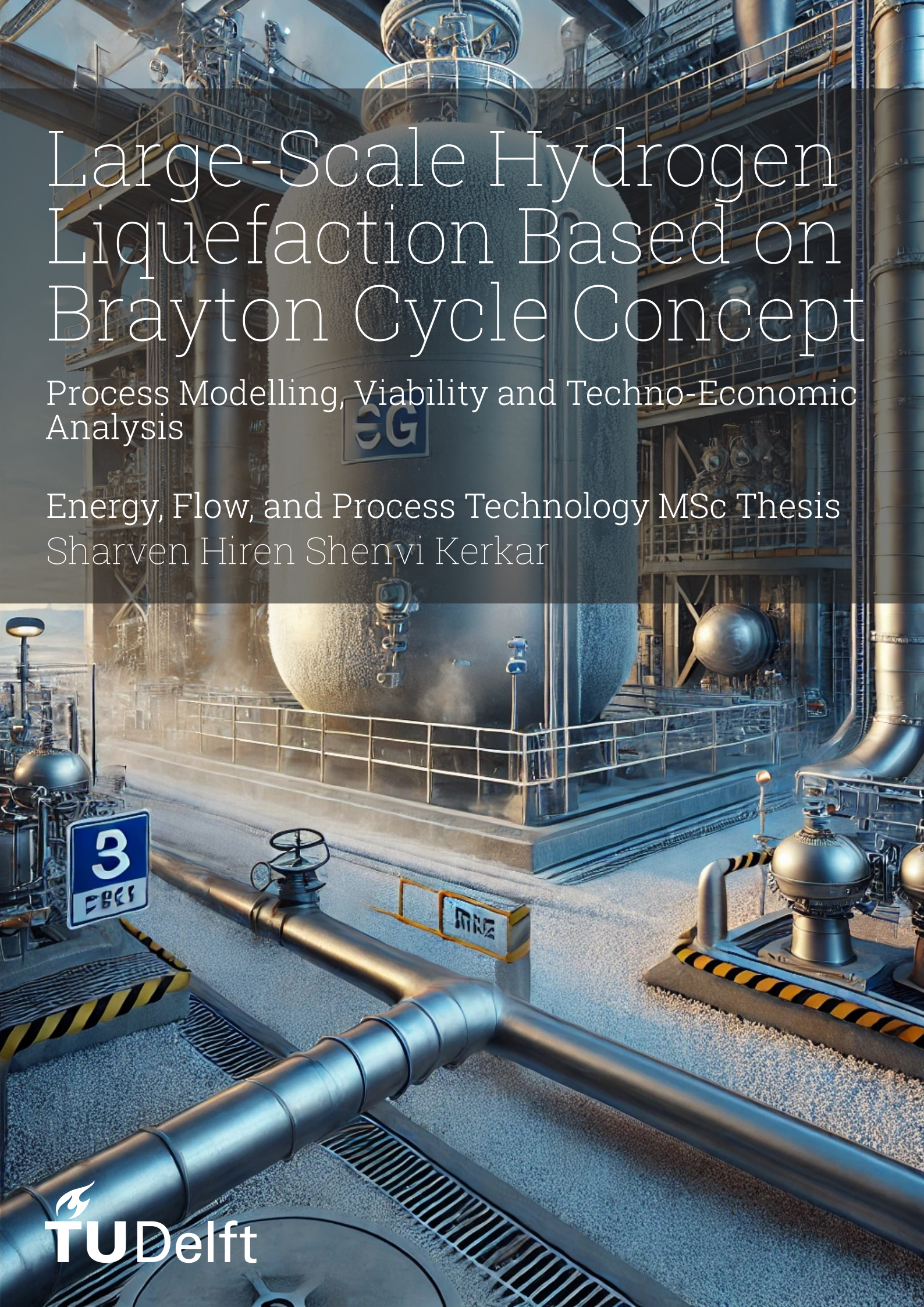


A detailed 3D rendering of an industrial hydrogen liquefaction plant. The scene features a large central storage tank with a 'EG' logo, surrounded by a complex network of pipes, valves, and safety railings. In the foreground, a large horizontal pipe runs across the frame, with a blue and white safety sign marked with the number '3' and the word 'EER' below it. The background shows more industrial structures under a clear sky.

Large-Scale Hydrogen Liquefaction Based on Brayton Cycle Concept

Process Modelling, Viability and Techno-Economic Analysis

Energy, Flow, and Process Technology MSc Thesis
Sharven Hiren Shenvi Kerkar

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Techno-Economic Analysis

by

Sharven Hiren Shenvi Kerkar

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Abstract

The viability of hydrogen as a sustainable energy carrier is significantly affected by the costs linked to its transportation and storage. Transporting and storing hydrogen in its liquid form offers remarkable advantages, as liquid hydrogen has unique characteristics, including lower weight and volume, as well as a higher energy content compared to gaseous hydrogen. However, current industrial hydrogen liquefaction processes face significant challenges related to efficiency and cost, with a second-law efficiency of less than 25% and costs ranging from 2.5-3.0 US\$/kg_{LH₂}.

Large energy storage systems can address the issue of energy demand fluctuations in renewable energy grids by storing excess energy produced and compensating for any energy shortfalls. The development of hydrogen energy storage systems will thus support the advancement and increased utilization of renewable energy sources. The demand for liquid hydrogen is expected to rise in the near future, driven by environmentally friendly applications and use in mobility sector. As a result, large-scale hydrogen liquefaction (LHL) plants will become increasingly important in the clean energy efficient hydrogen supply chain.

This thesis aims to develop a Large-scale Hydrogen Liquefaction (LHL) plant based on the Brayton-cycle concept of 86 TPD. The plant is modeled using Aspen HYSYS, with preliminary designs for key equipment—such as compressors, turbines, and plate-fin heat exchangers, ensuring compatibility with current technological constraints. State properties of the fluid used in the design of compressors and turbine equipment were obtained from REFPROP software, utilizing the Peng-Robinson Equation of State (EOS). For the design of plate-fin heat exchangers, Aspen Exchanger Design and Rating (EDR) was employed. Subsequently, a techno-economic analysis was conducted using the Aspen Process Economic Analyzer (APEA) to estimate both capital and operating expenditures, based on the process simulation model and preliminary equipment designs.

The specific energy consumption (SEC) of the plant, accounting for power recovery from turbine shafts, is determined to be 6.9025 kWh/kg_{LH₂}. The plant's exergy efficiency is calculated at 43.665%, and the specific liquefaction power is found to be 3.014 kWh/kg_{LH₂}. Assuming an electricity price of 0.1 €/kWh, modelled 86 TPD Brayton-cycle concept yielded specific liquefaction cost (SLC) of 1.57 €/kg_{LH₂}.

A sensitivity analysis was conducted to identify the parameters that influence the specific liquefaction cost (SLC) of the plant. The analysis focused on two key parameters: 1) electricity price and 2) feed pressure. The results reveal that fluctuations in electricity prices have a substantial impact on the plant's economic performance. Additionally, the analysis indicates that the plant's efficiency and economic viability are significantly sensitive to decreases in feed hydrogen pressure.

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Nomenclature

Abbreviations

Abbreviation	Definition
SEC	Specific Energy Consumption
APEA	Aspen Process Economic Analyzer
SLC	Specific Liquefaction Cost
TPD	Tons Per Day
LHL	Large Scale Hydrogen Liquefaction
IEA	International Energy Agency
COP	Coefficient of Performance
EOS	Equation of State
CAPEX	Capital Expenditure
OPEX	Operating Expenditure
TEA	Techno-Economic Analysis
EPC	Engineering, Procurement and Construction
CEPCI	Chemical Engineering Plant Cost Index
PFHX	Plate Fin Heat Exchanger
HEX	Heat Exchanger
EDR	Exchanger Design and Rating
OM	Operation and Maintenance Cost
PFC	Perfluorocarbon
NIST	National Institute of Standards and Technology
ISBL	Inside Battery Limits
OSBL	Outside Battery Limits
SMR	Small Modular Reactor
J-T	Joule-Thomson
LHC	Linde-Hampson Cycle
MR	Mixed Refrigerant

Symbols

Symbol	Definition	Unit
V	Volume	[m ³]
s	Specific entropy	Jkg ⁻¹ K ⁻¹
μ_{JT}	Joule-Thomson coefficient	
T	Temperature	K
W	Work	J
Q	Heat	J
h	Specific Enthalpy	Jkg ⁻¹
m_f	Mass Flow Rate	kgs ⁻¹
ω_s	Specific Speed	
z	Number of Stages	
n	Rotation per minute	RPM
φ	Flow Coefficient	
ψ	Work Coefficient	
R	Degree of Reaction	°

Symbol	Definition	Unit
δ_t	Rotor tip Diameter Ratio	
a_2	Rotor outlet absolute flow angle	°
β_2	Rotor Outlet relative flow angle	°
u_2	Impeller tip speed velocity	m/s
c_p	Specific heat at constant pressure	Jkg ⁻¹ K ⁻¹
v	Specific Volume	m ³ kg ⁻¹
p	Pressure	Pa
$\dot{W}$	Work per unit time	W
Re	Reynolds Number	
R	Universal gas constant, 8.314	J mol ⁻¹ K ⁻¹
U	Heat transfer coefficient	Wm ⁻² K ⁻¹
A	Area	m ²
η_{is}	isentropic efficiency	
U_a	Utilization Rate	
I_{fix}	Fixed Annual Interest rate	
t_p	Payment Period	year

Introduction

Hydrogen is already widely used in some industries, but it has not yet realised its potential to support clean energy transitions [1]. However, there are still many challenges preventing the widespread use of hydrogen. Transport and storage costs are critical to the competitiveness of hydrogen, as they can significantly increase the final price of hydrogen fuels. The low energy density of gaseous H₂ necessitates additional processes for storage and transportation over extended distances and time scales. Hydrogen liquefaction emerges as a viable solution to address these challenges, offering advantages such as enhanced purity, versatility for various end uses, and a higher volumetric hydrogen density compared to alternative vectors. Cryogenic liquid trucks make liquid hydrogen (LH₂) particularly cost-effective for long-distance delivery with moderate demands. However, the current production and logistic processes related to LH₂ face limitations, including economic and scale constraints, hindering its widespread global use.

Hydrogen liquefaction is an important thermodynamic process that has been fully developed for large-scale cryogenic applications. Most commercial hydrogen liquefaction plants have a capacity of less than 20 tons per day (TPD), while the largest one can liquefy up to 32 TPD [2]. The specific energy consumptions (SEC) of these liquefiers are between 10 and 20 kWh/kgLH₂ [3] which makes a significant contribution to the current specific liquefaction cost (SLC) range of 2.5-3 USD/kgLH₂ [4]. In contrast, the theoretical energy required to liquefy hydrogen from ambient conditions (300 K, 1.01 bar) is 3.9 kWh/kgLH₂, including the conversion of ortho to para-H₂, suggesting ample room for improvement. Recent studies indicate a trend of decreasing liquefaction costs with the expansion of plant capacity. Some estimates propose that, with increased capacity, liquefaction costs could potentially drop to less than 1 USD/kgLH₂. The Asia Pacific Energy Research Centre (APEREC) even projected that a liquefaction plant with an 800 TPD capacity could achieve costs as low as 0.53-0.78 USD/kgLH₂.

The GRAPE model, employed to assess global hydrogen deployment, indicates a substantial surge in demand, reaching 217 million tons (Mt) by the year 2050. This represents an almost threefold increase from the current market demand. Notably, the International Energy Agency (IEA) anticipates an even more pronounced growth trajectory, projecting a global demand surge to 520 Mt by the year 2070 under their Sustainable Development Scenario (SDS). Hydrogen Council expects that by 2050, about 10% of the hydrogen demand, just under 60,000 TPD, could be transported by sea [5].

This thesis endeavors to establish a robust framework for modeling an extensive hydrogen liquefaction process and assessing the economic viability of the plant, taking into account existing technical constraints. The research begins by focusing on modeling a high-capacity hydrogen liquefaction plant using a commercial process simulation tool. A systematic procedure is then developed for the preliminary design of key equipment as part of the technical evaluation. The results of these designs are incorporated back into the liquefier simulation model. Capital and operating costs are subsequently estimated

using a general cost estimation tool based on the developed procedure, followed by a comprehensive economic evaluation. Additionally, sensitivity and scale-up analyses are conducted to evaluate the impact of operational parameters and increased capacity on plant efficiency and economics. Finally, the study forecasts potential learning and scaling curves for the hydrogen liquefaction plant based on cost results and projections from relevant literature.

In summary, the main objective of this thesis is to provide a comprehensive assessment of the technical and economic viability of a conceptual large-scale hydrogen liquefaction process while developing modeling and cost estimation frameworks that incorporate technical considerations.

The frameworks formulated in this thesis are intended to offer a universal methodology for fellow researchers and plant designers to develop large-scale hydrogen liquefaction processes that focus not only on maximizing efficiency but also on the technical aspects and economic evaluation of the plant. The frameworks could serve as a foundation for establishing a general cost-optimization procedure for designing hydrogen liquefaction plants. The study's results and analyses improve understanding of technical limitations in hydrogen liquefaction technology and identify key factors for enhancing its competitiveness. Additionally, it offers valuable insights to policymakers and regulators in developing strategies and policies related to the integration of hydrogen as a clean energy carrier in various sectors.

1.1. Sub-Research Questions

- How can a conceptual high-capacity H₂ liquefaction plant be accurately modeled using the **Brayton Cycle** concept on a commercial process simulation tool?
- What is the technical evaluation procedure for the preliminary designs of the main equipment in a large-scale hydrogen liquefaction process, and how can the findings from these preliminary designs be incorporated into the overall plant design?
- How to effectively estimate the capital and operating costs of a conceptual hydrogen liquefier based on the process simulation model and equipment preliminary designs, and what are the key factors influencing the plant's economic feasibility?

