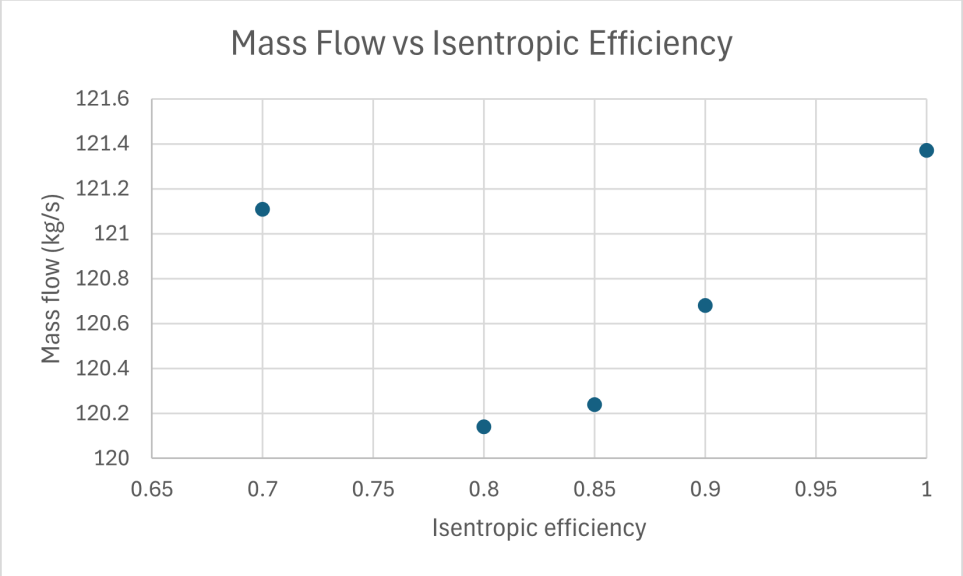


Figure 5.6: Variation of Mass Flow rate of helium in function of the isentropic efficiency

In the figure above the variation of the mass flow in function of the isentropic efficiency can be observed.

In normal circumstances it could be expected a decrease in the refrigerant flow, this would be to the bigger efficiency in some of the components in the system, leading to the need of less flow to do the same work.

In this work, the mass flow adopted a parabolic shape, with a minimal value in the efficiency of 0.8, and the biggest value when its an isentropic system.

This was unexpected, but can be explained, with the main reason being the flow distributions in the system to fulfil the cooling requirements, and is important to note that even though it varies, the variation is between 120.14 at its lowest and 121.31 at its highest, barely over 1 kg/s variation.

5.3.2 UA

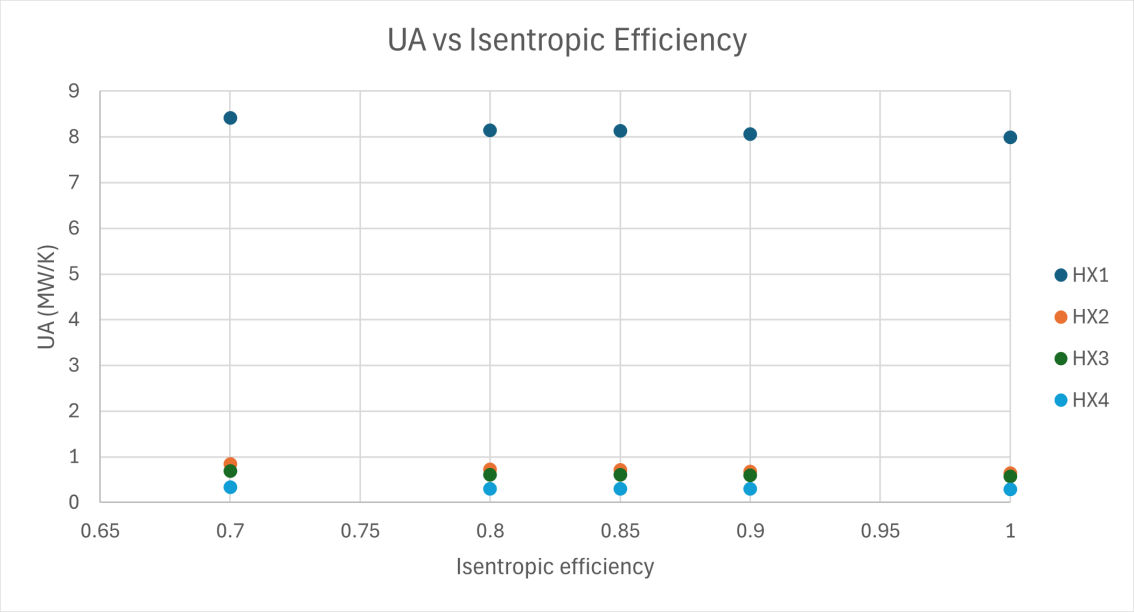


Figure 5.7: Variation of the heat exchanger's UA in function of the isentropic efficiency

In Figure 4.7, the variation of the UA of the heat exchangers in the system is shown according to isentropic efficiencies.

Normally, it could be considered that the UA would increase, since at the exit of the turbine the temperatures would be lower, enhancing the potential for greater temperature differences in the heat exchangers, which typically improves heat transfer efficiency.

The behavior of each heat exchanger will now be analyzed separately to determine if it follows the expected trend:

- **HX1**: The UA values progressively decrease. It varies from a maximum of 8.42 MW/K for 0.7 efficiency to 7.99 MW/K for an isentropic.
- **HX2**: The UA values progressively decrease. It varies from a maximum of 0.84 MW/K for 0.7 efficiency to 0.646 MW/K for an isentropic..
- **HX3**: The UA values progressively decrease. It varies from a maximum of 0.684 MW/K for 0.7 efficiency to 0.586 MW/K for an isentropic..
- **HX4**: The UA values progressively decrease. It varies from a maximum of 0.331 MW/K for 0.7 efficiency to 0.293 MW/K for an isentropic..

The observed trend of decreasing UA with increasing isentropic efficiency may differ from theoretical expectations due to the complex nature of the system, where many variables are involved,

introducing a certain randomness in the predictability of the UA values. The values behaving like this might be due to the fact that the overall heat absorbed will always be the same (from 300K to liquid saturation temperature at the specified temperature), making a temperature difference increase (LMTD) leading to a lower UA, as observed from equation 3.3. Another possible explanation is since in most cases the mass flow is lower, it will lead to a lower transfer rate, but this does not apply to all cases since the mass flow in the isentropic scenario is the larger value.

5.3.3 COP

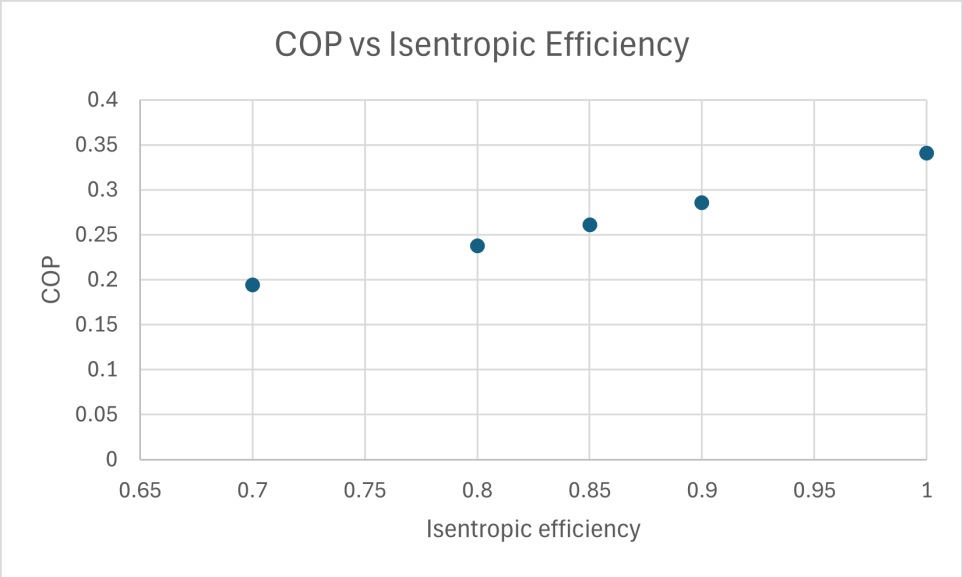


Figure 5.8: Variation of the Coefficient of Performance of the cycle in function of the isentropic efficiency

In the figure above it is presented the variation of the COP in function of the isentropic efficiency. It is expected that the value increases with the increase of the efficiency, a more efficient system will consume less energy to cool the same flow of hydrogen.

In this regard, the system behaved as expected, with a progressive increase of the COP. It is important to notice that the value almost doubled, from 0.194 at an efficiency of 0.7 to 0.341 when it is isentropic.

5.4 Influence on the Parameters

While the previous sections approached the influence of the variation of certain inputs in the cycle overall and the mass flows, the main goal of this work was minimizing the SEC of the cycle, in the next subsections two topics will be approached, the variation of the SEC and the Rejected Heat for the system.

5.4.1 SEC

In the parametric study (section 4.2), an analysis was conducted of how the SEC would vary with the variation of these inputs, these were the behaviours that would be expected from the system, since, in sensitivity analysis the values are not optimized, the mass flow, for example is the same in every run, this is to remove the mass flow as a possible influence in the results. The figures for the variation of the SEC in function of the inlet pressure and isentropic efficiency are presented, respectively, below.

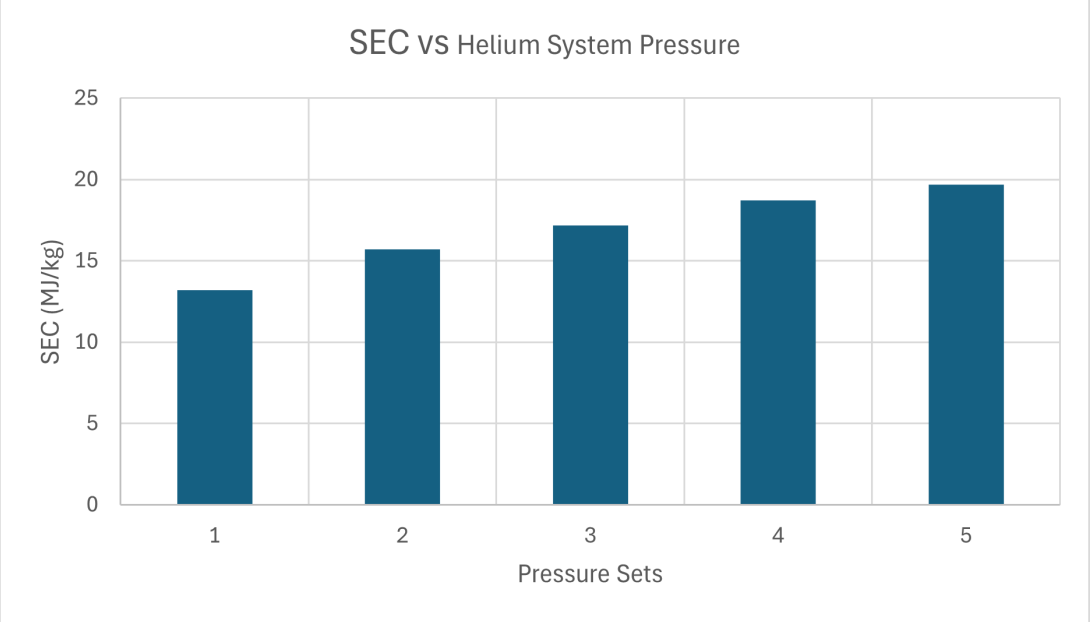


Figure 5.9: Variation of the Specific Energy Consumption of the cycle in function of the helium pressure sets

When analysing the COP, it was seen that the system was more effective when working at lower pressures, the SEC followed the same trend, it can be explained through the same reasons as the COP evolution, when the pressure is increased the system will acquire bigger temperatures, making the cooling of it essential, this part that will be approached ahead means that it cannot be said automatically that the system performs worse, because the systems heat rejection might increase significantly.