2

Literature Review

2.1. History of Hydrogen Liquefaction

James Dewar was the 1st scientist to liquefy hydrogen in 1897. This particular experiment was performed by him utilizing liquid air at -200°C and 200-atmosphere pressure and forcing it through a fine nozzle. The result was a jet of gas mixed with a liquid which unfortunately he could not collect. By spraying this jet on liquid air or oxygen he could only transform it into solids. In 1898, following the construction of a substantial regenerative cooling apparatus, he achieved success as liquefied hydrogen, cooled and compressed, escaped from the nozzle into the vacuum chamber.

2.2. Uses of Liquid Hydrogen

Liquefaction of hydrogen is important for increasing the energy density of the gas and obtaining higher purity. While hydrogen is more commonly used in the gaseous state, it is stored and transported in its liquid form. In space programs, liquid hydrogen is used as a primary rocket fuel for combustion with oxygen or fluorine and as a propellant for nuclear-powered rockets and space vehicles. For myriad chemical processes ranging from the manufacturing of high-density polyethylene and polypropylene to the hydrogenation of food-grade oils hydrogen is used as a raw material. In the metallurgical sector, hydrogen serves the purpose of diminishing metal oxides and safeguarding against oxidation during the heat treatment of specific metals and alloys. Additionally, semiconductor manufacturers employ hydrogen in their processes. In a refrigerator for the liquefaction application, the thermal load of the refrigerator is spread over the feed stream from gas at ambient temperature to liquid at cryogenic temperature [6].

2.3. Theoretical Information

2.3.1. IDEAL Liquefaction Process

The perfect refrigeration cycle is the Carnot cycle [7]. Liquefaction is fundamentally an open-system arrangement and an ideal liquefaction can be achieved only by the first two processes of the Carnot cycle which are a reversible isothermal compression followed by a reversible adiabatic (isentropic) expansion process as shown in Figure 2.1.

The input gas which has to be liquefied is compressed reversibly and isothermally to higher pressure from ambient conditions (point 1-2). This high pressure is selected such that the gas will reach the saturated liquid state (point f) after expansion in an adiabatic, reversible (isentropic) expander [7]. By applying the first law of thermodynamics to the system consisting of the compressor, expander, and liquid receiver, the following equation 2.1 is obtained:

$$Q_R - (W_c - W_e) = m_f(h_f - h_1) \quad (2.1)$$

By applying the second law of thermodynamics over the whole system the following equation is ob-

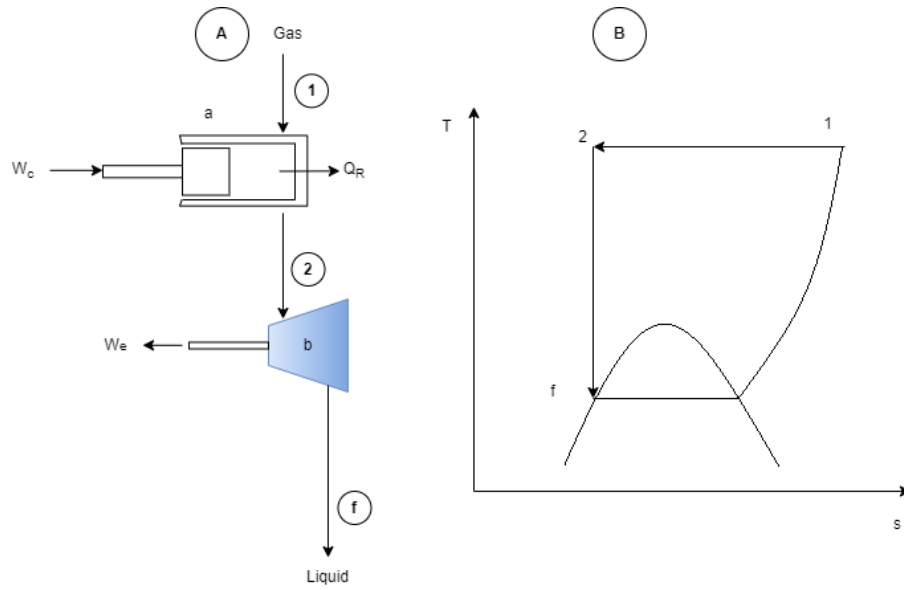


Figure 2.1: Thermodynamically Ideal System for gas liquefaction.
 A) Schematic: a) Isothermal Compressor; b) Isentropic expander.
 B) Liquefaction Thermodynamics.

tained:

$$Q_R = m_f T_1 (s_f - s_1) \quad (2.2)$$

By substituting reversible heat rejected in the isothermal compression process from equation 2.2 in the 1st law equation i.e 2.1, the expression for the ideal work being equal to the minimum work requirement for liquefaction of the gas:

$$\frac{-(W_c - W_e)}{m_f} = T_1 (s_1 - s_f) - (h_1 - h_f) \quad (2.3)$$

2.3.2. Joule-Thomson Effect

The phenomenon of fluid expansion, encountered during the traversal of an obstruction such as an expansion valve or a capillary tube, induces a consequential pressure drop within the fluid. This process, characterized by a lack of significant outer heat transfer and minimal alterations in kinetic energy, can be accurately described as isenthalpic. It is noteworthy that, in the absence of discernible work transfer between the fluid flow and its surroundings, the expansion of the fluid remains a predominantly isenthalpic process. A non-ideal Fluid will experience a temperature change. This phenomenon is called the Joule-Thomson (J-T) effect. The internal work done on attractive or repulsive interactions will result in a respective change of system temperature [7].

$$\mu_{JT} = \left(\frac{\partial T}{\partial p} \right)_h \quad (2.4)$$

The Joule-Thomson coefficient μ_{JT} of a fluid is an important parameter for the design of cryogenic refrigeration and liquefaction processes [8]. For an isenthalpic process, the change in temperature for change in pressure is represented by Joule-Thomson coefficient μ_{JT} . It is equivalent to the slope of the isenthalpic lines as shown in Figure 2.2. The region where μ_{JT} is greater than zero resembles an isenthalpic expansion which results in a decrease in temperature. Conversely, in regions where μ_{JT} is

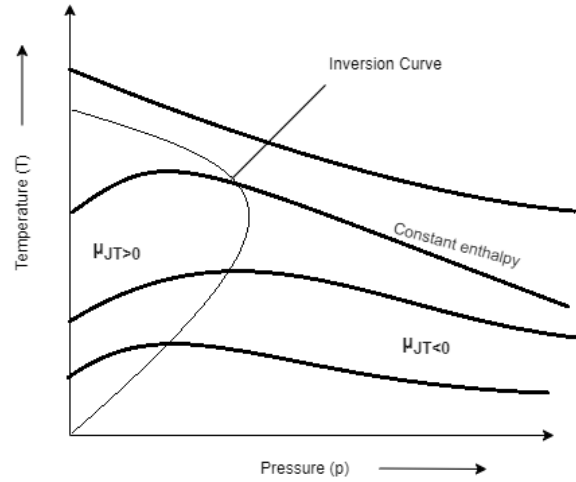


Figure 2.2: General temperature-pressure diagram for a real gas.

less than zero, the system exhibits characteristics indicating an isenthalpic expansion which increases the temperature. At the inversion points of the isenthalpic curves, the Joule-Thomson coefficient value is zero as the slope of the curves is zero.

2.3.3. Concept of Inversion Temperature for Real gas

Equation (2.5) expresses the Joule-Thomson coefficient in terms of volumetric and caloric properties. Since an ideal gas does not possess any intermolecular forces one can expect a value of zero for its Joule-Thomson coefficient [7]. For a real gas, the Joule-Thomson coefficient may be negative, zero, or positive, depending on the initial temperature and pressure of the material [7].

$$\mu_{JT} = \frac{1}{c_p} \left[T \left(\frac{\partial v}{\partial T} \right)_p - v \right] \quad (2.5)$$

In van der Waals equation of state constant a gives a measure of the intermolecular forces between the molecules and constant b provides a measure of the finite size of the gas molecules. The expression for the Joule-Thomson coefficient for real gases that follow the van der Waals equation of state is given by:

$$\mu_{JT} = \frac{(2a/RT)(1 - b/v)^2 - b}{c_p [1 - (2/vRT)(1 - b/v)^2]} \quad (2.6)$$

For larger values of the specific volume, Equation 2.6 simplifies to:

$$\mu_{JT} = \frac{1}{c_p} \left(\frac{2a}{RT} - b \right) \quad (2.7)$$

This expression shows that the Joule-Thomson coefficient is positive when $T < 2a/bR$ and negative when $T > 2a/bR$ [7]. All the points on the inversion curve 2.3 resemble the J-T coefficient to be zero. Hence equation 2.6 will be simplified to:

$$T_i = \frac{2a}{bR} (1 - b/v)^2 \quad (2.8)$$

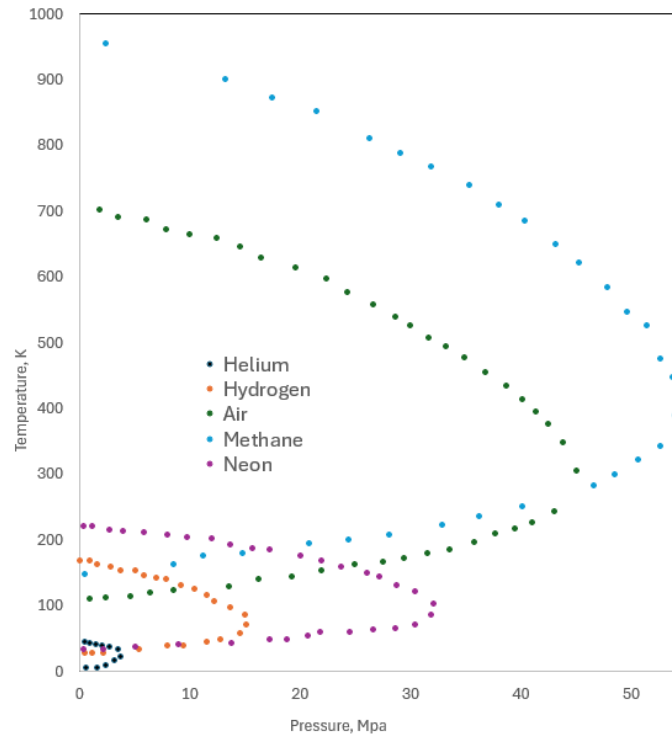


Figure 2.3: J-T inversion curves of common cryogenic fluids
a) Methane; b) Air; c) Neon; d) Hydrogen; e) Helium
Cooling by isenthalpic expansion is only possible left (inside) of the respective inversion curve.

Table 2.1: Maximum Inversion Temperature for Several Gases [7]

Gas Type	Inversion Temperature (K)
Helium [^4He]	45
Carbon monoxide	652
Hydrogen	205
Neon	250
Argon	794
Air	603
Oxygen	761
Nitrogen	621
Methane	939

2.3.4. Properties of Hydrogen

Hydrogen is considered to be an alternative future energy carrier that can potentially facilitate the transition from fossil fuels to sources of clean energy because of its advantages such as high-energy density, variety of potential sources (for example water, biomass, organic matter), lightweight, and especially low environmental impact (water is the sole combustion product) [9]. Hydrogen's naturally occurring isotopes, protium, deuterium, and tritium, can combine and form diatomic molecules. However, since tritium is unstable and radioactive, and deuterium is incredibly scarce compared to protium (which has an abundance of more than 99.98%), only the properties of hydrogen molecules comprising protium are considered for industrial applications [10]. The specific mass evaporation heat (in kJ/kg) seems to be relatively high, but the volumetric evaporation heat (in kJ/l) is essentially lower because of the very low hydrogen density [11].

2.3.5. Ortho and Para modification of Hydrogen

Hydrogen can be regarded as a binary mixture of spin isomers, which are ortho-H₂ and para-H₂, and an equilibrium composition of ortho-H₂ and para-H₂ varies with temperature [12]. Ortho-Hydrogen (o-H₂) and Para-Hydrogen (p-H₂) represent two allotropic forms of the hydrogen molecule, differentiated by the spin states of the protons in the hydrogen atoms. Ortho-hydrogen (o-H₂) is when the two proton nuclear spins of the hydrogen molecule are aligned in parallel, while Para-hydrogen (p-H₂) is when the nuclear spins are in the opposite direction [13]. In Figure 2.4 the schematic representation of these two isomers is indicated. From the liquefaction perspective, the most important fact is that the energy content of ortho-hydrogen is higher than that of para-hydrogen. This means that the conversion from ortho into para hydrogen leads to heat generation [11]. The ratio of the average number of all hydrogen molecules in the p-H₂ form and that in the o-H₂ form at equilibrium conditions varies with temperature. The equilibrium mixture at a given temperature is called the equilibrium-hydrogen (e-H₂) [14]. At 25°C, molecular hydrogen consists of 75 % ortho-hydrogen and 25 % of para-hydrogen. This type of hydrogen molecule is termed as normal Hydrogen (n-H₂). At the normal boiling point, hydrogen essentially exists in the para-state, which is preferred because of its lower boil-off gas rate.

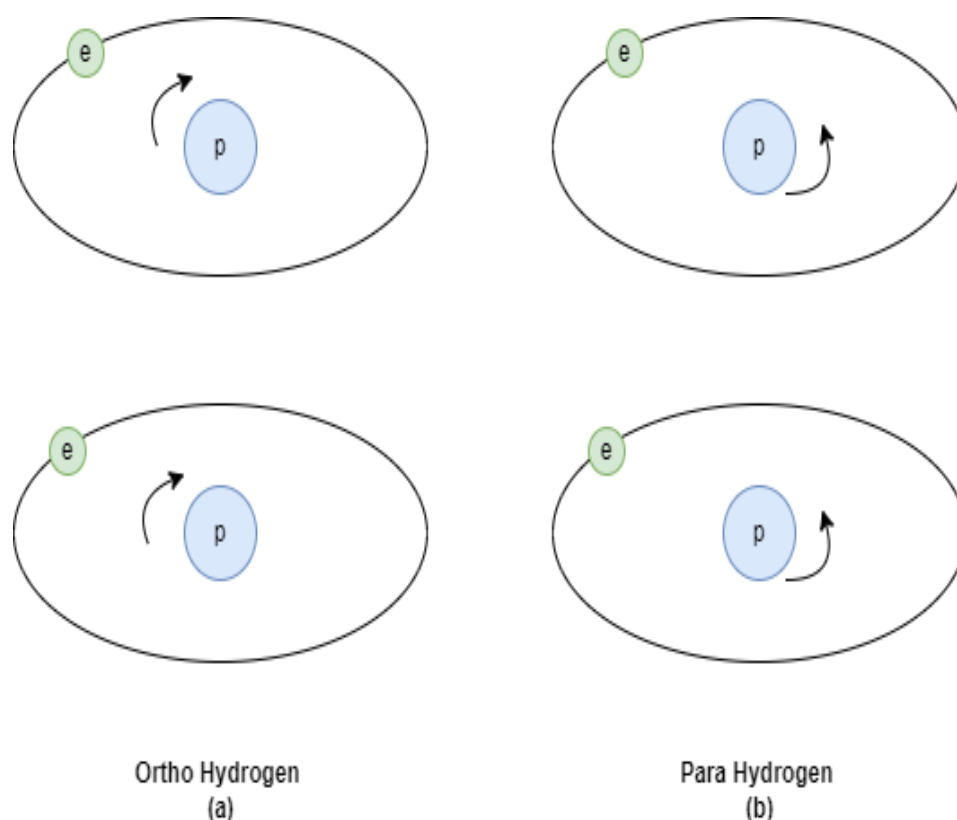
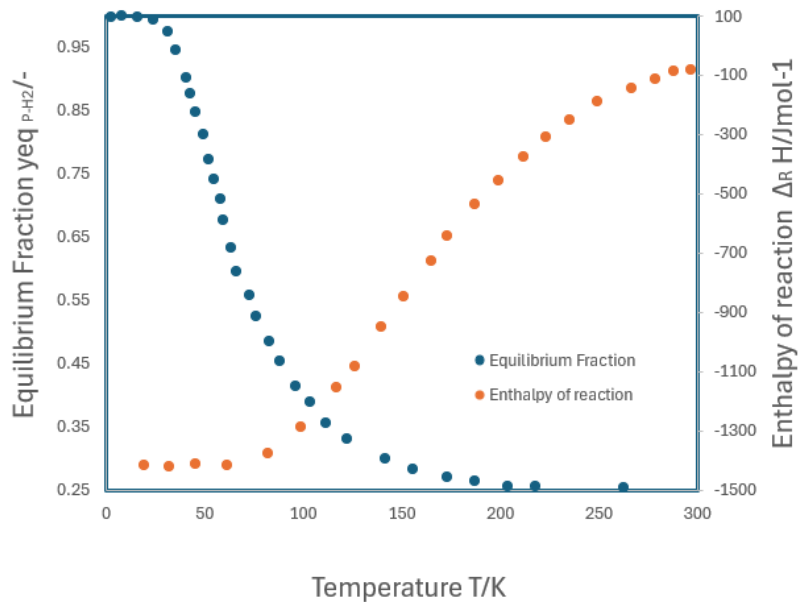


Figure 2.4: Ortho - Hydrogen (a) and Para - Hydrogen (b); p – proton, e – electron, the arrows correspond to the spin direction of the nucleus.

As hydrogen transitions from room temperature to a temperature near its typical boiling point of approximately 20.27 Kelvin, a transformation occurs, shifting the molecular configuration from ortho-hydrogen to para-hydrogen. These characteristics are seen in Table 2.2 and Figure 2.5. During the transition, the original o-H₂ molecules drop to a lower molecular-energy level, thus, releasing a quantity of energy (an exothermic reaction) called the heat of conversion [15]. Unfortunately, in the absence of a catalyst, the process of converting ortho- to para-hydrogen happens very slowly [15].

Table 2.2: Equilibrium concentration of para-Hydrogen in equilibrium Hydrogen [16]

Temperature [K]	Mole fraction of p-H ₂
20.27	0.9980
30	0.9702
40	0.8873
50	0.7796
60	0.6681
70	0.5588
80	0.4988
100	0.3947
120	0.3296
140	0.2980
160	0.2796
200	0.2597
250	0.2526
300	0.2507

**Figure 2.5:** Equilibrium composition & enthalpy of reaction of ortho- & para-hydrogen mixtures

2.3.6. Fundamental Liquefaction Systems

Linde-Hampson System

The Linde-Hampson cycle (LHC) exhibits a promising future as a cooling method to achieve cooling temperatures below -40°C and is highly desirable in commercial refrigeration [17]. The Linde-Hampson system, also called the Joule-Thomson cycle when used as a refrigerator, is considered the simplest liquefaction system as shown in Figure 2.6. In this cycle, the working gas is first compressed to a pressure of 20 MPa and passed through a recuperative heat exchanger where the returning cold vapour stream cools the warm high-pressure working gas. Further, this high-pressure gas will be expanded in a Joule-Thomson valve, and the stream will be in a partial gas-liquid phase at ambient pressure. The liquified gas is the product that will be stored and the cold gas vapors will be sent for recuperation in the heat exchanger.

The maximum inversion temperature of hydrogen is less than the standard ambient conditions hence the Linde-Hampson liquefier system is not applicable. To make use of the Linde-Hampson principle, hydrogen needs to be precooled below 205 K. This can be achieved via a Precooled Linde-Hampson liquefaction system. The precooling process in Linde-Hampson systems involves employing distinct refrigeration systems with different refrigeration fluids. The objective is to precool the primary gas stream, specifically hydrogen, before it enters the initial (two-stream) heat exchanger, ensuring that the hydrogen temperature is considerably lower than the ambient temperature. Another variation of the Linde-Hampson system, known as the precooled dual-pressure configuration, has been developed for hydrogen liquefaction. This modification has the potential to decrease the overall work input, albeit with a marginal reduction in the liquid yield of the system.

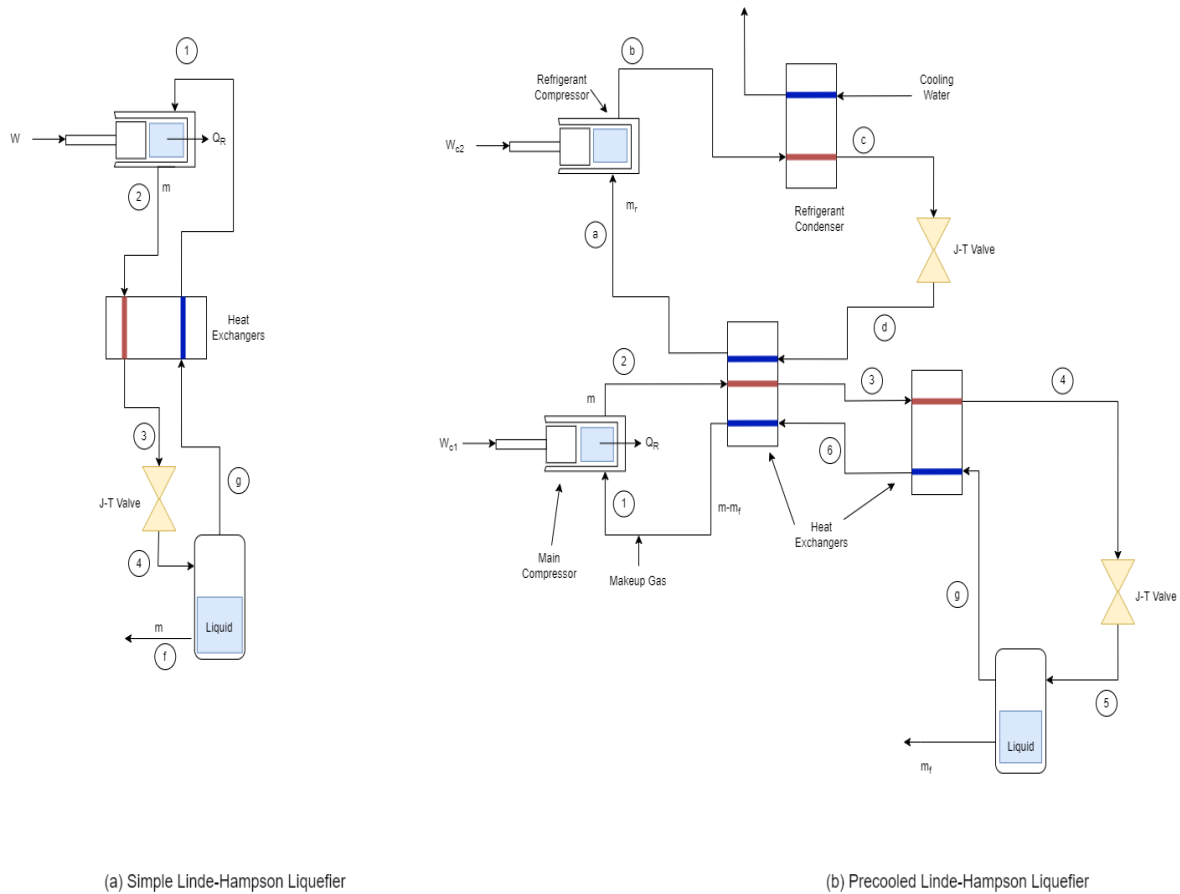


Figure 2.6: Schematic of Linde-Hampson refrigeration and liquefaction systems

Claude cycle

In the Linde-Hampson cycle, the expansion through the J-T valve is an irreversible process. Hence to improve the performance of the liquefaction system an isentropic process of expansion can be implemented instead of the isenthalpic process. This can be done by the usage of a turbine or expander which would remove the energy from the liquefying stream of fluid as shown in Figure 2.7.

If a rotary expander is utilized the cycle is sometimes also referred to as the Kapitza cycle [7]. The FOM of a Claude-type liquefier is substantially higher than for all Linde-Hampson cycles without additional work performing expansion: (1) Refrigeration effect is produced directly at cold temperatures by the withdrawal of work (enthalpy) in the expander, (2) sub-cooling of the flow at the inlet of the J-T valve greatly reduces entropy production during the isenthalpic expansion, and (3) the cold end temperature spread between the high and low-pressure stream is reduced by the direct bypass of mass flow through the expander [7].

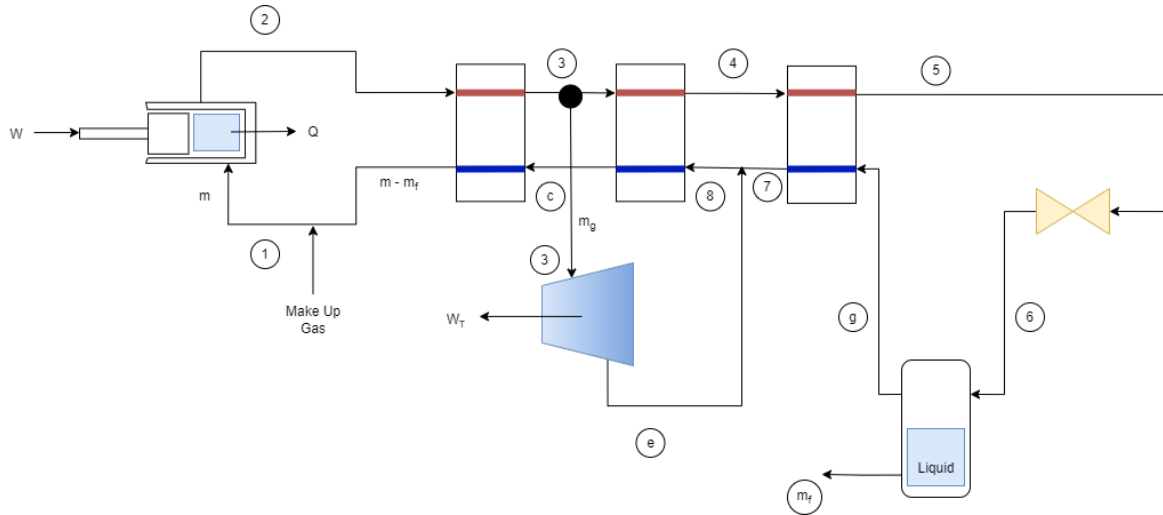


Figure 2.7: Claude Liquefaction system

Reverse Turbo-Brayton Cycle

In the Reverse Turbo-Brayton cycle, the working fluid undergoes pressurization by a compressor and simultaneous pre-cooling within a counterflow heat exchanger, commonly referred to as a recuperator is shown in Figure 2.8. Subsequently, the fluid, having exited the heat exchanger outlet, experiences an isentropic expansion in a turbine. This expansion process yields a cooling effect, and the resultant cooling power is harnessed at the cooling interface. This system employs a closed refrigeration cycle containing a pure or mixed refrigerant (MR) as the working fluid to cool the stream of the fluid to be liquefied. The technical work extracted by the turbine is used to contribute to driving the compressor, therefore the thermodynamic cycle efficiency is higher than that of the cycles where the fluid undergoes isenthalpic Joule-Thomson expansion. This cycle serves as an effective means of generating cooling power through a carefully orchestrated combination of compression, pre-cooling, and expansion processes.