Regarding the values, it was a significant and steady increase, from the first to the last point, proving that the pressure of helium has a significant impact in the energy consumption of the system. The increase was from 13.2 MJ/kg to 19.67 MJ/kg. It is also important to point out that as the pressure increases the energy consumption increase decreases, there might be a point in which increasing the pressures barely has an impact of the energy consumption.

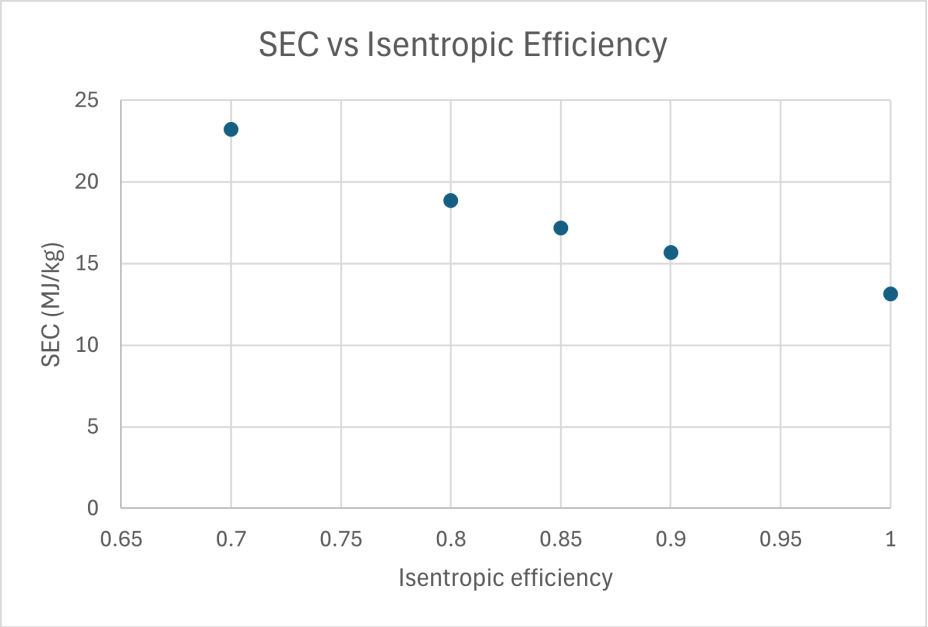


Figure 5.10: Variation of the Specific Energy Consumption of the cycle in function of the isentropic efficiency

Similar to the previous situation, a decrease was expected but a more significant one compared to the inlet pressure variation. When analysing figure 4.10 it is possible to see that it behaves like expected, it has a great reduction from a maximum SEC at 0.7 efficiency, valued at 23.31 MJ/kg, until the isentropic scenario at 13.13 MJ/kg, almost halving the energy consumption.

As expected, the components of the system requiring less energy to compress and producing more energy leads to a much better performance in the system, even if the mass flow barely changes throughout the isentropic efficiency variation.

5.4.2 Rejected Heat

Like with the SEC, the same kind of analysis was made in section 4.2, so the behaviour was expected to be equal to the one presented in that section. The figures for the variation of the rejected heat in function of the helium pressure sets and isentropic efficiency are presented, respectively, below.

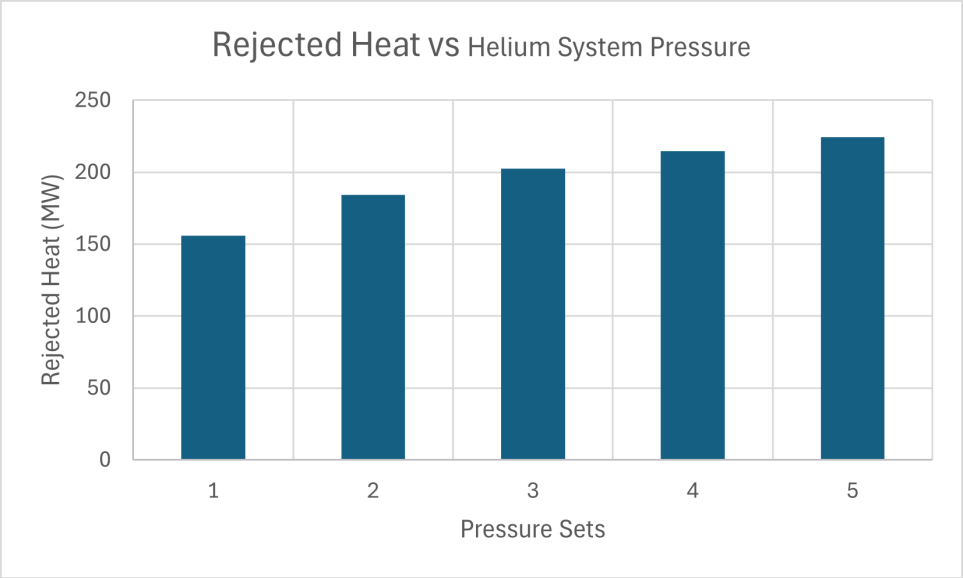


Figure 5.11: Variation of the Rejected Heat of the cycle in function of the helium pressure sets

Thermodynamically speaking, it could be said that it was predicted that the heat in the system would increase, bigger working pressures would lead to higher temperatures in the cycle, leading to a bigger heat absorption by the water in the intercoolers.

This behaviour was what can be seen in figure 5.11, a steady increase in the rejected heat in the system, from 155.72 MW to 224.45 MW, this increase could be studied further by analysing the temperatures in the system, a subject of further analysis in the next section, due to the adjustment of the water mass flow to maximize the heat rejection in the system.

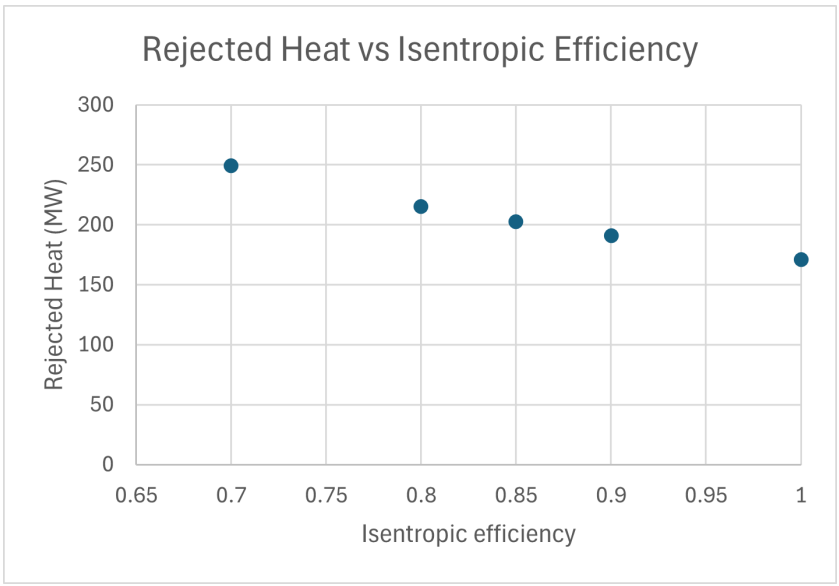


Figure 5.12: Variation of the Rejected Heat of the cycle in function of the isentropic efficiency

Like with the SEC, an increase in the isentropic efficiency leads to a much lower rejected heat amount, the components working with less flaw, lead to less heat being produced in the system, because as seen before, a compressor that has an isentropic efficiency below 1 compresses to higher temperatures and a turbine decompresses with the exit being a higher temperature than predicted.

The values rapidly decrease from 249.25 on 0.7 efficiency to 171.05 on a isentropic situation, leading to a great decrease in the rejected heat, almost halving the value.

5.5 Study of District Heating Network integration

After analysing the values obtained, it was decided to study a possible usage of the heat that is being produced by the system, therefore making it useful and in theory, increasing the efficiency of the plant. The conditions for the usage were based on the integration of the intercoolers in a District Heating Network (DHN), in which the system's coolers would be connected to the network, and making it possible for the integration of a single system cooler, or a full intercooler's coolers.

After deciding that the system would be integrated in parallel, allowing a certain level of independence between all intercoolers, it was decided the working conditions, the water would need to enter the network at 333 K and the return water would be at 313 K, as in the case of low temperature DHN.

There were two scenarios studied, one under the normal working conditions, and a study of how could all of the rejected heat be useful.

5.5.1 Integration under normal circumstances

In all simulations it was analyzed the temperature of the water outlet, if the temperature was higher than the minimum, it was considered that the heat exchanged was useful, in all of the scenarios only in the third intercooler, in which all of the coolers reached the minimum temperature, managed to be considered as useful heat. Below is presented the useful heat variation, in percentage, in function of the inlet pressure.

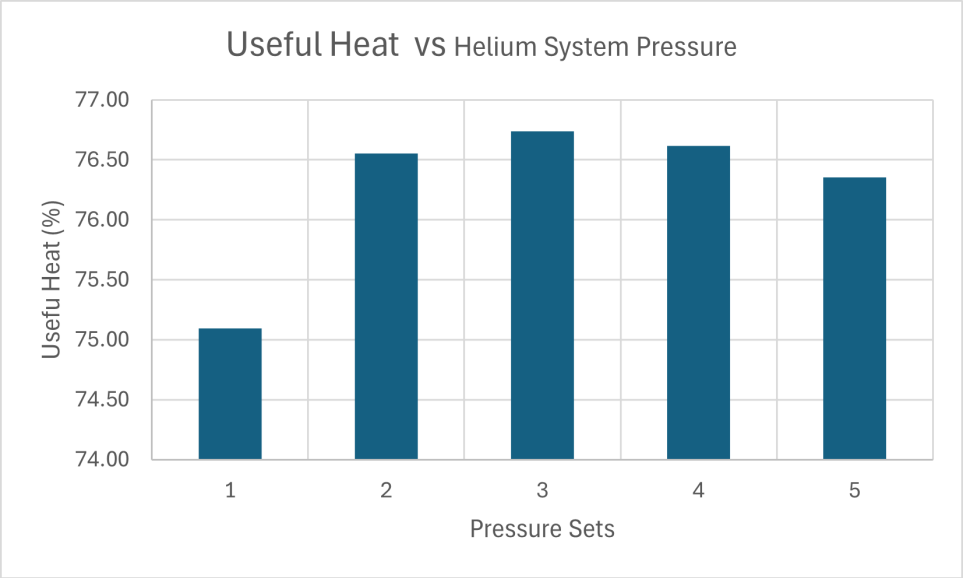


Figure 5.13: Variation of the Useful Heat of the cycle in function of the helium pressure set points

After analysing the figure, the trendline assumes a parabolic, in which the maximum useful heat is at set point 3, the value of the useful heat itself does not vary much between the minimum and the maximum, a 1.64% increase, when analysing this, on of the reason in which the useful heat is bigger is due to the aforementioned mass flow distribution, if the flow is redistributed to be bigger in the third intercooler, it would drive the value high, another reason could be the total heat be in fact higher, leading to a reduced fraction, a lower percentage does mean that the absolute value in fact is smaller, specially with such little differences.