Theoretically, the minimum operating temperature of a J-B refrigerator is limited by the refrigerant's freezing temperature [14]. A further practical limit to T_{min} is given by the turbine design [8]. A two-phase flow in the turbine is technically challenging and is typically avoided. Therefore, Brayton Cycles are often operated only in the gas phase [8]. However, the cycle can be useful as a precooler system for Linde-Hampson and Claude liquefaction systems. Numerous gas liquefaction system designs have incorporated the JB refrigeration cycle throughout the conceptual and real applications. Traditionally, the reverse Joule-Brayton cycle has only been considered for small-scale hydrogen liquefaction plants, but lately, there has been growing interest in its application in high-capacity systems [14].

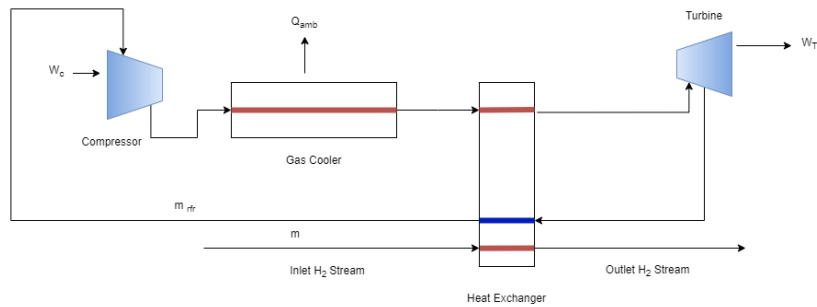


Figure 2.8: Joule-Brayton Refrigeration cycle for Hydrogen liquefaction

The Brayton liquefaction process, depicted in Figure 2.9, involves pre-cooling hydrogen using liquid nitrogen, mirroring the flow rate employed in the Claude liquefier. Subsequently, the Brayton refrigeration cycle facilitates further cooling and liquefaction of hydrogen. In this cycle, helium serves as the

refrigerant and undergoes compression through a three-stage system with interstage cooling. The compressed helium is then split into two streams, each undergoing pre-cooling to different temperatures in HX-4 and HX-5, respectively. These streams contribute to cooling hydrogen after its expansion in each refrigeration loop. Following passage through a conversion reactor to enhance the proportion of para-hydrogen and a J-T valve to sequentially reduce pressure, the liquefied hydrogen is stored. This integrated process ensures efficient hydrogen liquefaction through the synergistic utilization of liquid nitrogen and a sophisticated Brayton refrigeration cycle.

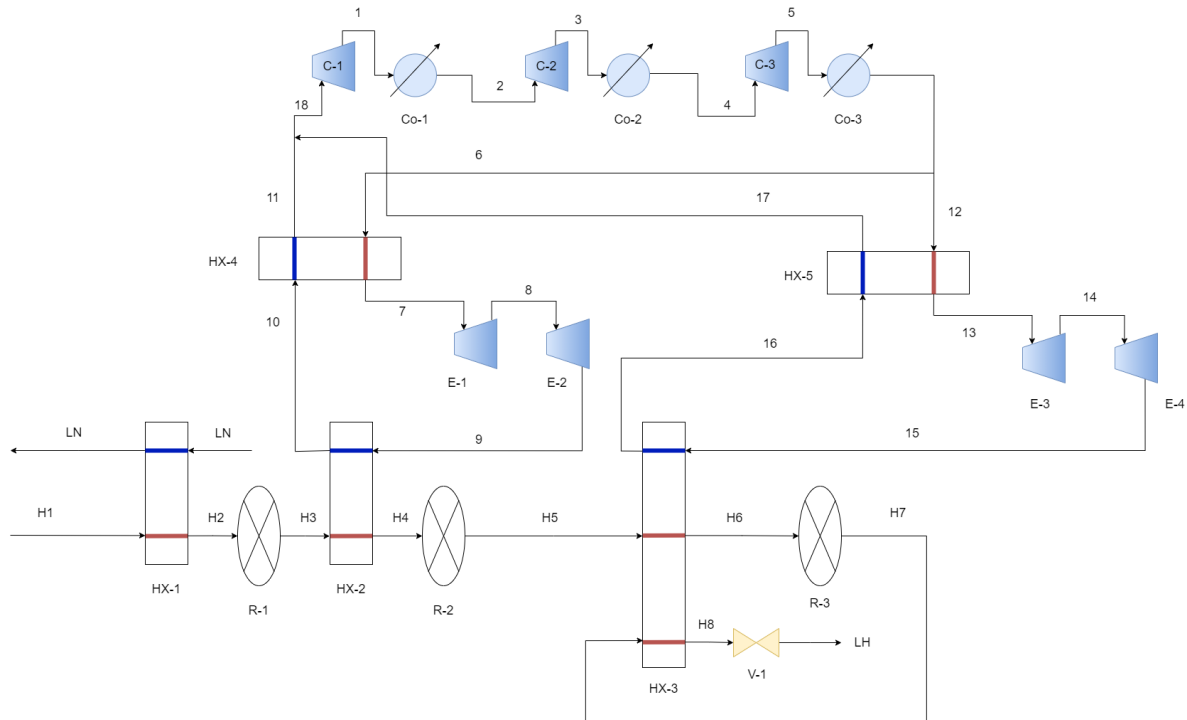


Figure 2.9: Schematic Diagram of the Brayton Liquefier

2.4. Existing Liquid Hydrogen Production

The SEC of existing industrial hydrogen liquefiers ranges from (10 to 15) kWh/kg_{LH₂} or (35 to 45) % of the lower heating value of hydrogen, with exergy efficiencies ranging from 20–30% [2]. This high energy demand is partially due to the relatively small size (capacity) of the existing liquefiers (less than approximately 32 TPD per liquefaction train), the design of which has focussed on lower capital cost (CAPEX) rather than high efficiency [2]. More than fifty industrial hydrogen liquefaction plants have been constructed since 1952, with more than fifteen industrial plants constructed or proposed since 2000. Recently-constructed plants are based on modified Claude cycles and use catalyst-packed heat exchangers (for continuous ortho–para conversion). Commercial catalysts are used in both the pre-cooling stage (where LN₂ is often used as the refrigerant) and the cryogenic stages before the final expansion [2].

In industrial hydrogen liquefaction, diverse processes are employed, utilizing coolants such as helium, hydrogen, or gas mixtures. Hydrogen liquefaction for small-scale plants with a maximum capacity of 2.5 tons per day (TPD) is accomplished with a Brayton refrigeration cycle using helium as a refrigerant. This technology is characterized by low investment costs but lower process efficiency and hence higher operating costs. In view of energy consumption, the Reverse Brayton cycle is more efficient than the Claude cycle. A key factor contributing to the lower efficiency of the Claude cycle is the presence of an expansion valve, which is absent in the Reverse Brayton cycle. The expansion valve is a significant source of efficiency loss, generating considerable entropy through throttling. This leads to increased circulation flow rates of the refrigerant, higher power consumption, and reduced pressure ratio due to leakage.

2.4.1. Linde-Leuna Hydrogen Liquefaction plant

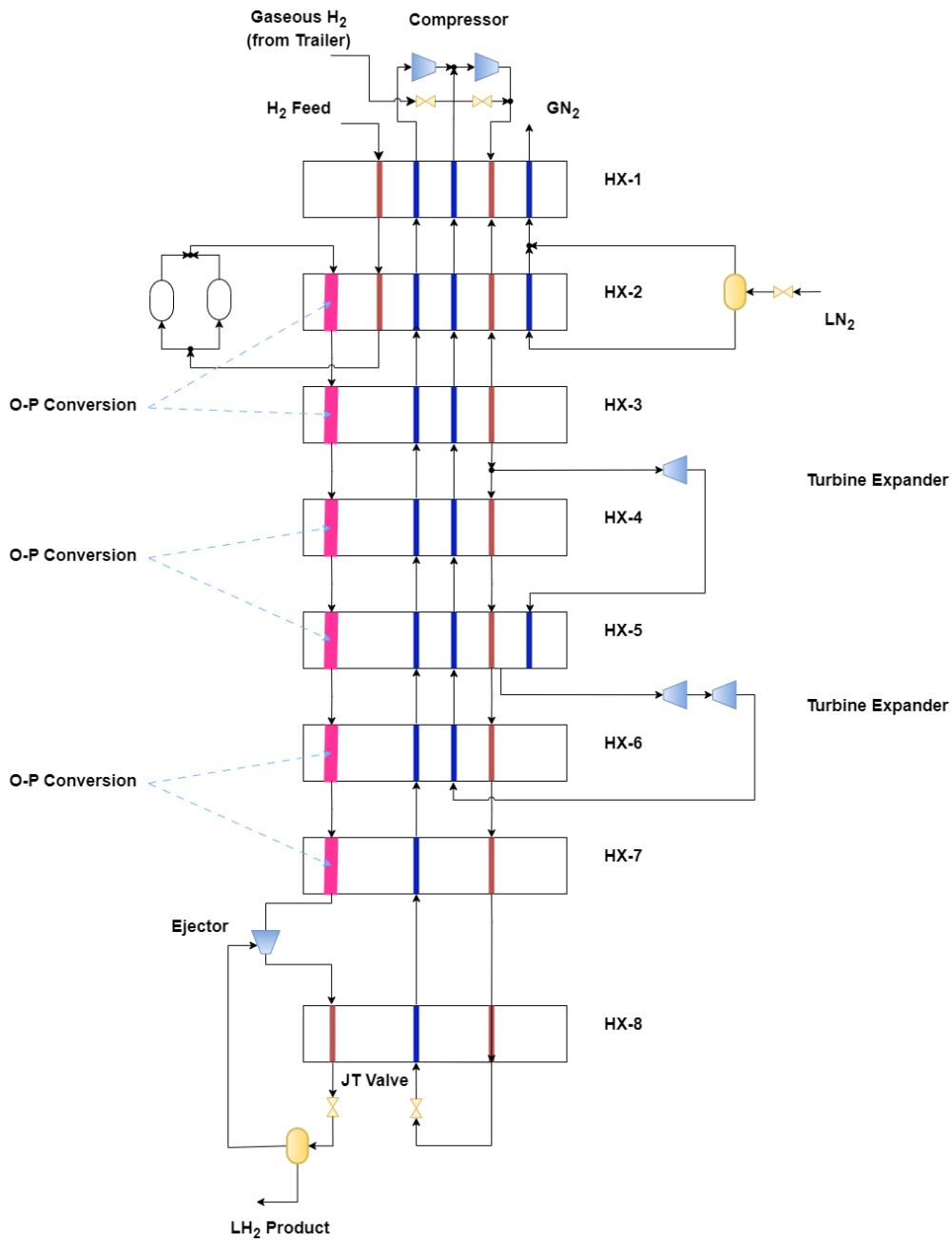


Figure 2.10: Process block diagram for the Linde hydrogen liquefier at Leuna

The Linde hydrogen liquefaction facility located in Leuna, Germany, employs a customized pre-cooled Claude cycle as shown in Figure 2.10. In this process, the pre-cooling stage utilizes recycled streams of liquid nitrogen, while the cryogenic stages involve the use of recycled streams of hydrogen. It reaches higher efficiency than a similar decommissioned plant at Ingolstadt [18]. The improvements are due to the use of continuous ortho–para conversion, oil-free advanced dynamic gas bearing turbines, and an ejector to re-liquefy boil-off gas and flash gas [2]. The cryogenic cooling system comprises a sequence of three turbines operating at speeds of 102,000 rpm and functioning within a pressure range of (0.52 to 2.0) MPa. 7 The reported SEC for the Leuna plant is 11.9 kWh/kg_{LH₂} and the exergy efficiency is 23.6 % [17].

2.4.2. Praxair Hydrogen Liquefaction plant

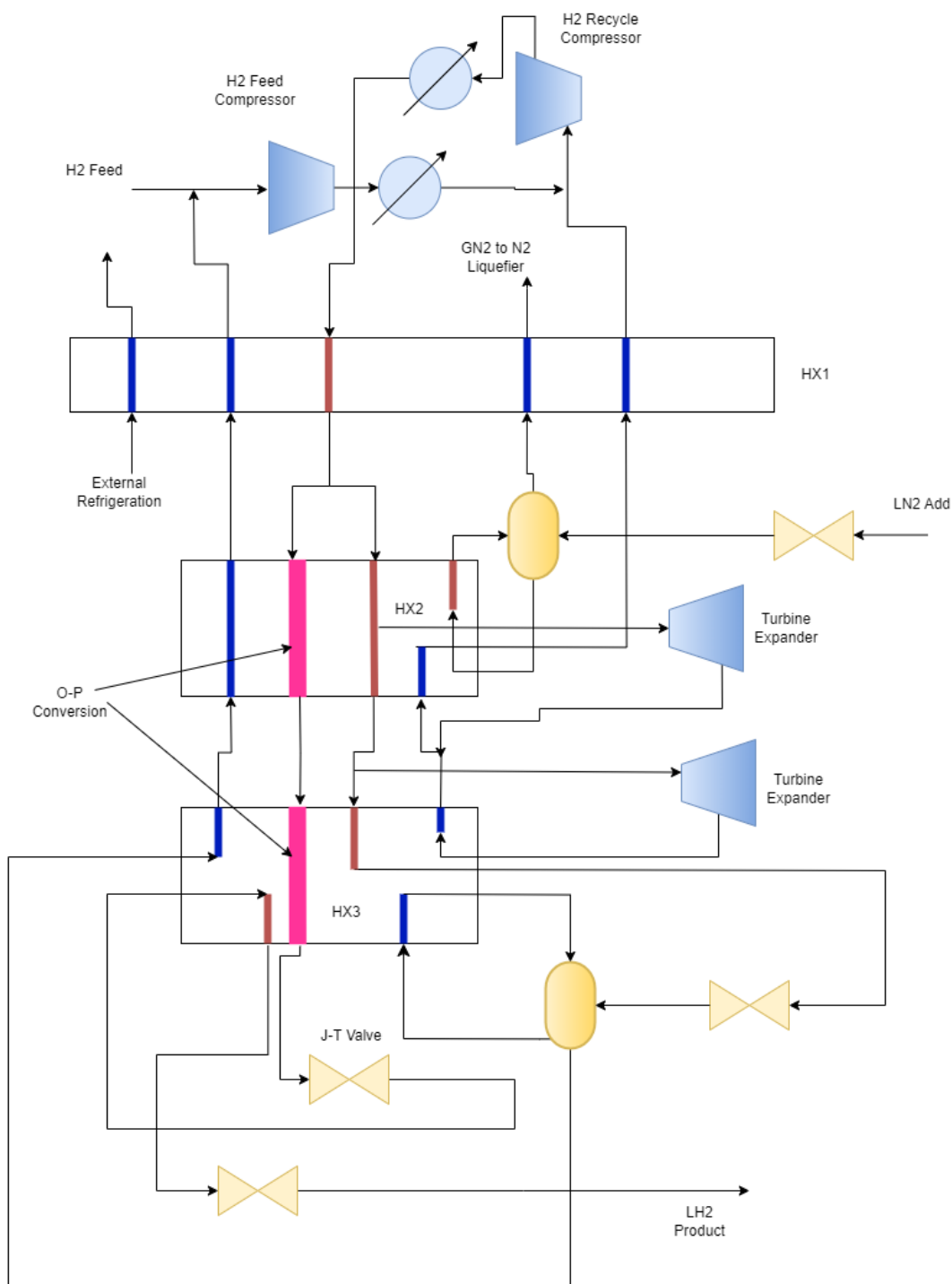


Figure 2.11: Process block diagram for a typical Praxair plant.

Praxair has five hydrogen liquefaction plants, all located in the USA, with capacities between 18 and 32 TPD. These plants also implement modified pre-cooled Claude cycles that include three heat exchangers Figure 2.11: the first cools the hydrogen feed with both nitrogen gas and a refrigerant from an external cycle, the second uses liquid nitrogen, and the hydrogen recycle stream as coolants, while the third exchanger is cooled with the hydrogen recycle stream alone. The cryogenic cooling system comprises two turbines preceding a conclusive isenthalpic (Joule–Thomson) expansion. The system

incorporates continuous ortho-to-para conversion. The Standard Energy Consumption (SEC) values for Praxair plants typically range between (12.5 and 15) kWh/kg_{LH₂}, while the exergy efficiency falls within the range of 19.3% to 24%.

2.4.3. Kimitsu Japan Hydrogen Liquefaction plant

Nippon Steel Corporation (NSC), a participant in the "Japan Hydrogen & Fuel Cell Demonstration Project" supported by the Ministry of Economy, Trade and Industry, has established a demonstration facility at its Kimitsu Works. This facility is designed for the production of liquid hydrogen, intended for use as a fuel in fuel cell vehicles. The demonstration plant was the world's first attempt to separate hydrogen from coke oven gas (COG) a by-product of steelworks and liquefy it [19] as shown in Figure 2.12. This plant has a capacity of 0.2 TPD and employs the usage of Helium Brayton cycle for the hydrogen liquefaction process. The plant employs the pressure swing adsorption (PSA) method to adsorb, separate, and refine hydrogen, which accounts for some 55% of coke oven gas (COG) [19]. This process eliminates the generation of exhaust gas and waste heat that would typically arise from chemical reactions like reformation. The residual gas is fed back to COG or used as a fuel for steel making process.

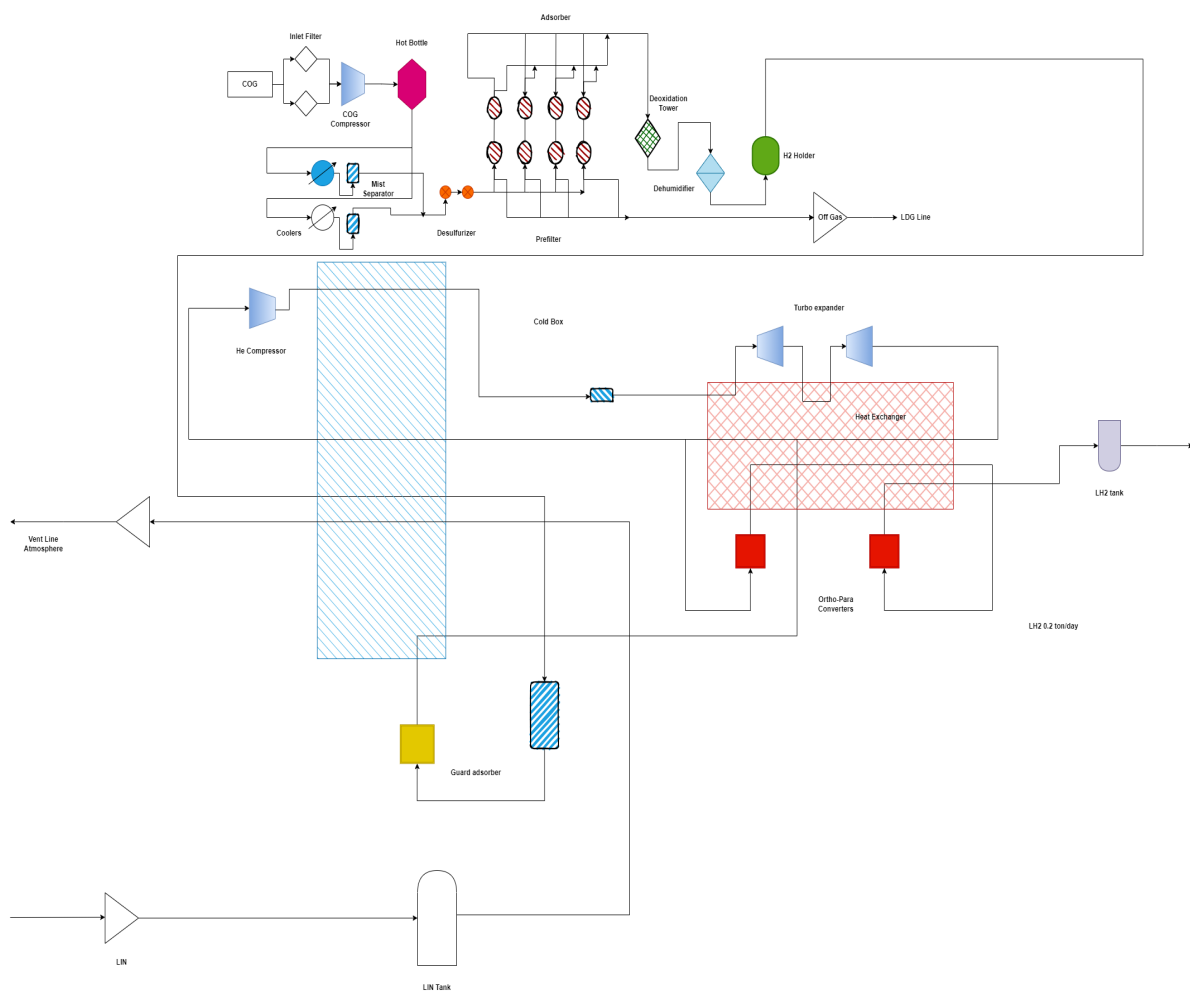


Figure 2.12: Schematic of Kimitsu Japan Hydrogen Liquefaction plant.

2.4.4. Other H₂ Liquefaction Plants based on Brayton cycle

India has adopted two major commercial hydrogen liquefaction technology plants at Mahendragiri, established in 1992 with a capacity of 0.3 TPD, and Saggonda, established in 2004 with a capacity of 1.2 TPD, organized by ISRO and Andhra sugar, respectively [9].

2.5. Conceptual Hydrogen Liquefaction Systems based on Brayton cycle

2.5.1. IDEALHY Project

The IDEALHY project is a conceptual design of a 50 TPD liquefier based on an MR pre-cooled 'nelium' (75% helium, 25% neon) mixed refrigerant in a dual Brayton refrigeration cycle [20] is depicted in Figure 2.13. The feed hydrogen is compressed from (2 to 8) MPa and this occurs in two reciprocating piston compressors. After that precooling up to 130K is achieved using four heat exchangers and a mixed refrigerant cycle comprising nitrogen, methane, ethane, propane, and n-butane. In the context of cryogenic cooling, a refrigerant known as the "nelium" mixer is employed within a dual Brayton refrigeration cycle. During the pre-cooling stage from (130 to 85)K, the conversion of ortho to para hydrogen occurs in four adiabatic converters and then continuously in subsequent catalyst-packed heat exchangers for temperature of the Hydrogen main stream less than 85K. Final expansion of the hydrogen stream to the liquid phase is achieved through two expansion turbines from (8 to 0.2) MPa [2].

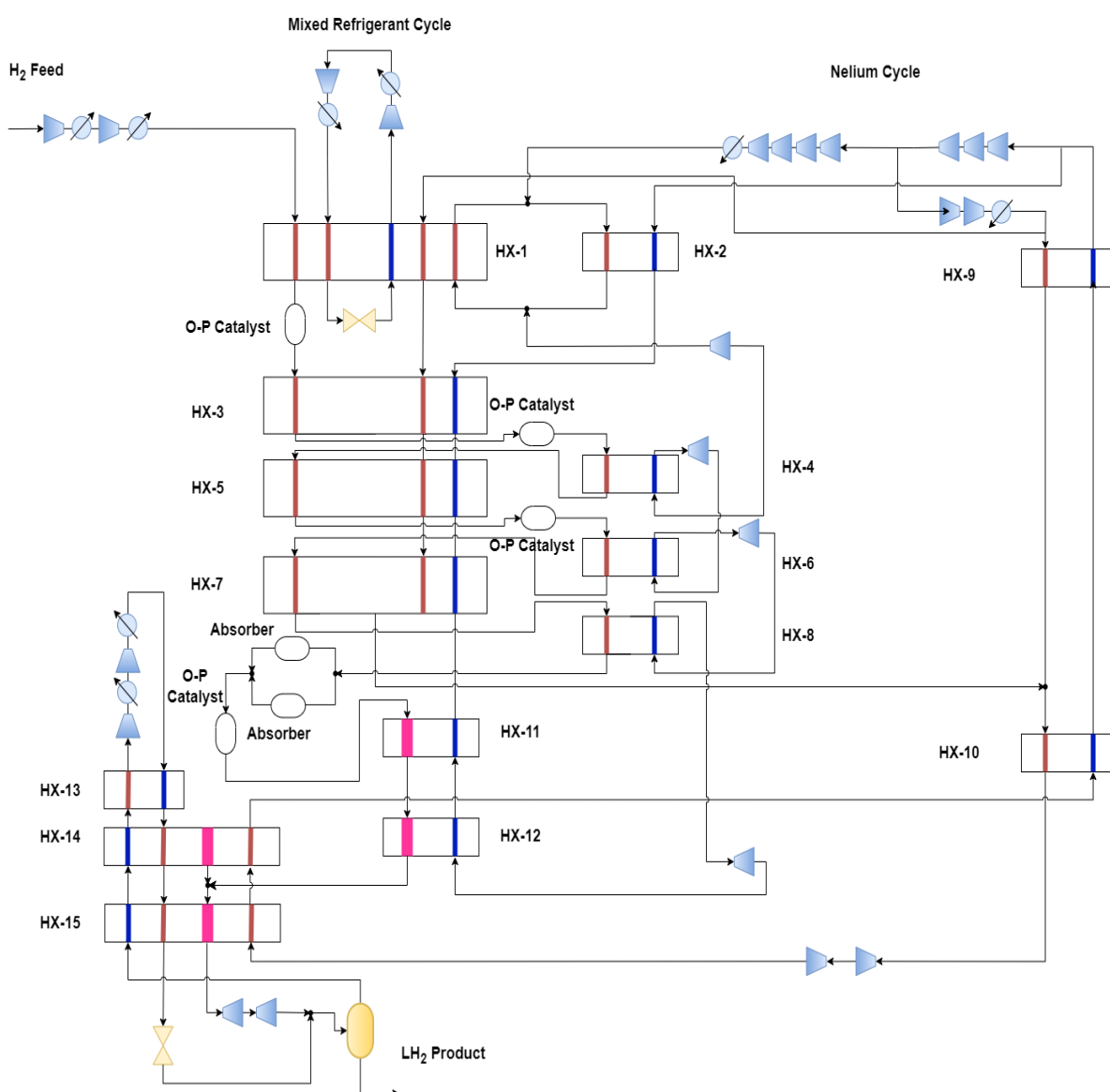


Figure 2.13: Process Block Diagram of IDEALHY Project.

2.5.2. High Efficiency Large Capacity Hydrogen Liquefier by Quack.

To investigate the conceptual design of large scale hydrogen liquefaction Quack et al.[21] had developed a 172 TPD capacity plant as shown in Figure 2.14. The overall efficiency of the plant was 53.8% considering the power recovery from the shafts of the turbine expanders.