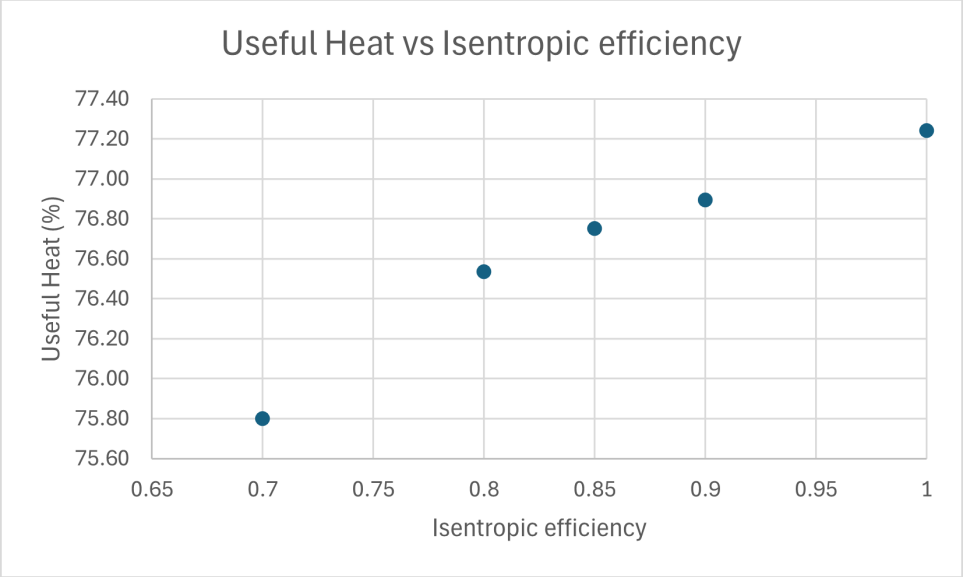


Figure 5.14: Variation of the Useful Heat of the cycle in function of the isentropic efficiency

When analysing the impact of the isentropic efficiency, there is an increase in the percentage

of the useful heat, and a sizeable one, of 1.44 %, like with the similar situation, it could be due to several reasons, but the main one is most likely the fact of the total heat rapidly decreases when increasing the efficiency, adding to that the mass flow distribution and it leads to a bigger share of the heat being useful.

5.5.2 Maximizing the useful heat usage

After investigation possible ways to approach the problem, one of the solutions found was adjusting the pressure ratios in the intercoolers, to manage to give out 100% useful heat, this will naturally lead to some differences in the values obtained in the optimization, the other path chosen was through the adjustment of the mass flow of water in the intercoolers, both of these solutions will naturally lead to different values on the SEC and rejected heat, each case will be presented and talked about separately.

5.5.2.1 Pressure Variation

Table 5.1: Variation of values compared to base case through the adjustment of the pressure in the intercoolers

				Pressure Variation			
		Base Case		Values		Percentage	
SEC (MJ/kg)		17.18		14.34		16.53%	
Q_rej (MW)	IC1	19.91	202.53	41.9	171.67	110.45%	15.24%
	IC2	27.2		38.73		42.39%	
	IC3	155.42		91.04		41.42%	
Helium Mass Flow (kg/s)		120.14		122.09		1.62%	
Water Mass Flow (kg/s)		120		120		———	

In table 4.1 is presented the variation of the values through the adjustment of the pressure in each intercooler. The values were changed to allow each of the heat exchangers to reach the minimum temperature required of 333 K. The values changed from:

- **IC1**: 400 kPa to 1100 kPa (1.1 MPa).
- **IC2**: 750 kPa to 2500 kPa (2.5 MPa).
- **IC3**: 4 MPa to 7 MPa.

The change lead to a decrease in SEC and Rejected Heat, while the mass flow of Helium slightly increased.

The decrease in the SEC was unexpected, one of the reasons might be due to the assumption of a constant isentropic efficiency, which in reality does not happen, leading to a better performing

system, in reality, the polytropic efficiency is the one constant and the isentropic efficiency varies according to the transformation made.

The decrease in rejected heat was also unexpected, the increase in pressures should lead to a bigger amount of rejected heat but this might be explained through an insufficient mass flow of water in the system, leading to much less heat being absorbed by the coolers than previously expected. The higher temperature differential between the helium and water flows lead to an insufficient cooling in the system.

The slight increase in the refrigerant mass flow could not be deemed as significant thermodynamically, since there seems to be no major reason for the value to change, this change might be attributed to the mass flow distribution and optimization method.

5.5.2.2 Flow Variation

Table 5.2: Variation of values compared to base case through the adjustment of the water mass flow in the intercoolers

				Flow Variation			
		Base Case		Values		Percentage	
SEC (MJ/kg)		17.18		19.15		11.47%	
Q_rej (MW)	IC1	19.91	202.53	19.71	186.12	1.00%	8.10%
	IC2	27.2		24.33		10.55%	
	IC3	155.42		142.08		8.58%	
Helium Mass Flow (kg/s)		120.14		120.06		0.07%	
Water Mass Flow (kg/s)		120		55		54%	

In table 4.2 is presented the variation of the values through the adjustment of the water mass flow in the system. The value was changed to allow each of the heat exchangers to reach the minimum temperature required of 333 K. The minimum mass flow that fulfilled this objective was 55 kg/s.

The increase in the SEC was expected, such as the decrease in the rejected heat, the system with a lower water mass flow is unable to absorb as much heat as previously, this lower cooling power will lead to higher temperatures in the system, increasing the work necessary to compress the helium.

The Helium mass flow did not change, meaning that the system was able to cool without need for an increase on the refrigerant flow, it was a possibility to be able to have lower temperatures in the system.

Chapter 6

Conclusion and Future Works

6.1 Conclusion

A model was developed to simulate the liquefaction of hydrogen on a large-scale plant using MATLAB. It was subsequently used to find the optimal mass flow under different helium pressures and isentropic efficiencies. For each of the results, different parameters were studied: the Specific Energy Consumption (SEC), Rejected Heat, Heat Exchanger's UA, and Coefficient of Performance (COP). During the simulations, the mass flow of the refrigerant, in this case, helium, was adjusted and redistributed across the system to achieve the minimum SEC. Subsequently, the rejected heat of the system was analyzed, including its potential incorporation into a district heating network and possible ways to modify the cycle to maximize this incorporation into useful heat for the network, such as by decreasing the mass flow of water in the intercoolers or increasing the pressure in them.

Key findings from these studies include:

- The optimal mass flow of refrigerant is not significantly influenced by the pressures of the refrigerant or the isentropic efficiency.
- The UA values decrease with a more efficient system and are not significantly impacted by the refrigerant pressure.
- The COP is significantly influenced by these variables; it decreases with higher refrigerant pressure and increases with higher isentropic efficiency.
- The SEC is also significantly influenced by these variables but behaves in the opposite manner to the COP.
- The rejected heat significantly decreases with an increase in isentropic efficiency and significantly increases with an increase in the refrigerant pressure.

Additionally, the research revealed:

- Increasing isentropic efficiencies in turbines and compressors leads to more efficient cooling processes, as evidenced by decreasing UA values of heat exchangers.
- Higher pressures enhance the thermal conductivity and density of helium, improving heat transfer capabilities.
- Despite the expectation, the increase in heat rejection was not consistently observed, likely due to limitations in the cooling water mass flow.

Regarding the incorporation of rejected heat into the district heating network, it was found that:

- Varying the pressure in the intercoolers decreased both the SEC and rejected heat, while slightly increasing the mass flow.
- Varying the flow of the refrigerant increased the SEC and decreased the rejected heat, while maintaining the refrigerant flow unchanged.

These findings suggest that optimizing the refrigerant mass flow and pressure settings can enhance the efficiency of the hydrogen liquefaction process and its integration with district heating networks, potentially leading to significant energy savings and reduced CO_2 emissions. The study also highlights potential areas for future exploration and improvement, such as better control of mass flow rates and pressure settings to maximize the efficiency of heat exchangers and the overall liquefaction process.

6.2 Future works

In order to continue and enrich the research carried out in this dissertation, some of the possible suggestions for future work are:

- Experimenting with a different refrigerant, for example a mix of He/Ne (80/20).
- Using a ordinary differential equation to solve the heat exchangers in the system.
- Aiming for optimization of the compression ratio, especially when taking into account the useful heat usage.
- Studying the exergetic efficiency, to see possible points of improvement.
- Using the polytropic effciciency for the system, which replicates much more realistically the behaviours of the system also incorporating its pressure ratio formula, more complex but a better predictor of the pressure in all the points of an intercooler, but it requires estimation of the temperature of the points inside the intercoolers.
- Study the same model with pressure loss included and a more robust hydrogen properties model, to see if the values are closer.