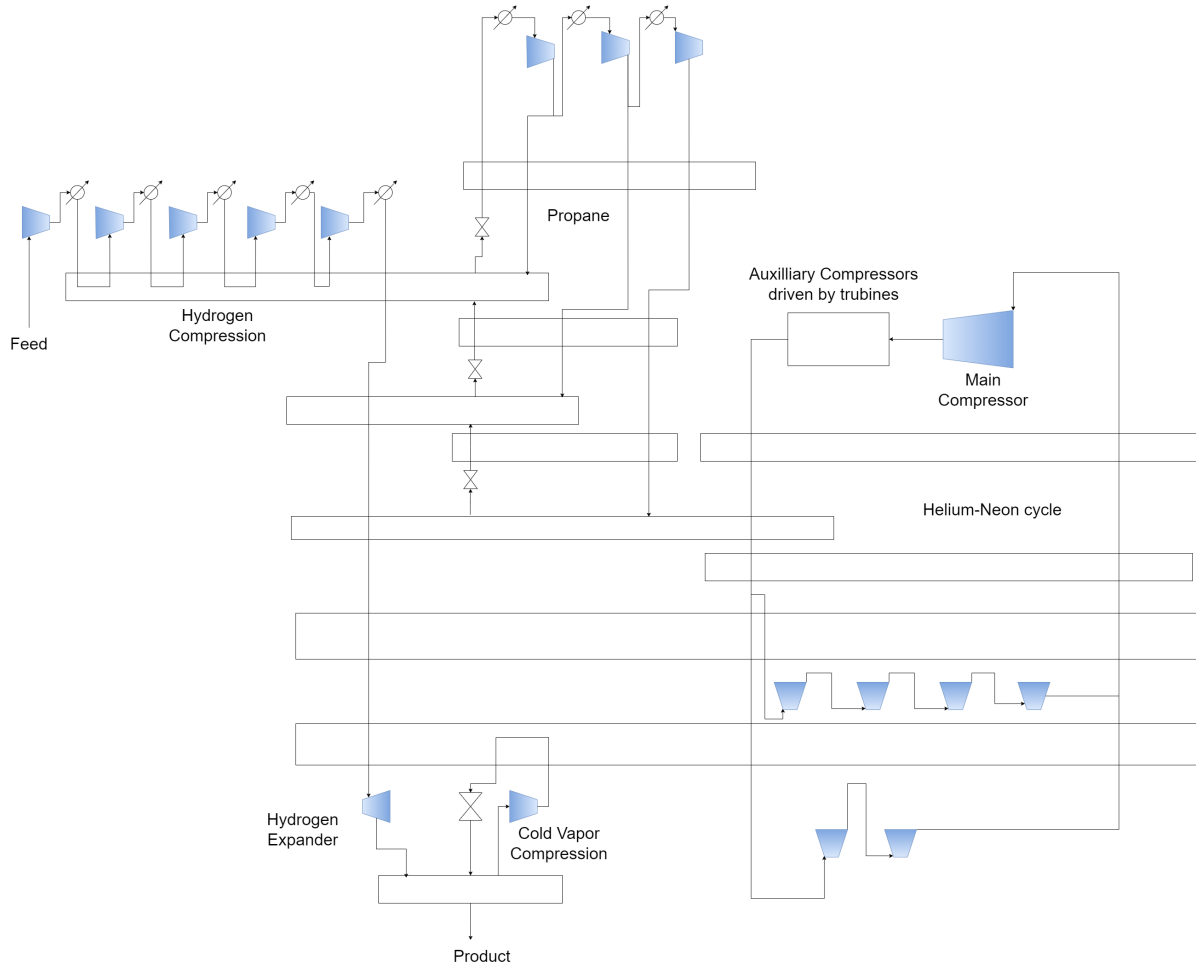


Figure 2.14: Conceptual design of a high efficiency large capacity hydrogen liquefier

2.5.3. Large-Scale Hydrogen Liquefier utilizing Mixed-Refrigerant Pre-Cooling by Berstad

A 86 TPD liquid hydrogen plant was developed by Berstad et al.[22] utilizing mixed refrigerant pre-cooling cycle to achieve a temperature of 75K in the hydrogen gas stream (H-6) as shown in Figure 2.15. The mixed refrigerant consisted of nine components i.e. Pentane, Butane, Propane, Ethylene, Ethane, Methane, Nitrogen, Neon, and R14. The cryogenic liquefaction cycle is based on Brayton cycle concept and the refrigerant used is Nelium which is 80% helium and 20% neon. This Brayton cycle is equipped with fifteen stage compressor unit with a recuperator. The isentropic efficiencies assumed in the feed and MR is 85% and in that of H₂ flash gas compressors is 80%. The exergy efficiency of this plant is 45.8% and the noted SEC is 23.343 MW considering the recovery from the shaft generators of turbines utilized in the plant. This plant diagram and details of the all streams have been used as a reference case in this thesis research.

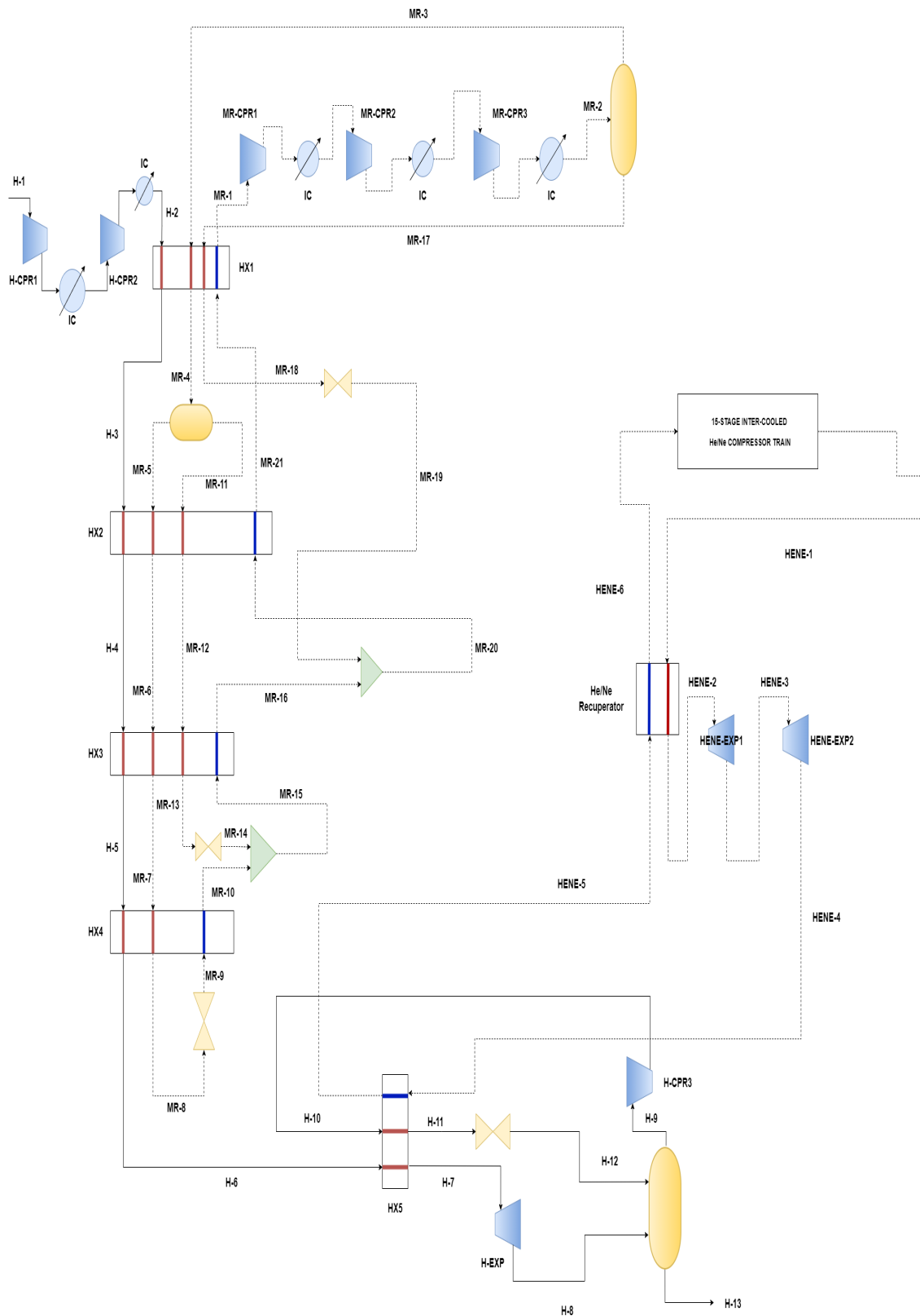


Figure 2.15: Process flow diagram, modified MR process with J–T throttling.

2.6. Equipment for Hydrogen Liquefaction

This section outlines the primary technical design considerations related to process equipment in hydrogen liquefaction processes, with a specific emphasis on the capacity and performance limitations of the equipment. The core process equipment of industrial hydrogen liquefaction processes are:

- Heat Exchangers
- Compressors
- Turbine expanders

These components will be the main focus of the equipment design part of this thesis. Other essential equipment in the hydrogen liquefaction process are the cryogenic coldbox and Joule-Thompson valve. Further standard process equipment of industrial process plants that are not described herein include, among others, pumps, coolers, chillers, phase separator vessels, drums, piping, valves, instrumentation, analyzers, and measuring devices.

2.6.1. Heat Exchangers

Heat exchangers play a crucial role in low-temperature liquefaction and refrigeration systems. In the realm of industrial hydrogen liquefaction, aluminum plate-fin heat exchangers (PFHX) are extensively employed. Their widespread usage is attributed to their versatility in accommodating various process channels and capacities. Furthermore, they offer a substantial surface area for efficient heat exchange, minimizing internal temperature differences and pressure drops. Importantly, these heat exchangers require relatively little space and involve lower capital expenditure. Aluminium PFHX can be designed to withstand a maximum pressure of approximately 115-130 bar [14]. The main hydrogen passages in the PFHX are often filled with catalyst particulates to promote the continuous and thermodynamically more efficient conversion of ortho- to para-hydrogen within the heat exchangers [2]. Hydrous ferric oxide, $\text{Fe}(\text{OH})_3$, is the commonly used catalyst material for this application [14].

According to Donaubauer [16] et al., perforated fins are preferred to give an improved catalyst distribution in the reacting hydrogen stream passages. According to Linde AG, the practical fin height is between 4-10 mm while the fin thickness varies between approximately 0.2-0.6 mm. Ohlig and Decker [4] 5.44 reported that the total exergy losses in the heat exchangers could be up to 21.6 % of the total exergy input to a typical hydrogen liquefaction process. More recently, Berstad et al. [21] calculated that the cryogenic heat exchangers contributed to approximately 21% of the total irreversibilities in a conceptual liquefaction plant with a capacity of 125 TPD. Generally, increasing the size of the PFHX would provide more heat transfer surface area and volume, which would eventually result in a higher exergy efficiency and increase the capital expenditure of the plant [23]. Linde A.G. reported the maximum geometrical dimensions for hydrogen liquefaction application is approximately 8.2 m x 3.4 m x 1.5 m, with a core volume of 15-30 m^3 and a specific surface of 500-2,000 m^2/m^3 [7].

Design of Heat exchanger

The general heat transfer equation between streams across heat exchanger is:

$$Q = U \cdot A \cdot \Delta T_m \quad (2.9)$$

In process simulation, the heat transfer rate (Q) is ascertained by employing the first law of energy balances. Concurrently, the temperature difference (ΔT_m) is conventionally derived from the composite curves of the cold and warm streams. Subsequently, the product of the overall heat transfer coefficient (U) and heat transfer area (A) is determined accordingly. The assumed heat transfer coefficients for the PFHX inside the hydrogen liquefier coldbox and the precooling coldbox are 0.1 kW/m^2 and 0.2 kW/m^2 , respectively.

2.6.2. Compressors

The task of supplying refrigeration to facilitate the hydrogen liquefaction process is accomplished through the operation of compressors. Feed compression and compression required in the refrigeration cycle account for over 90% of overall power consumption [24]. Higher feed pressure can reduce the work needed in the liquefaction system [25]. Additionally, Berstad et al.[26] reported that the compression system, which comprises compressors and intercoolers, contributes to a large portion of the exergy losses in a conceptual hydrogen Claude cycle liquefier. Within industrial cryogenic refrigeration process plants, the prevailing compressors employed are reciprocating piston compressors, rotary screw compressors, and turbo compressors. In-built hydrogen liquefiers, reciprocating piston compressors, or rotary screw compressors are typically used. In the conceptualization of hydrogen liquefaction processes, extensive consideration has been given to the utilization of reciprocating pistons as well as turbo/centrifugal compressors. Compressor capacity is constrained to its maximum feasible limit. The selection of the compressor type is contingent upon the process design, and conversely, the process design is influenced by the availability of compressors. Typically, hydrogen is delivered at a pressure above 15 bar from SMR and electrolysis plants. Owing to the notable impact of irreversibilities, the operational efficiency of compressors plays a crucial role in determining the overall operating expenses of the plant. Nevertheless, enhanced compression performance comes at the expense of higher capital costs. A compression system has the potential to constitute a substantial portion, up to 50%, of the total investment in equipment expenditures.

The exergy efficiency of the hydrogen liquefaction process is significantly impacted by the compressor's efficiency. The isentropic efficiency of the compressor is dictated by factors such as its type, capacity, and design. In hydrogen liquefaction systems, compressors are typically driven by electric motors, boasting mechanical efficiencies of up to 0.96. Conversely, the utilization of large motors can yield electrical efficiencies of up to 0.97.

The refrigerant fluid to be compressed, the required compressor capacity, and the required compression pressure ratio are the main compressor selection criteria. For the up-scaling of hydrogen liquefaction processes, the maximum feasible compressor inlet volumetric flow rate $\dot{V}_{in, max}$ and the feasible compression pressure ratio are the compressor design limiting parameters that need to be considered [8]. Figure 2.16 shows the type and application conditions of compressors that are commonly found in process industry.