Appendix A

Matlab Code

A.1 paracontent.m

```
%calculates the equilibrium para content for particular temperature
%input temp must be in [K]
function outputpara = paracontent(inputtemp)
%o-p equilibrium / H2 properties
%interpolated data comes from para.csv.
original data is from Woolley et al.
M=readmatrix('para.csv');
T=M(:,1)';
para_fract=(M(:,2)')/100;
outputpara=interp1(T,para_fract,inputtemp,'linear');
```

A.2 H2props

```
function [enthalpy, entropy] = H2props(T, P, paracontent)
% Add CoolProp MATLAB wrapper path
coolprop_path = 'C:\Users\acer\Documents\CoolProp-master\wrappers\MATLAB';
addpath(coolprop_path);

%Input
%P = Pa
%T = K
%paracontent = dimensionless
%Output
%enthalpy = kJ/kg
%entropy = kJ/kg.K

% REFERENCE STATE
```

```
T_ref = 298.15; % K
P_ref = 101325; % Pa

% DESIRED VALUES AT REFERENCE STATE
% first, find the difference between normal and para:

R = 8.314; % J/mol-K
MW_H2 = 2.0159; % g/mol
RH2 = R / MW_H2; % J/g-K

h_para_ref = PropsSI('H', 'T', T_ref, 'P', P_ref, 'PARAHYD');
s_para_ref = PropsSI('S', 'T', T_ref, 'P', P_ref, 'PARAHYD');

% [J/kg], enthalpy
% [J/kg-K], entropy


% These are what the values of h and s at the reference state ARE,
as they're called from PropsSI:

h_normal_ref_RAW = PropsSI('H', 'T', T_ref, 'P', P_ref, 'HYDROGEN');
s_normal_ref_RAW = PropsSI('S', 'T', T_ref, 'P', P_ref, 'HYDROGEN');

% [J/kg], enthalpy
% [J/kg-K], entropy

% Now, the h and s offsets are found by subtracting
the RAW values from the "should be" values:
h_offset = h_para_ref - h_normal_ref_RAW;
s_offset = s_para_ref - s_normal_ref_RAW;

% Now, find the hydrogen properties at the input T, P, and para fraction:
ortho = 1 - paracontent;
h_n = PropsSI('H', 'T', T, 'P', P, 'HYDROGEN');
s_n = PropsSI('S', 'T', T, 'P', P, 'HYDROGEN');

h_n=h_n+h_offset;
s_n=s_n+s_offset;

h_p = PropsSI('H', 'T', T, 'P', P, 'PARAHYD');
s_p = PropsSI('S', 'T', T, 'P', P, 'PARAHYD');


enthalpy = h_p * (paracontent - ortho / 3) + 4 / 3 * ortho * h_n;
entropy = s_p * (paracontent - ortho / 3) + 4 / 3 * ortho *
```

```
(s_n - RH2 * 0.562336) - RH2 * (ortho * log(ortho) +
paracontent * log(paracontent));


% Remove the path after using CoolProp to avoid conflicts
rmpath(coolprop_path);
```

A.3 compressor.m

```
function [work_done, T_out] = compressor(eta, P_HP, P_LP, T_ent, m_dot)

%Input
%eta = isentropic efficency (dimensionless)
%P_HP, P_LP = Pressure High (Exit), Pressure Low(entrance) (Pa)
%m_dot = mass flows (g/s)
%T = Temperature entrance (K)
%Output
%WorkProd = Work required in the compressor (W)
%T_final = Temperature at the exit (K)


coolprop_path = 'C:\Users\acer\Documents\CoolProp-master\wrappers\MATLAB';
addpath(coolprop_path);

h_in = PropsSI('H', 'T', T_ent, 'P', P_LP, 'helium');
s_in = PropsSI('S','T', T_ent, 'P', P_LP, 'helium');
h_out_ideal = PropsSI('H', 'P', P_HP, 'S', s_in, 'helium');
h_out = h_in + (h_out_ideal - h_in)/eta;
T_out = PropsSI('T', 'P', P_HP, 'H', h_out, 'helium');
work_done = m_dot*(h_out - h_in);


% Remove the path after using CoolProp to avoid conflicts
rmpath(coolprop_path);


% fprintf('The value for the Compression Work was: %f kW\n', work_done
    /10^3);
% fprintf('The value for the T_out was: %f K\n', T_out);
end
```

A.4 expander.m

```
function [WorkProd, T_final] =
expander(eta_s, P_LP, P_HP, T,m_dot, coolprop_path)

coolprop_path = 'C:\Users\acer\Documents\CoolProp-master\wrappers\MATLAB';
addpath(coolprop_path);

%Input
%eta = isentropic efficency (dimensionless)
%P_HP, P_LP = Pressure High(entrance), Pressure Low(exit) (Pa)
%m_dot = mass flows (g/s)
%T = Temperature entrance (K)
%Output
%WorkProd = Work Produced in the turbine (W)
%T_final = Temperature at the exit (K)




h_in = PropsSI('H', 'T', T, 'P', P_HP, 'helium');
s_in = PropsSI('S', 'T', T, 'P', P_HP, 'helium');
h_out_s = PropsSI('H', 'P', P_LP, 'S', s_in, 'helium');
h_out = h_in - eta_s * (h_in - h_out_s);
T_final = PropsSI('T', 'P', P_LP, 'H', h_out, 'helium');
WorkProd = m_dot * (h_out-h_in);


% Remove the path after using CoolProp to avoid conflicts
rmpath(coolprop_path);


% fprintf('The value for the Work created was: %f kW\n', WorkProd/10^3);
% fprintf('The value for the exit temperature was: %f K\n', T_final);


end
```

A.5 wetexpander.m

```
function [WorkProd, T_ext] = wetexpander(m_dot, P_LP, P_HP,T_ent,eta,
    para_H2)
```

```
%Input
%eta = insetropic efficiency (dimensionless)
%P_HP,P_LP = Pressure High (entrance), Pressure Low (exit) (Pa)
%T_ent , T_ext = Temperature entrance, Temperature exit(K)
%m_dot = mass flow (g/s)
%Output
%WorkProd = Work Produced (W)



[h_in, s_in] = H2props(T_ent, P_HP,para_H2);

h_out_s = py.CoolProp.CoolProp.PropsSI('H', 'P', P_LP, 'S', s_in, 'PARAHYD
    ');

h_out = h_in - eta * (h_in - h_out_s);
T_ext = py.CoolProp.CoolProp.PropsSI('T', 'P', P_LP, 'H', h_out, 'PARAHYD
    ');


WorkProd = m_dot* (h_out-h_in);

% fprintf('The value for the Work created was: %f kW\n', WorkProd/10^3);
% fprintf('The value for the exit temperature was: %f K\n', T_ext);

end
```

A.6 CalculateUA.m

```
function UA = CalculateUA(T_ent, T_ext, P, m_dot, para_H2,type)

%Input
%para_h2 = Para hydrogen content (dimensionless)
%P = Pressure (Pa)
%T_ent,T_ext = Temperature entrance, Temperature exit (K)
%m_dot = mass flows (kg/s)
%Output
%UA = Heat transfer coefficient (W/K)
if type == "HX"

LMTD = (T_ent(1) - T_ext(2) - (T_ext(1) - T_ent(2))) /
log((T_ent(1) - T_ext(2)) / (T_ext(1) - T_ent(2)));
```

```
h_ent_1 = H2props(T_ent(1), P(1),para_H2);
h_ent_2 = py.CoolProp.CoolProp.PropsSI('H','P',P(2),'T',T_ent(2),'helium')
    ;
h_ext_1 = H2props(T_ext(1), P(1),para_H2);
h_ext_2 = py.CoolProp.CoolProp.PropsSI('H','P',P(2),'T',T_ext(2),'helium')
    ;




Q_1 = m_dot(1)*(h_ent_1-h_ext_1);
Q_2 = m_dot(2)*(h_ext_2-h_ent_2);

Q_guess = (Q_1+Q_2)/2;

UA=abs(Q_guess/LMTD);

end
if type == "Reg"

LMTD = (T_ent(1) - T_ext(2) - (T_ext(1) - T_ent(2))) /
log((T_ent(1) - T_ext(2)) / (T_ext(1) - T_ent(2)));
h_ent_1 = py.CoolProp.CoolProp.PropsSI('H','P',P(1),'T',T_ent(1),'helium')
    ;
h_ent_2 = py.CoolProp.CoolProp.PropsSI('H','P',P(2),'T',T_ent(2),'helium')
    ;
h_ext_1 = py.CoolProp.CoolProp.PropsSI('H','P',P(1),'T',T_ext(1),'helium')
    ;
h_ext_2 = py.CoolProp.CoolProp.PropsSI('H','P',P(2),'T',T_ext(2),'helium')
    ;


Q_1 = m_dot(1)*(h_ent_1-h_ext_1);
Q_2 = m_dot(2)*(h_ext_2-h_ent_2);

Q_guess = abs(Q_1+Q_2)/2;

UA=Q_guess/LMTD;



end
if type == "Cooler"

LMTD = (T_ent(1) - T_ext(2) - (T_ext(1) - T_ent(2))) /
```

```
log((T_ent(1) - T_ext(2)) / (T_ext(1) - T_ent(2)));
h_ent_1 = py.CoolProp.CoolProp.PropsSI('H','P',P(1),'T',T_ent(1),'helium')
    ;
h_ent_2 = py.CoolProp.CoolProp.PropsSI('H','P',P(2),'T',T_ent(2),'air');
h_ext_1 = py.CoolProp.CoolProp.PropsSI('H','P',P(1),'T',T_ext(1),'helium')
    ;
h_ext_2 = py.CoolProp.CoolProp.PropsSI('H','P',P(2),'T',T_ext(2),'air');


Q_1 = m_dot(1)*(h_ent_1-h_ext_1);
Q_2 = m_dot(2)*(h_ext_2-h_ent_2);

Q_guess = (Q_1+Q_2)/2;

UA=abs(Q_guess/LMTD);

end

end
```

A.7 HX.m

```
    function [Q_rej, T_ext, m_dot_corr] = HX(UA_guess, m_dot, T_ent, P,
        para_content,T_design, type)
coolprop_path = 'C:\Users\acer\Documents\CoolProp-master\wrappers\MATLAB';
addpath(coolprop_path);

%Input
%UA = Temperatures at point 1 and 2 (K)
%P= Pressure (Pa)
%m_dot = mass flows (kg/s)
%T_ent = Temperature entrance (K)
%Para_content = Content of para hydrogen (used in HX) (dimensionless)
%type = defines the use of the HX, either H2-He HX, Regenerator or Cooler
%Output
%Q_rej = Rejected heat in the HX, used to evaluate the rejected heat by
    the coolers (W)
%T_ext = Temperature at the exit (K)

UA_diff= 200;
tol = 100;

m_dot_1 = m_dot(1);
m_dot_2 = m_dot(2);
```

```
T_ent1 = T_ent(1);
T_ent2 = T_ent(2);

P_1 = P(1);
P_2 = P(2);

if type == "HX"
    % while UA_diff > tol
        h_ent1 = H2props(T_ent1, P_1,para_content);
        h_ent2 = py.CoolProp.CoolProp.PropsSI('H', 'T', T_ent2, 'P', P_2,
            'helium');


        %Q_max and NTU Calculation
        deltaT_max = T_ent1 - T_ent2;

        Cp_H2 = py.CoolProp.CoolProp.PropsSI('C', 'T', T_ent1, 'P', P_1, '
            PARAHYD');
        Cp_He = py.CoolProp.CoolProp.PropsSI('C', 'T', T_ent2, 'P', P_2, '
            helium');

        C_min = min(m_dot_1*Cp_H2,m_dot_2*Cp_He);
        C_max = max(m_dot_1*Cp_H2,m_dot_2*Cp_He);

        Q_dot_max = C_min*deltaT_max;

        NTU = UA_guess/C_min;

        c = C_min/C_max;

        if c == 1
            epsilon = NTU/(1+NTU);
        end
        if c < 1
            epsilon = (1-exp(-NTU*(1-c)))/(1-c*exp(-NTU*(1-c)));
        end


        Q_dot = epsilon * Q_dot_max;


        h_ext1 = h_ent1 - Q_dot/m_dot_1;
        h_ext2 = Q_dot/m_dot_2 + h_ent2;
```

```
        T_ext1= py.CoolProp.CoolProp.PropsSI('T', 'H', h_ext1, 'P', P_1, '
            PARAHYD');
        T_ext2= py.CoolProp.CoolProp.PropsSI('T', 'H', h_ext2, 'P', P_2, '
            helium');

        % UA_new = CalculateUA([T_ent1 T_ent2],[T_ext1 T_ext2],[P_1 P_2],[
            m_dot_1 m_dot_2],para_content,'HX');
        % UA_diff = abs(UA_guess - UA_new);
        % UA_guess = UA_new;

        m_dot_corr = m_dot_2;

        if T_ext2 > T_design
            h_ext2 = py.CoolProp.CoolProp.PropsSI('H', 'T', T_design, 'P',
                 P_2, 'helium');
            m_dot_2 = Q_dot/(h_ext2-h_ent2);
            m_dot_corr = m_dot_2;
            T_ext2 = T_design;
        end

        if T_ext2 > T_ent1
            T_ext2 = 0.95 * T_ent1;
            h_ext2 = py.CoolProp.CoolProp.PropsSI('H', 'T', T_ext2, 'P',
                P_2, 'helium');
            m_dot_2 = Q_dot/(h_ext2-h_ent2);
            m_dot_corr = m_dot_2;
        end

        if T_ext1 < T_ent2
            T_ent2 = 0.95 * T_ent1;
            h_ent2 = py.CoolProp.CoolProp.PropsSI('H', 'T', T_ent2, 'P',
                P_2, 'helium');
            m_dot_2 = Q_dot/(h_ext2-h_ent2);
            m_dot_corr = m_dot_2;
        end


     % end


    T_ext = [T_ext1, T_ext2];
    Q_rej = Q_dot;

end
```

```
if type == "Reg"

   % while UA_diff > tol
        h_ent1 = py.CoolProp.CoolProp.PropsSI('H', 'T', T_ent1, 'P', P_1,
            'helium');
        h_ent2 = py.CoolProp.CoolProp.PropsSI('H', 'T', T_ent2, 'P', P_2,
            'helium');

        %Q_max and NTU Calculation
        deltaT_max = T_ent1 - T_ent2;

        Cp_He1 = py.CoolProp.CoolProp.PropsSI('C', 'T', T_ent1, 'P', P_1,
            'helium');
        Cp_He2 = py.CoolProp.CoolProp.PropsSI('C', 'T', T_ent2, 'P', P_2,
            'helium');

        C_min = min(m_dot_1*Cp_He1,m_dot_2*Cp_He2);
        C_max = max(m_dot_1*Cp_He1,m_dot_2*Cp_He2);

        Q_dot_max = C_min*deltaT_max;

        NTU = UA_guess/C_min;

        c = C_min/C_max;

        if c == 1
            epsilon = NTU/(1+NTU);
        end
        if c < 1
            epsilon = (1-exp(-NTU*(1-c)))/(1-c*exp(-NTU*(1-c)));
        end


        Q_dot = epsilon * Q_dot_max;


        h_ext1 = h_ent1 - Q_dot/m_dot_1;
        h_ext2 = Q_dot/m_dot_2 + h_ent2;

        T_ext1= py.CoolProp.CoolProp.PropsSI('T', 'H', h_ext1, 'P', P_1, '
            helium');
        T_ext2= py.CoolProp.CoolProp.PropsSI('T', 'H', h_ext2, 'P', P_2, '
            helium');
```

```
        % UA_new = CalculateUA([T_ent1 T_ent2],[T_ext1 T_ext2],[P_1 P_2],[
            m_dot_1 m_dot_2],para_content,'Reg');
        % UA_diff = abs(UA_guess - UA_new);
        % UA_guess = UA_new;


    %end


    T_ext = [T_ext1, T_ext2];
    Q_rej = Q_dot;
    m_dot_corr = m_dot_2;

end



if type == "Cooler"
    %while UA_diff > tol
        h_ent1 = py.CoolProp.CoolProp.PropsSI('H', 'T', T_ent1, 'P', P_1,
            'helium');
        h_ent2 = py.CoolProp.CoolProp.PropsSI('H', 'T', T_ent2, 'P', P_2,
            'water');

        %Q_max and NTU Calculation
        deltaT_max = T_ent1 - T_ent2;

        Cp_He = py.CoolProp.CoolProp.PropsSI('C', 'T', T_ent1, 'P', P_1, '
            helium');
        Cp_water = py.CoolProp.CoolProp.PropsSI('C', 'T', T_ent2, 'P', P_2
            , 'water');

        C_min = min(m_dot_1*Cp_He,m_dot_2*Cp_water);
        C_max = max(m_dot_1*Cp_He,m_dot_2*Cp_water);

        Q_dot_max = C_min*deltaT_max;

        NTU = UA_guess/C_min;

        c = C_min/C_max;

        if c == 1
            epsilon = NTU/(1+NTU);
        end
        if c < 1
```

```
            epsilon = (1-exp(-NTU*(1-c)))/(1-c*exp(-NTU*(1-c)));
        end


        Q_dot = epsilon * Q_dot_max;


        h_ext1 = h_ent1 - Q_dot/m_dot_1;
        h_ext2 = Q_dot/m_dot_2 + h_ent2;

        T_ext1= py.CoolProp.CoolProp.PropsSI('T', 'H', h_ext1, 'P', P_1, '
            helium');
        T_ext2= py.CoolProp.CoolProp.PropsSI('T', 'H', h_ext2, 'P', P_2, '
            water');

        %
        % UA_new = CalculateUA([T_ent1 T_ent2],[T_ext1 T_ext2],[P_1 P_2],[
            m_dot_1 m_dot_2],para_content,'Cooler');
        % UA_diff = abs(UA_guess - UA_new);
        % UA_guess = UA_new;

    %end


    T_ext = [T_ext1, T_ext2];
    Q_rej = Q_dot;
    m_dot_corr = m_dot_2;




end
% fprintf('The value for the T_ext1 was: %f K\n', T_ext1(1));
% fprintf('The value for the T_ext2 was: %f K\n', T_ext(2));
% fprintf('The value for the Q_rej was: %f KW\n', Q_rej/10^3);
% fprintf('The value for the m_dot was: %f kg/s\n', m_dot_corr);
end
```

A.8 mix.m

```
    function[T_3, h_3]  = Mix(T_1,P_1,m_dot_1 ,T_2, P_2,m_dot_2,m_dot_3,
        P_3)

coolprop_path = 'C:\Users\acer\Documents\CoolProp-master\wrappers\MATLAB';
```

```
addpath(coolprop_path);

%Input
%T_1, T_2 = Temperatures at point 1 and 2 (K)
%P_1,P_2,P_3 = Pressure at all the points (Pa)
%m_dot_1,m_dot_2,m_dot_3 = mass flows (g/s)
%Output
%T_3 = Temperature at point 3 (K)
%h_3 = Enthalpy at point 3 (J/g)


h_1 = PropsSI('H','T',T_1,'P',P_1,'Helium');
h_2 = PropsSI('H','T',T_2,'P',P_2,'Helium');
h_3 = (m_dot_1*h_1 + m_dot_2*h_2)/(m_dot_1+m_dot_2);

T_3=PropsSI('T','H',h_3,'P',P_3,'Helium');

% Remove the path after using CoolProp to avoid conflicts
    rmpath(coolprop_path);

end
```