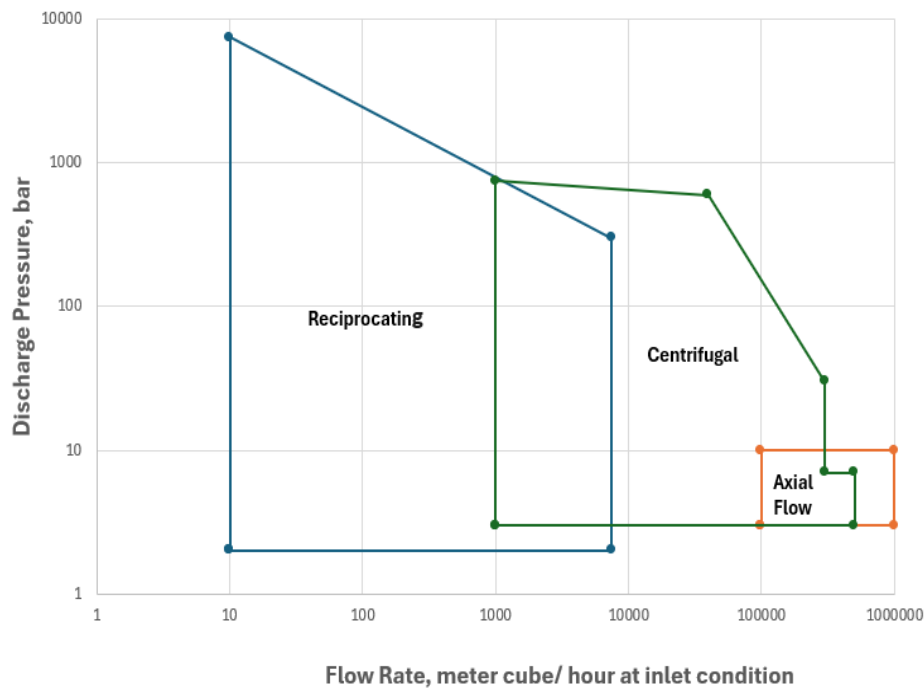


Figure 2.16: Compressor Operating Range

Rotary Screw Compressors

Oil-injected rotary screw compressors require relatively lower CAPEX; however, the efficiencies of these machines are low ($\eta_{is} = 0.65 - 0.75$) and have not seen significant improvements over time. Hence, to this day, the use of rotary screw compressors are limited to small-scale hydrogen liquefaction plant (< 3 TPD). For this reason only reciprocating piston compressors and turbo compressors are considered for the large-scale hydrogen liquefaction processes developed in this work.

Reciprocating Piston Compressors

In hydrogen liquefiers, reciprocating piston compressors are the state-of-the-art for the compression of the hydrogen feed gas stream and the hydrogen in the cryogenic refrigeration cycle. Large reciprocating piston compressors can achieve high isentropic efficiencies in the range of ($\eta_{is} = 0.75 - 0.92$). A further advantage of reciprocating piston compressors is the high compression pressure ratios that are feasible per stage, even for fluids with a low molar mass like hydrogen and helium [8]. The typical pressure ratio per stage is 1.6-2.5 [27]. Multi-stage reciprocating piston compressors with up to 4 compressor stages with inter-cooling are typically installed. However, reciprocating compressors have relatively high maintenance demands and most cannot meet the minimum requirement of continuous, uninterrupted operation for two years. Therefore, if the required flow is sufficient for a centrifugal compressor, or if the necessary head is not so high that it would not require an excessive number of stages, a centrifugal compressor is typically preferred.

Turbo Compressors

Turbo compressors stand out as the most efficient compressor type currently available in the market, typically delivering superior throughput compared to piston compressors. As a result, they prove to be more aptly suited for large-scale applications. Turbo compressors can be classified into two main types: centrifugal (also known as radial-flow) and axial-flow turbo compressors. In managing substantial volume flows, axial compressors demonstrate higher efficiency compared to centrifugal compressors. Nevertheless, centrifugal compressors exhibit greater reliability, reduced susceptibility to fouling, and broader operational flexibility. Additionally, axial-flow compressors typically entail higher capital expenditures (CAPEX) than centrifugal counterparts, although this may be justified by their smaller diameter size and efficiency at elevated volumetric rates. Hermetically-sealed compressors can be used with a much higher initial investment to achieve near-zero losses during operation. Furthermore, hermetically-sealed compressors are currently limited to applications with low maximum feasible capacity and power efficiency [28].

In reciprocating compressors, high discharge temperatures can cause problems with any sealing element (any non-metallic component in contact with the compressed gas), lubrication, and failure of the cylinder valve. Therefore, the discharge temperature should be checked for all possible working conditions, at least for the average and maximum suction temperature [29]. As recommended by API std 618 [30], the maximum predicted discharge temperature shouldn't exceed 150°C or 135°C for hydrogen-rich services (molecular weight of 12 or less). The latest trend is to hold the gas discharge temperatures below 120°C to extend the life of wearing parts [31]. On the other hand, the maximum discharge temperature of centrifugal compressors depends on the compressor design and is usually between 200 and 230°C [32].

2.6.3. Turbine/ Turbo Expanders

Expansion turbines, or turbo expanders, achieve greater cooling through isentropic expansion compared to the Joule-Thomson valve's throttling effect. However, turbines require a higher initial investment [2]. Consequently, the utilization of turbine expanders increase the exergy efficiency of the liquefier significantly when the mechanical energy from the rotation of the turbine is recovered. Berstad et al.[20] reported that for large-scale liquefier plants, recovering 80% of the power from the turbines for compression, could reduce the SEC by up to 7%. Due to the additional CAPEX, energy recovery is only economically attractive for large turbines (> 100 kW) when the electricity cost is high. In the existing hydrogen liquefaction methods, turbine power is typically dissipated using braking systems, such as air or oil brakes. However, there is potential for implementing turbine power recovery systems in the medium term, which can increase overall energy efficiency. Despite this, several technical challenges must be addressed to successfully integrate turbine power recovery technology. These challenges include optimizing the recovery system to operate efficiently under varying load conditions, ensuring

compatibility with existing liquefaction infrastructure, and managing the integration of the recovered power into the broader energy system. Addressing these issues will be critical to realizing the benefits of turbine power recovery in hydrogen liquefiers.

In the design of a turbo expander, key considerations revolve around crucial parameters such as the isentropic enthalpy drop across the expander and the volume flow rate at the expander discharge. These parameters play a pivotal role in establishing the rotor speed and wheel flow area. Within the constraints of stress and mechanical limitations, these factors collectively dictate the configuration of the hydraulic channel, thereby influencing the overall efficiency of the expander. As reported in the literature, the isentropic efficiency of cryogenic expanders is in the range of 80-90% [2]. In turbo expander design, the important parameters are the isentropic enthalpy drop across the expander and the volume flow rate at the expander discharge, which determine the rotor speed and wheel flow area, respectively. Within stress and mechanical limits, these two determine the configuration of the hydraulic channel and, thus, the expander efficiency [33].

2.7. Process Economics

In the course of developing the large-scale hydrogen liquefaction concept, a key goal in process economics evaluation involves the computation and assessment of the specific liquefaction cost (SLC). The SLC serves as a comprehensive measure encompassing all ownership costs associated with the hydrogen liquefaction plant. Its utility extends to facilitating straightforward cost-benefit analyses and supporting in-depth assessments of the hydrogen supply chain. The SLC of existing hydrogen liquefaction plants is between 2.5 and 3.0 USD/kgLH₂ [8]. Recent studies have shown that large-scale hydrogen liquefiers should be able to attain an SLC of less than 1 USD/kgLH₂ without requiring novel technologies.

$$SLC = \frac{CAPEX_a + OPEX_a + OM_a}{\dot{m}_{LH_2,a}}. \quad (2.10)$$

As shown in Equation 2.10, to determine the cost of liquefaction for the facility, it is necessary to take into account both the capital expenditure (CAPEX) and operating expenditure (OPEX). The following sections will briefly explain both terms and associated cost estimation models found in the literature.

2.7.1. Capital Expenditure

Capital expenditure (CAPEX), commonly known as capital expenses or fixed capital investment, encompasses the total costs associated with the planning, construction, and installation of a plant, along with any essential modifications required to prepare the plant site. Numerous scientific literature [34] offer methodologies, correlations, and models to facilitate the estimation of "Class 4" capital costs [34]. In the realm of cost estimation, as defined by the Association for the Advancement of Cost Estimating International (AACE International), "Class 4" cost estimates are considered preliminary and fall under categories such as "approximate," "study," and "feasibility." These estimates provide an accuracy level of approximately $\pm 30\%$.

According to Sinot and Towler, CAPEX consists of the following costs. The investment in the Inside Battery Limits (ISBL) of the plant encompasses both direct and indirect field costs. Direct field costs involve major process equipment, bulk items like piping and instruments, civil works, and installation labor. Indirect field costs include construction equipment, temporary construction, utilities, field expenses, insurance, labor benefits, miscellaneous overhead items, and services. The Offsite costs or Outside Battery Limits (OSBL) investment pertains to necessary modifications for site infrastructure, such as power generation plants, cooling towers, and maintenance facilities. Engineering costs, also known as home office costs, encompass detailed design, procurement, construction supervision, administrative charges, bonding, and contractor's profit. Contingency charges are additional funds allocated in the project budget to accommodate unforeseen discrepancies or deviations from the estimated costs.

Following Towler & Sinnott,[16] offsite costs are typically estimated as a percentage of ISBL costs during the early design phase, usually ranging from 10% to 100% depending on the project scope and its impact on-site infrastructure. In the context of petrochemical projects, offsite costs typically range from

20% to 50% of Inside Battery Limits (ISBL) costs. An initial estimate of 40% is often applied when specific site details are unknown. Established sites, as observed in "brownfield" projects with mature infrastructure, tend to have comparatively lower offsite costs. Conversely, entirely new areas, as seen in "greenfield" projects, are likely to incur higher offsite costs.

A rule of thumb for estimating engineering costs is 30% of ISBL plus OSBL costs for relatively smaller projects and 10% of ISBL plus OSBL costs for larger projects. On the other hand, the contingency charge should be at least 10% of ISBL plus OSBL costs for any projects. If the plant's technological readiness is low, higher contingency charges should be used. In this case, contingency costs can be as high as 50% of ISBL plus OSBL costs.

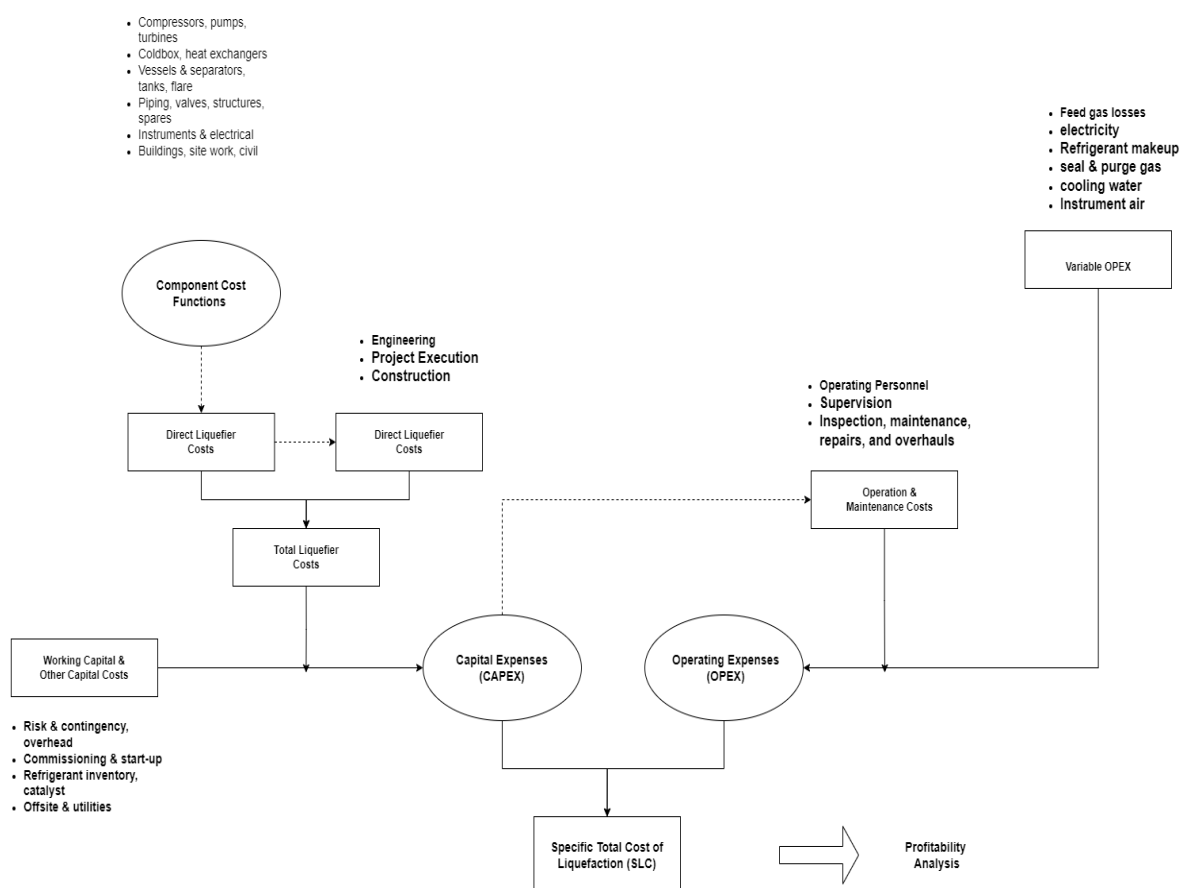


Figure 2.17: Schematic procedure for the liquefier SLC estimation proposed by Cardella [8]

Syed et al.[35] and Cardella et al. [8] conducted capital cost estimations specific for hydrogen liquefaction systems. Both employ a cost estimation model based on process equipment cost functions and adapted factors from literature to estimate ISBL investment. However, Cardella et al. [8] have developed and fitted most of their cost correlations specifically for hydrogen liquefier equipment and validated the model with cost data from industrial manufacturers. The resulting correlations from the fittings remain unpublished. Figure 2.17 shows the schematic procedure for the process economics of hydrogen liquefaction plants proposed by Cardella et al.[34]

Cost Escalation

Any approach to cost estimation relies on past data to predict future expenses. However, material prices and labor costs are susceptible to inflation. Consequently, a means must be employed to rejuvenate outdated cost data for estimating during the design phase and to project the plant's forthcoming construction expenses. Typically, historical cost data is refreshed using publicly available cost indices [16]. The following equation provides a means to adjust equipment and process plant construction costs from one period to another using cost indices:[34]

$$\text{Cost in Year A} = \text{Cost in Year B} \times \left(\frac{\text{Cost Index in Year B}}{\text{Cost Index in Year A}} \right) \quad (2.11)$$

2.7.2. Operating Expenditure

The operating expenditure (OPEX), also termed as the cash cost of production (CCOP), [34] is the expense of operating the process plant to manufacture a product, which can include up to the packaging, shipping, selling and distribution as well as the general overhead expenses [36]. In general, OPEX can be classified into variable and fixed costs of production [34]. Variable production costs encompass expenses associated with a plant's output or operational rate. These costs include raw materials utilized or transformed within the process plant, utilities like fuels, steam, cooling water, electricity, and consumables such as solvents, acids, inert materials, and catalysts that necessitate regular or frequent replacement.