A.9 cycle.m

```
    %cycle test
function [SEC, Q_rej] = cycle(T_ent, P_ent, P_storage, m_dot, eta)

    global H_H2;
    global S_H2;
    global H_He;
    global S_He;


%initialization
P_H2 = zeros(6,1);
P_He = zeros(51,1);
T_H2 = P_H2;
T_He = P_He;
m_dot_H2_total = m_dot(1);
m_dot_He_total = m_dot(2);
H_H2 = zeros(6,1);
S_H2 = zeros(6,1);
H_He = zeros(51,1);
S_He = zeros(51,1);
```

```
m_dot_H2 =zeros(6,1);
m_dot_He =zeros (51,1);


%NORMAL INITIAL FLOWS
m_dot_He_1 = m_dot_He_total/4;
m_dot_He_2 = m_dot_He_total/4;
m_dot_He_3 = m_dot_He_total/4;
m_dot_He_4 = m_dot_He_total/4;


%CASE STUDY
% m_dot_He_1 = 27.35;
% m_dot_He_2 = 40.81;
% m_dot_He_3 = 41.25;
% m_dot_He_4 = 23.56;


%COOLER FLUID CHARATERISTICS
T_water = zeros(15,1);
T_water(1:15) = 313;
m_dot_water = zeros(15,1);
P_water = 100000;


%UNCOMMENT FOR ADJUSMENT OF FLOW FOR EACH COOLER
% m_dot_water(1) = 2;
% m_dot_water(2) = 19.49;
% m_dot_water(3) = 82.77;
% m_dot_water(4) = 84.33;
% m_dot_water(5) = 60.74;
% m_dot_water(6) = 191;
% m_dot_water(7) = 160.4;
% m_dot_water(8) = 56.8;
% m_dot_water(9) = 381;
% m_dot_water(10) = 321;
% m_dot_water(11) = 271.4;
% m_dot_water(12) = 298;
% m_dot_water(13) = 262.8;
% m_dot_water(14) = 316.6;
% m_dot_water(15) = 23.7;
```

```
%uncomment and comment above if same flow for every cooler
m_dot_water(1:15) = 120;



%Temperatures
T_H2(1)=T_ent;
T_H2(6)=30;
T_He(33)=300;
T_He(35)= 89;
T_He(38)=40;
T_He(43)=27;
T_He(49)=18;

T_He(34)=T_He(33);
T_He(36)=T_He(33);
T_He(41)=T_He(33);
T_He(47)=T_He(33);

%Pressures
P_H2(1)=P_ent;
P_H2(2:5)=P_H2(1);
P_H2(6)=P_storage;
P_He(35)= 150000;
P_He(1)=P_He(35);

P_reg = P_He(35);
P_stage1 = 350000;
P_stage2 = 650000;
P_stage3 = 3000000;

rp1 = P_stage1/P_reg;
rp2 = P_stage2/P_stage1;
rp3 = P_stage3/P_stage2;

P_He(2:3)= P_He(1)*rp1^(1/4);
P_He(4:5)=P_He(3)*rp1^(1/4);
P_He(6:7)=P_He(5)*rp1^(1/4);
P_He(8:9)=P_He(7)*rp1^(1/4);

P_He(38:40) = P_He(9);
P_He(10)= P_He(9);

P_He(11:12)= P_He(10)*rp2^(1/3);
P_He(13:14)=P_He(12)*rp2^(1/3);
```

```
P_He(15:16)=P_He(14)*rp2^(1/3);
P_He(17)=P_He(16);


P_He(18:19)= P_He(17)*rp3^(1/8);
P_He(20:21)=P_He(19)*rp3^(1/8);
P_He(22:23)=P_He(21)*rp3^(1/8);
P_He(24:25)=P_He(23)*rp3^(1/8);
P_He(26:27)=P_He(25)*rp3^(1/8);
P_He(28:29)=P_He(27)*rp3^(1/8);
P_He(30:31)=P_He(29)*rp3^(1/8);
P_He(32:33)=P_He(31)*rp3^(1/8);

P_He(34)=P_He(33);
P_He(36:37)=P_He(33);
P_He(41:42)=P_He(33);
P_He(47:48)=P_He(33);


P_He(43:46)=P_He(16);
P_He(49:51)=P_He(16);

%mass  balance
m_dot_H2(1:6)=m_dot_H2_total;


m_dot_He(34:35) = m_dot_He_1;
m_dot_He(1:9)= m_dot_He_1;

m_dot_He(36:40) = m_dot_He_2;

m_dot_He(41:45) = m_dot_He_3;
m_dot_He(47:51) = m_dot_He_4;

m_dot_He(46) = m_dot_He(45)+ m_dot_He(51);
m_dot_He(10)=m_dot_He(9)+m_dot_He(40);
m_dot_He(11:16) = m_dot_He(10);
m_dot_He(17)=m_dot_He(16)+m_dot_He(46);
m_dot_He(18:33)=m_dot_He(17);


while T_H2(6) > py.CoolProp.CoolProp.PropsSI('T', 'P', P_storage, 'Q', 0,
    'PARAHYD') && T_diff > 1
%HX1
para_content_1=paracontent(T_H2(1));
```

```
UA_HX1 = CalculateUA([T_H2(1) T_He(35)], [92.65 296.43], [P_H2(1) P_He(35)
    ], [m_dot_H2_total m_dot_He(1)], para_content_1,'HX');
[Q_cooling1, T_out_1,m_dot_corr1]= HX(UA_HX1,[m_dot_H2_total m_dot_He(1)
    ],[T_H2(1) T_He(35)],[P_H2(1) P_He(35)],para_content_1,296.4,'HX');
T_H2(2)=T_out_1(1);
T_He(1)=T_out_1(2);
m_dot_He_1 = m_dot_corr1;

%rebalance%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
m_dot_He(34:35) = m_dot_He_1;
m_dot_He(1:9)= m_dot_He_1;
m_dot_He(36:40) = m_dot_He_2;
m_dot_He(41:45) = m_dot_He_3;
m_dot_He(47:51) = m_dot_He_4;
m_dot_He(46) = m_dot_He(45)+ m_dot_He(51);
m_dot_He(10)=m_dot_He(9)+m_dot_He(40);
m_dot_He(11:16) = m_dot_He(10);
m_dot_He(17)=m_dot_He(16)+m_dot_He(46);
m_dot_He(18:33)=m_dot_He(17);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%



%IC1(water 3,4 and helium 1,2)

[Work_IC1_1, T_IC1_1]=compressor(eta,P_He(2),P_He(1),T_He(1),m_dot_He(1));
T_He(2)=T_IC1_1;
UA_Cooler1 = CalculateUA([T_He(2) T_water(1)],[298.15 350],[P_He(2)
    P_water],[m_dot_He(1) m_dot_water(1)],0,'Cooler');
[Q_rej_IC1_1, T_out_IC1_1,~]=HX(UA_Cooler1,[m_dot_He(1) m_dot_water(1)],[
    T_He(2) T_water(1)],[P_He(2) P_water],0,0,'Cooler');
T_He(3)=T_out_IC1_1(1);
T_water(1)=T_out_IC1_1(2);

[Work_IC1_2, T_IC1_2]=compressor(eta,P_He(4),P_He(3),T_He(3),m_dot_He(1));
T_He(4)=T_IC1_2;
UA_Cooler2 = CalculateUA([T_He(4) T_water(2)],[298.15 350],[P_He(4)
    P_water],[m_dot_He(1) m_dot_water(2)],0,'Cooler');
[Q_rej_IC1_2, T_out_IC1_2,~]=HX(UA_Cooler2,[m_dot_He(1) m_dot_water(2)],[
    T_He(4) T_water(2)],[P_He(4) P_water],0,0,'Cooler');
T_He(5)=T_out_IC1_2(1);
T_water(2)=T_out_IC1_2(2);

[Work_IC1_3, T_IC1_3]=compressor(eta,P_He(6),P_He(5),T_He(5),m_dot_He(1));
T_He(6)=T_IC1_3;
```

```
UA_Cooler3 = CalculateUA([T_He(6) T_water(3)],[298.15 350],[P_He(6)
    P_water],[m_dot_He(1) m_dot_water(3)],0,'Cooler');
[Q_rej_IC1_3, T_out_IC1_3,~]=HX(UA_Cooler3,[m_dot_He(1) m_dot_water(3)],[
    T_He(6) T_water(3)],[P_He(6) P_water],0,0,'Cooler');
T_He(7)=T_out_IC1_3(1);
T_water(3)=T_out_IC1_3(2);

[Work_IC1_4, T_IC1_4]=compressor(eta,P_He(8),P_He(7),T_He(7),m_dot_He(1));
T_He(8)=T_IC1_4;
UA_Cooler4 = CalculateUA([T_He(8) T_water(4)],[298.15 350],[P_He(8)
    P_water],[m_dot_He(1) m_dot_water(4)],0,'Cooler');
[Q_rej_IC1_4, T_out_IC1_4,~]=HX(UA_Cooler4,[m_dot_He(1) m_dot_water(4)],[
    T_He(8) T_water(4)],[P_He(8) P_water],0,0,'Cooler');
T_He(9)=T_out_IC1_4(1);
T_water(4)=T_out_IC1_4(2);

Q_rej_IC1_tot = Q_rej_IC1_1 + Q_rej_IC1_2 + Q_rej_IC1_3 + Q_rej_IC1_4;
Work_IC1_tot= Work_IC1_1 + Work_IC1_2 + Work_IC1_3 + Work_IC1_4;


%HX2
para_content_2=0.95;
UA_HX2 = CalculateUA([T_H2(2) T_He(38)], [45.16 86.90], [P_H2(2) P_He(38)
    ], [m_dot_H2_total m_dot_He(38)], para_content_2,'HX');
[Q_cooling2 , T_out_2,m_dot_corr2]= HX(UA_HX2,[m_dot_H2(2) m_dot_He(38)],[
    T_H2(2) T_He(38)],[P_H2(2) P_He(38)],para_content_2,91.92,'HX');
T_H2(3)=T_out_2(1);
T_He(39)=T_out_2(2);
m_dot_He_2 = m_dot_corr2;

%rebalance%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
m_dot_He(34:35) = m_dot_He_1;
m_dot_He(1:9)= m_dot_He_1;
m_dot_He(36:40) = m_dot_He_2;
m_dot_He(41:45) = m_dot_He_3;
m_dot_He(47:51) = m_dot_He_4;
m_dot_He(46) = m_dot_He(45)+ m_dot_He(51);
m_dot_He(10)=m_dot_He(9)+m_dot_He(40);
m_dot_He(11:16) = m_dot_He(10);
m_dot_He(17)=m_dot_He(16)+m_dot_He(46);
m_dot_He(18:33)=m_dot_He(17);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


%REG1
```

```
UA_Reg1 = CalculateUA([T_He(36) T_He(39)],[91.92 294.15],[P_He(36) P_He
    (39)],[m_dot_He(36) m_dot_He(44)],0,'Reg');
[~, T_reg_1,~] = HX(UA_Reg1,[m_dot_He(36) m_dot_He(44)],[T_He(36) T_He(39)
    ],[P_He(36) P_He(39)],0,0,'Reg');
T_He(37)=T_reg_1(1);
T_He(40)=T_reg_1(2);

%IC2
[T_mix_1, ~] = Mix(T_He(9),P_He(9),m_dot_He(9),T_He(40),P_He(40),m_dot_He
    (40),m_dot_He(10),P_He(10));

%h_9 = PropsSI('H','T','P',P_He(9),'Helium');
%h_40 = PropsSI('H','T',T_He(40),'P',P_He(40),'Helium');
%h_10 = (m_dot_He(9)*h_9 + m_dot_He(40)*h_40)/m_dot_He(10);

%T_He(10)=PropsSI('T','H',h_10,'P',P_He(10),'Helium');


T_He(10) = T_mix_1;


[Work_IC2_1, T_IC2_1]=compressor(eta,P_He(11),P_He(10),T_He(10),m_dot_He
    (10));
T_He(11)=T_IC2_1;
UA_Cooler5 = CalculateUA([T_He(11) T_water(5)],[298.15 350],[P_He(11)
    P_water],[m_dot_He(10) m_dot_water(5)],0,'Cooler');
[Q_rej_IC2_1, T_out_IC2_1,~]=HX(UA_Cooler5,[m_dot_He(10) m_dot_water(5)],[
    T_He(11) T_water(5)],[P_He(11) P_water],0,0,'Cooler');
T_He(12)=T_out_IC2_1(1);
T_water(5)=T_out_IC2_1(2);


[Work_IC2_2, T_IC2_2]=compressor(eta,P_He(13),P_He(12),T_He(12),m_dot_He
    (10));
T_He(13)=T_IC2_2;
UA_Cooler6 = CalculateUA([T_He(13) T_water(6)],[298.15 350],[P_He(13)
    P_water],[m_dot_He(10) m_dot_water(6)],0,'Cooler');
[Q_rej_IC2_2, T_out_IC2_2,~]=HX(UA_Cooler6,[m_dot_He(10) m_dot_water(6)],[
    T_He(13) T_water(6)],[P_He(13) P_water],0,0,'Cooler');
T_He(14)=T_out_IC2_2(1);
T_water(6)=T_out_IC2_2(2);

[Work_IC2_3, T_IC2_3]=compressor(eta,P_He(15),P_He(14),T_He(14),m_dot_He
    (10));
```

```
T_He(15)=T_IC2_3;
UA_Cooler7 = CalculateUA([T_He(15) T_water(7)],[298.15 350],[P_He(15)
    P_water],[m_dot_He(10) m_dot_water(7)],0,'Cooler');
[Q_rej_IC2_3, T_out_IC2_3,~]=HX(UA_Cooler7,[m_dot_He(10) m_dot_water(7)],[
    T_He(15) T_water(7)],[P_He(15) P_water],0,0,'Cooler');
T_He(16)=T_out_IC2_3(1);
T_water(7)=T_out_IC2_3(2);

Q_rej_IC2_tot = Q_rej_IC2_1 + Q_rej_IC2_2 + Q_rej_IC2_3;
Work_IC2_tot= Work_IC2_1 + Work_IC2_2 + Work_IC2_3;

%HX3

para_content_3=0.95;
UA_HX3 = CalculateUA([T_H2(3) T_He(43)], [29.05 43.16], [P_H2(3) P_He(43)
    ], [m_dot_H2_total m_dot_He(3)], para_content_3,'HX');
[Q_cooling3, T_out_3,m_dot_corr3]= HX(UA_HX3,[m_dot_H2(3) m_dot_He(43)],[
    T_H2(3) T_He(43)],[P_H2(3) P_He(43)],para_content_3,48.7,'HX');
T_H2(4)=T_out_3(1);
T_He(44)=T_out_3(2);
m_dot_He_3 = m_dot_corr3;

%rebalance%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
m_dot_He(34:35) = m_dot_He_1;
m_dot_He(1:9)= m_dot_He_1;
m_dot_He(36:40) = m_dot_He_2;
m_dot_He(41:45) = m_dot_He_3;
m_dot_He(47:51) = m_dot_He_4;
m_dot_He(46) = m_dot_He(45)+ m_dot_He(51);
m_dot_He(10)=m_dot_He(9)+m_dot_He(40);
m_dot_He(11:16) = m_dot_He(10);
m_dot_He(17)=m_dot_He(16)+m_dot_He(46);
m_dot_He(18:33)=m_dot_He(17);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%



%REG2

UA_Reg2 = CalculateUA([T_He(41) T_He(44)],[48.7 294.15],[P_He(41) P_He(44)
    ],[m_dot_He(41) m_dot_He(44)],0,'Reg');
[~, T_reg_2,~] = HX(UA_Reg2,[m_dot_He(41) m_dot_He(44)],[T_He(41) T_He(44)
    ],[P_He(41) P_He(44)],0,0,'Reg');
T_He(42)=T_reg_2(1);
T_He(45)=T_reg_2(2);
```

```
%HX4

para_content_4=0.95;
UA_HX4 = CalculateUA([T_H2(4) T_He(49)], [20.57 27.05], [P_H2(4) P_He(49)
    ], [m_dot_H2_total m_dot_He(4)], para_content_4,'HX');
[Q_cooling4, T_out_4,m_dot_corr4]= HX(UA_HX4,[m_dot_H2(4) m_dot_He(49)],[
    T_H2(4) T_He(49)],[P_H2(4) P_He(49)],para_content_4,32.97,'HX');
T_H2(5)=T_out_4(1);
T_He(50)=T_out_4(2);
m_dot_He_4 = m_dot_corr4;

%rebalance%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
m_dot_He(34:35) = m_dot_He_1;
m_dot_He(1:9)= m_dot_He_1;
m_dot_He(36:40) = m_dot_He_2;
m_dot_He(41:45) = m_dot_He_3;
m_dot_He(47:51) = m_dot_He_4;
m_dot_He(46) = m_dot_He(45)+ m_dot_He(51);
m_dot_He(10)=m_dot_He(9)+m_dot_He(40);
m_dot_He(11:16) = m_dot_He(10);
m_dot_He(17)=m_dot_He(16)+m_dot_He(46);
m_dot_He(18:33)=m_dot_He(17);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


%REG3

UA_Reg3 = CalculateUA([T_He(47) T_He(50)],[32.97 294.15],[P_He(47) P_He
    (50)],[m_dot_He(47) m_dot_He(50)],0,'Reg');
[~, T_reg_3,~] = HX(UA_Reg3,[m_dot_He(47) m_dot_He(50)],[T_He(47) T_He(50)
    ],[P_He(47) P_He(50)],0,0,'Reg');
T_He(48)=T_reg_3(1);
T_He(51)=T_reg_3(2);

%%

%IC3

[T_mix_2, ~] = Mix(T_He(51),P_He(51),m_dot_He(51),T_He(45),P_He(45),
    m_dot_He(45),m_dot_He(46),P_He(46));


T_He(46) = T_mix_2;
```

```
[T_mix_3, ~] = Mix(T_He(46),P_He(46),m_dot_He(46),T_He(16),P_He(16),
    m_dot_He(16),m_dot_He(17),P_He(17));

T_He(17)=T_mix_3;

[Work_IC3_1, T_IC3_1]=compressor(eta,P_He(18),P_He(17),T_He(17),m_dot_He
    (17));
T_He(18)=T_IC3_1;
UA_Cooler8 = CalculateUA([T_He(18) T_water(8)],[298.15 350],[P_He(18)
    P_water],[m_dot_He(17) m_dot_water(8)],0,'Cooler');
[Q_rej_IC3_1, T_out_IC3_1,~]=HX(UA_Cooler8,[m_dot_He(17) m_dot_water(8)],[
    T_He(18) T_water(8)],[P_He(18) P_water],0,0,'Cooler');
T_He(19)=T_out_IC3_1(1);
T_water(8)= T_out_IC3_1(2);

[Work_IC3_2, T_IC3_2]=compressor(eta,P_He(20),P_He(19),T_He(19),m_dot_He
    (19));
T_He(20)=T_IC3_2;
UA_Cooler9 = CalculateUA([T_He(20) T_water(9)],[298.15 350],[P_He(20)
    P_water],[m_dot_He(19) m_dot_water(9)],0,'Cooler');
[Q_rej_IC3_2, T_out_IC3_2,~]=HX(UA_Cooler9,[m_dot_He(19) m_dot_water(9)],[
    T_He(20) T_water(9)],[P_He(20) P_water],0,0,'Cooler');
T_He(21)=T_out_IC3_2(1);
T_water(9)=T_out_IC3_2(2);

[Work_IC3_3, T_IC3_3]=compressor(eta,P_He(22),P_He(21),T_He(21),m_dot_He
    (21));
T_He(22)=T_IC3_3;
UA_Cooler10 = CalculateUA([T_He(22) T_water(10)],[298.15 350],[P_He(22)
    P_water],[m_dot_He(21) m_dot_water(10)],0,'Cooler');
[Q_rej_IC3_3, T_out_IC3_3,~]=HX(UA_Cooler10,[m_dot_He(21) m_dot_water(10)
    ],[T_He(22) T_water(10)],[P_He(22) P_water],0,0,'Cooler');
T_He(23)=T_out_IC3_3(1);
T_water(10)=T_out_IC3_3(2);


[Work_IC3_4, T_IC3_4]=compressor(eta,P_He(24),P_He(23),T_He(23),m_dot_He
    (23));
T_He(24)=T_IC3_4;
UA_Cooler11 = CalculateUA([T_He(24) T_water(11)],[298.15 350],[P_He(24)
    P_water],[m_dot_He(24) m_dot_water(11)],0,'Cooler');
[Q_rej_IC3_4, T_out_IC3_4,~]=HX(UA_Cooler11,[m_dot_He(24) m_dot_water(11)
    ],[T_He(24) T_water(11)],[P_He(24) P_water],0,0,'Cooler');
T_He(25)=T_out_IC3_4(1);
```

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T_water(11)=T_out_IC3_4(2);

[Work_IC3_5, T_IC3_5]=compressor(eta,P_He(26),P_He(25),T_He(25),m_dot_He
    (25));
T_He(26)=T_IC3_5;
UA_Cooler12 = CalculateUA([T_He(26) T_water(12)],[298.15 350],[P_He(26)
    P_water],[m_dot_He(26) m_dot_water(12)],0,'Cooler');
[Q_rej_IC3_5, T_out_IC3_5,~]=HX(UA_Cooler12,[m_dot_He(26) m_dot_water(12)
    ],[T_He(26) T_water(12)],[P_He(26) P_water],0,0,'Cooler');
T_He(27)=T_out_IC3_5(1);
T_water(12)=T_out_IC3_5(2);

[Work_IC3_6, T_IC3_6]=compressor(eta,P_He(28),P_He(27),T_He(27),m_dot_He
    (27));
T_He(28)=T_IC3_6;
UA_Cooler13 = CalculateUA([T_He(28) T_water(13)],[298.15 350],[P_He(28)
    P_water],[m_dot_He(28) m_dot_water(13)],0,'Cooler');
[Q_rej_IC3_6, T_out_IC3_6,~]=HX(UA_Cooler13,[m_dot_He(28) m_dot_water(13)
    ],[T_He(28) T_water(13)],[P_He(28) P_water],0,0,'Cooler');
T_He(29)=T_out_IC3_6(1);
T_water(13)=T_out_IC3_6(2);

[Work_IC3_7, T_IC3_7]=compressor(eta,P_He(30),P_He(29),T_He(29),m_dot_He
    (29));
T_He(30)=T_IC3_7;
UA_Cooler14 = CalculateUA([T_He(30) T_water(14)],[298.15 350],[P_He(30)
    P_water],[m_dot_He(30) m_dot_water(14)],0,'Cooler');
[Q_rej_IC3_7, T_out_IC3_7,~]=HX(UA_Cooler14,[m_dot_He(30) m_dot_water(14)
    ],[T_He(30) T_water(14)],[P_He(30) P_water],0,0,'Cooler');
T_He(31)=T_out_IC3_7(1);
T_water(14)=T_out_IC3_7(2);

[Work_IC3_8, T_IC3_8]=compressor(eta,P_He(32),P_He(31),T_He(31),m_dot_He
    (31));
T_He(32)=T_IC3_8;
UA_Cooler15 = CalculateUA([T_He(32) T_water(15)],[298.15 350],[P_He(32)
    P_water],[m_dot_He(32) m_dot_water(15)],0,'Cooler');
[Q_rej_IC3_8, T_out_IC3_8,]=HX(UA_Cooler15,[m_dot_He(32) m_dot_water(15)
    ],[T_He(32) T_water(15)],[P_He(32) P_water],0,0,'Cooler');
T_He(33)=T_out_IC3_8(1);
T_water(15)=T_out_IC3_8(2);

Q_rej_IC3_tot = Q_rej_IC3_1 + Q_rej_IC3_2 + Q_rej_IC3_3 + Q_rej_IC3_4 +
    Q_rej_IC3_5 + Q_rej_IC3_6 + Q_rej_IC3_7 + Q_rej_IC3_8;
```

```
Work_IC3_tot= Work_IC3_1 + Work_IC3_2 + Work_IC3_3 + Work_IC3_4 +
    Work_IC3_5 + Work_IC3_6 + Work_IC3_7 + Work_IC3_8;


%turbines

[W_turb_1, T_turb_1] = expander(eta,P_He(35),P_He(34),T_He(34),m_dot_He
    (34));
[W_turb_2, T_turb_2] = expander(eta,P_He(38),P_He(37),T_He(37),m_dot_He
    (37));
[W_turb_3, T_turb_3] = expander(eta,P_He(43),P_He(42),T_He(42),m_dot_He
    (42));
[W_turb_4, T_turb_4] = expander(eta,P_He(49),P_He(48),T_He(48),m_dot_He
    (48));

W_turb_tot = W_turb_1 + W_turb_2 + W_turb_3 + W_turb_4;

T_diff1 = abs(T_He(35)-T_turb_1);
T_diff2 = abs(T_He(38)-T_turb_2);
T_diff3 = abs(T_He(43)-T_turb_3);
T_diff4 = abs(T_He(49)-T_turb_4);

T_diff = max([T_diff1 T_diff2 T_diff3 T_diff4]);




%wet expander

[Expander_work, T_H2(6)]= wetexpander(m_dot_H2(6),P_H2(6),P_H2(5),T_H2(5),
    eta,para_content_4);
W_exp = Expander_work;


%Parameters

W_total = abs(W_exp + W_turb_tot + Work_IC1_tot + Work_IC2_tot +
    Work_IC3_tot);

SEC = W_total/m_dot_H2_total;



Q_rej = Q_rej_IC1_tot + Q_rej_IC2_tot + Q_rej_IC3_tot;
```

```
Q_cooling = Q_cooling1+Q_cooling2+Q_cooling3+Q_cooling4;

COP = Q_cooling/W_total;

for i = 1:numel(T_He)
    % Calculate enthalpy and entropy for helium at each temperature and
       pressure
    H_He(i) = py.CoolProp.CoolProp.PropsSI('H', 'T', T_He(i), 'P', P_He(i)
       , 'helium');
    S_He(i) = py.CoolProp.CoolProp.PropsSI('S', 'T', T_He(i), 'P', P_He(i)
       , 'helium');
end
for i = 1:5
    % Calculate enthalpy and entropy for helium at each temperature and
       pressure
    [H_H2(i), S_H2(i)] = H2props(T_H2(i),P_H2(i),0.95);
end
    H_H2(6)=py.CoolProp.CoolProp.PropsSI('H', 'P', P_storage, 'Q', 0, '
       PARAHYD');
    S_H2(6)=py.CoolProp.CoolProp.PropsSI('S', 'P', P_storage, 'Q', 0, '
       PARAHYD');




T_He(35)=T_turb_1;
T_He(38)=T_turb_2;
T_He(43)=T_turb_3;
T_He(49)=T_turb_4;

%%
T_He(34) = T_He(33);
T_He(36) = T_He(33);
T_He(41) = T_He(33);
T_He(47) = T_He(33);



%rebalance%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
m_dot_He(34:35) = m_dot_He_1;
m_dot_He(1:9)= m_dot_He_1;
m_dot_He(36:40) = m_dot_He_2;
m_dot_He(41:45) = m_dot_He_3;
m_dot_He(47:51) = m_dot_He_4;
m_dot_He(46) = m_dot_He(45)+ m_dot_He(51);
```

```
m_dot_He(10)=m_dot_He(9)+m_dot_He(40);
m_dot_He(11:16) = m_dot_He(10);
m_dot_He(17)=m_dot_He(16)+m_dot_He(46);
m_dot_He(18:33)=m_dot_He(17);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

fprintf('UA1 = %f MW/K\n', UA_HX1/10^6)
fprintf('UA2 = %f MW/K\n', UA_HX2/10^6)
fprintf('UA3 = %f MW/K\n', UA_HX3/10^6)
fprintf('UA4 = %f MW/K\n', UA_HX4/10^6)

fprintf('m_dot_He 1 = %f\n', m_dot_He_1)
fprintf('m_dot_He 2 = %f\n', m_dot_He_2)
fprintf('m_dot_He 3 = %f\n', m_dot_He_3)
fprintf('m_dot_He 4 = %f\n', m_dot_He_4)
fprintf('m_dot_H2 = %f\n', m_dot_H2_total)

for i = 1:numel(T_He)
    fprintf('T_He(%d) = %f\n', i, T_He(i));
end
for i = 1:numel(T_H2)
    fprintf('T_H2(%d) = %f\n', i, T_H2(i));
end

% for i = 1:numel(T_water)
% fprintf('T_water(%d) = %f\n', i, T_water(i));
% end
fprintf('QIC1=%f',Q_rej_IC1_tot/10^6)
fprintf('QIC2=%f',Q_rej_IC2_tot/10^6)
fprintf('QIC3=%f',Q_rej_IC3_tot/10^6)


fprintf('The value for the Q_cooling was: %f MW\n', Q_cooling/10^6);
fprintf('Desired T_H2 is = %f\n', py.CoolProp.CoolProp.PropsSI('T', 'P',
    P_storage, 'Q', 0, 'PARAHYD'));
fprintf('The value for the COP was: %f \n', COP);
fprintf('The value for the SEC was: %f MJ/kg\n', SEC/10^6);
fprintf('The value for the Q_rej was: %f MW\n', Q_rej/10^6);
fprintf('m_dot_He total = %f\n', sum([m_dot_He_1 m_dot_He_2 m_dot_He_3
    m_dot_He_4]))


end
```

```
end
```

A.10 mdotfinder.m

```
function [m_dot_opt, SEC_opt, Q_rej_opt] = mdotfinder(~, ~, ~,~)

global H_H2;
global S_H2;
global H_He;
global S_He;

% Define the objective function to be minimized, it was chosen to
% change the values below
T_ent = 300;
P_ent = 6000000;
P_storage = 150000;
eta = 0.85;
objective_function = @(m_dot) cycle(T_ent, P_ent, P_storage, [10 m_dot
    ], eta);

% Set the initial guess for m_dot
m_dot_init = 120; % Example initial guess

% Perform the optimization using fminsearch

m_dot_opt = fminsearch(objective_function,m_dot_init);

[SEC_opt, Q_rej_opt] = cycle(T_ent, P_ent, P_storage, [10, m_dot_opt],
     eta);

% Plot enthalpy vs entropy
figure;
plot(S_He, H_He, 'b', 'LineWidth', 1.5);
xlabel('Entropy (J/kg-K)');
ylabel('Enthalpy (J/kg)');
title('Enthalpy vs Entropy of Helium');
for i = 1:numel(H_He)
    text(S_He(i), H_He(i), num2str(i), 'HorizontalAlignment', 'center
        ', 'VerticalAlignment', 'middle', 'Color', 'magenta');
end

% Plot enthalpy vs entropy
figure;
plot(S_H2, H_H2, 'b', 'LineWidth', 1.5);
```

```
    xlabel('Entropy (J/kg-K)');
    ylabel('Enthalpy (J/kg)');
    title('Enthalpy vs Entropy of Hydrogen');
    for i = 1:numel(H_H2)
        text(S_H2(i), H_H2(i), num2str(i), 'HorizontalAlignment', 'center
            ', 'VerticalAlignment', 'middle', 'Color', 'magenta');
    end

    % fprintf('Optimal m_dot: %.2f kg/s\n', m_dot_opt);
    fprintf('Optimal SEC: %.2f MJ/kg\n', SEC_opt/10^6);
    fprintf('Optimal Q_rej: %.2f MW\n', Q_rej_opt/10^6);


end
```

A.11 plotvariable.m

```
   % Initialization
%here you can choose the number of points and which variable is going to
    be
%studied, lb and ub are the max and min values
num_points=5;
lb = 0.7;
ub = 1;
range = linspace(lb, ub, num_points);
SEC_values = zeros(size(range));
T_ent = 300;
P_storage = 150000;
P_ent = 6000000;
m_dot = [10 130];
%eta = 0.85;

% Iteration
for i = 1:numel(range)
    % Initial value
     x1 = range(i);

 %Iteration, [SEC_values(i),~] for SEC, [~,Qrej_values(i)] for rejected
 %heat
[SEC_values(i),~] = cycle(T_ent, P_ent , P_storage ,m_dot,x1);

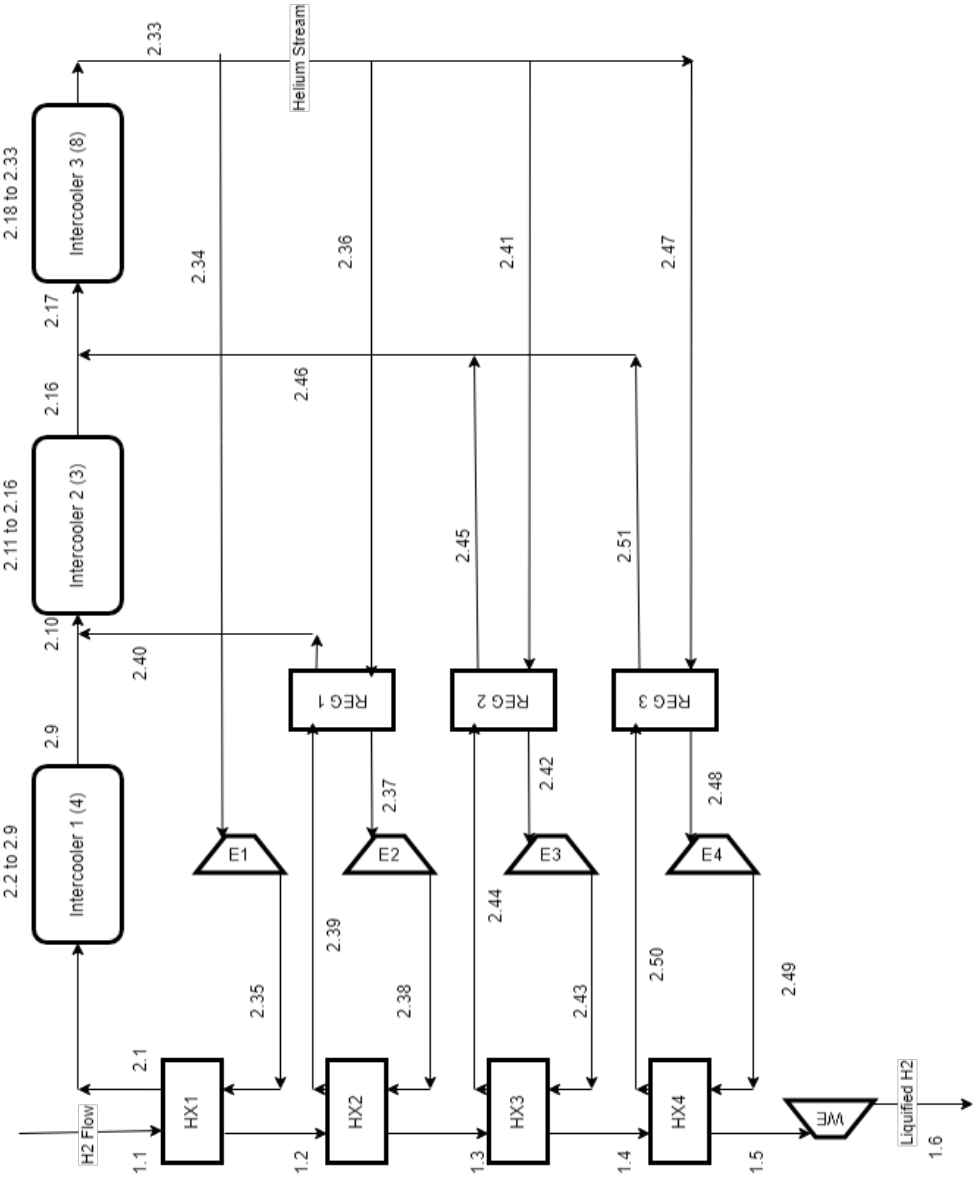
% Plot vs. variable
plot(range, SEC_values/10^6, 'o-');
xlabel('Efficiency');
```

```
ylabel('SEC (MW/kg)');
title('SEC vs. Efficiency');

end
```

Appendix B

Design Points of the cycle



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