In chemical plants, costs of raw materials are usually the major component of the overall operating costs, which are typically around 80-90% of the OPEX [34]. Utility costs are generally about 5-10% of the OPEX [34]. The number of raw materials and utilities required to make the desired product at the plant's design capacity can be estimated from the process model's mass and energy balances [34]. Consumables typically cost less than 3% of the OPEX [34].

In contrast, fixed production costs remain constant regardless of the plant's operational level or production output [16]. These costs do not decrease even if the plant reduces its production. The components of fixed production costs include: [16]

- Operating labor: Dependent on the number of shift positions and salaries of each operator, with operator salaries varying based on region and experience level.
- Supervision: Typically considered as 25% of operating labor costs.
- Direct salary overhead: Usually falls within the range of 40% to 60% of operating labor plus supervision expenses.
- Maintenance: Typically estimated at (3-5)% of ISBL (Inside Battery Limits) investments, contingent on the expected reliability of the plant.
- Property taxes and insurance: Generally around (1-2)% of ISBL fixed capital.
- Rent of land and buildings: Typically around (1-2)% of ISBL plus OSBL (Outside Battery Limits) cost.
- General plant overhead: Charges covering corporate overhead functions, such as human resources, research and development (R&D), information technology, finance, etc.
- Allocated environmental charges: Intended to cover superfund payments, typically around (1-2)% of ISBL plus OSBL cost.
- Running license fees and royalty payments.
- Capital charges: These include interest payments on any debt or loans used to finance the project but exclude expected returns on invested equity capital.
- Sales and marketing costs: Near zero for commodities, but for branded items (food, drug, cosmetics, etc.), these costs can be as high as millions of US dollars annually.

Process Plant Modelling

3.1. Reference Process

Based on the literature review, it can be presumed that most large-scale H₂ liquefaction concepts are developed by adopting either one of the basic systems:

- Precooled Claude Cycle
- Joule-Brayton Cycle
- Integration with LNG Production

The primary aim of this thesis is to explore the application of the Brayton cycle for large-scale hydrogen liquefaction. The use of the MR pre-cooling system eliminates the need for the LN₂ pre-cooling system, which requires a considerable portion of the total H₂ liquefaction energy [2], [37]. Mixed refrigerants (MR) are advantageous because their compositions can be easily adjusted to match the evaporation curve with the cooling requirements of hydrogen gas. Based on this data, the large-scale hydrogen liquefier utilizing the mixer-refrigerant pre-cooling has been selected to be the base process for the case study in this thesis. The reference plant used to conduct the modelling is **Process flow diagram, modified MR process with J–T throttling** from Berstad et al.[22]. The plant capacity is 86 TPD i.e.1 kg/s of liquid hydrogen as the output.

3.2. Process Description

The hydrogen liquefaction plant, depicted in Figure 3.1, utilizes the Brayton cycle and has been modelled using Aspen HYSYS software. Hydrogen gas is introduced into the process at a flow rate of 86 TPD, with an initial pressure of 21 bar and a temperature of 310 K. In this system, the H-1 stream, containing hydrogen at 21 bar, is compressed to 80 bar through a two-stage compression system comprising compressors HPC-1 and HPC-2, achieving an overall pressure ratio of 4. Post-compression, each stage incorporates an aftercooler to decrease the gas temperature to 310 K. Subsequently, the H-2 hydrogen gas stream, at 80 bar and 310 K, enters the heat exchanger HEX1, where it is precooled to 255 K by exchanging heat with the precooling cycle.

The refrigerant of the precooling cycle consists of eight components with different mole fractions as mentioned in Table 3.2. The reference plant utilized 2.15 had a mixture of nine components as a refrigerant as depicted in Table 3.1

$$\text{COP} = \frac{\dot{Q}_L}{\dot{W}_{in}} \quad (3.1)$$

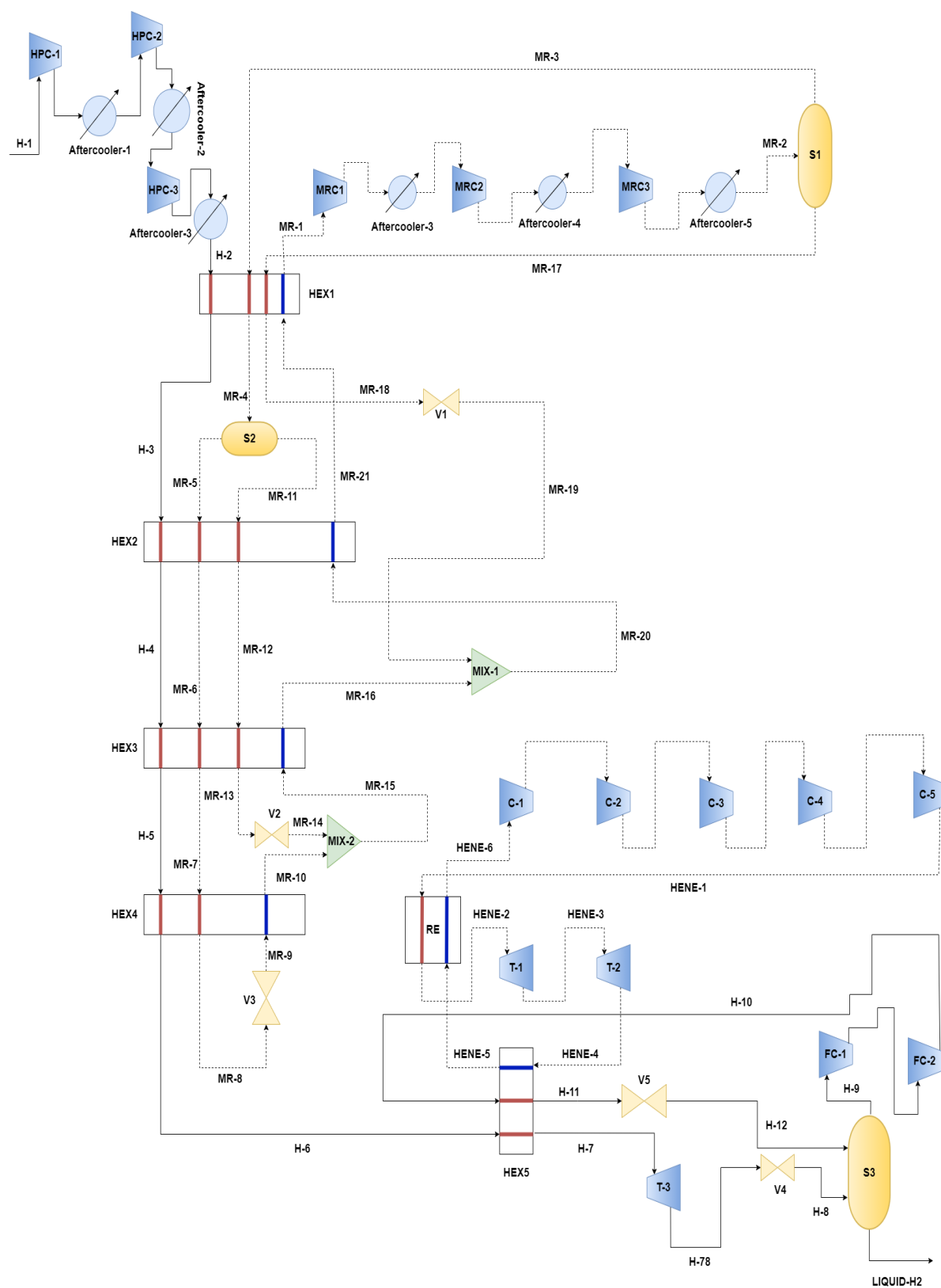


Figure 3.1: High-Pressure H₂ Brayton Cycle Liquefier Process Flow Diagram.

When R14 is included in the pre-cooling mixed refrigerant, the work input required is 8,385 kW. In contrast, when R14 is not considered, the work input increases to 9,173 kW. The useful energy output in the absence of R14 is 21,123 kW, resulting in a COP of 2.30. When R14 is included, the useful energy output decreases to 19,733 kW, with a COP of 2.35, calculated using equation (3.1). Even though the COP of both cycle is similar, R14 is a perfluorocarbon (PFC) that is not a natural refrigerant and poses environmental concerns due to its ozone depletion potential and contribution to global warming. The temperature of the H-6 stream is -175°C when R14 is used, but achieves -195°C for a flow rate of 35 kg/s in the pre-cooling cycle without R14. Achieving -195°C with R14 would require a higher flow rate, which would further reduce the COP of the cycle. Therefore, R14 was removed from the mixture.

Table 3.1: Mixed Refrigerant Composition [22]

Component	Mole Fraction [%]
Pentane	11.80
Butane	06.60
Propane	19.40
Ethylene	11.80
Ethane	08.60
Methane	16.60
Nitrogen	15.60
Neon	02.40
R14	07.20

Table 3.2: New Mixed Refrigerant Composition

Component	Mole Fraction [%]
Pentane	12.70
Butane	07.50
Propane	20.30
Ethylene	12.70
Ethane	09.50
Methane	17.50
Nitrogen	16.50
Neon	03.30

The mixed refrigerant in the precooling cycle is pressurised to 24.8 bar with three compressor units i.e. MRC-1, MRC-2, and MRC-3 and the flow rate required for the cooling duty purpose is 35 kg/s to bring down the temperature of gas hydrogen to 78 K and 75 bar in H-6. The pre-cooling cycle refrigerant in the MR-2 line is in vapour and liquid form. Hence it has to be sent in the separator unit where MR-3 is in the vapour phase and MR-17 is in the liquid phase. The number of heat exchangers required for precooling purposes is four i.e. HEX1, HEX2, HEX3, and HEX4. The stream data of both hydrogen gas being cooled down and the precooling cycle used to cool the hydrogen gas is provided in Tables 3.3 and 3.5.

After the hydrogen gas has been precooled to 78 K and 75 bar by the precooling cycle. This hydrogen enters the second refrigeration cycle i.e. for cryogenic liquefaction using the Brayton cycle concept. The refrigerant used in this cryogenic cycle is a helium-neon mixture (Nelium) with a mole fraction distribution of 80% and 20%. The Nelium refrigerant is pressurised from 2.4 bar to 73 bar using an intercooler compression system of 5 units i.e. (C-1, C-2, C-3, C-4, and C-5). The recuperator is used for cooling the compressed refrigerant from 310 K to 75 K utilizing the cooling duty from the incoming Nelium refrigerant stream (HENE-5) after it has cooled the hydrogen streams i.e. (H-6 and H-10) for cryogenic liquefaction.

The hydrogen gas in H-6 which is at 78 K is cooled down to 33 K in H-7 in HEX5. After it is cooled down to 33 K this gas stream (H-7) is isentropically expanded in a turbine (T-3) with an isentropic efficiency of 86.6% to a pressure of 4 bar and further expanded in an isenthalpic valve for Joule-Thompson effect to take place so that liquid hydrogen is formed. The vapour quality in the H-8 stream is 0.3085 which is compressed to 11 bar from 1 bar using the Flash Compressor (FC). After compression, H-10 is cooled down to 26.44 K by the usage of cooling duty from the Nelium refrigeration cycle (HENE-4 to HENE-5) and further expanded in an isenthalpic valve to recycle the liquid hydrogen to get the desired output of 86 TPD.

3.3. Process Simulation

Aspen process simulation software, developed by Aspen Technology, is extensively utilised across the process industries for the sophisticated design, rigorous optimisation, and comprehensive management of chemical processes. In this thesis, process modelling and simulation have been performed in the steady-state process simulator Aspen HYSYS V12.

Table 3.3: Hydrogen Stream State Points

Stream	Temp.[K]	Press.[bar]	Flowrate[kg/s]	Vapour Quality
H-1	310	20	1	1
H-2	310	80	1	1
H-3	255	78.7	1	1
H-4	235	77.5	1	1
H-5	145	76.2	1	1
H-6	78	75	1	1
H-7	33	73.8	1	1
H-78	26	4	1	0.1551
H-8	20.2	1	1	0.3085
H-9	20.2	1	0.3834	1
H-10	45.6	11	0.3834	1
H-11	26.44	10.5	0.3834	0
H-12	20.2	1	0.3834	0.196
Liquid-H2	20.2	1	1	0

Table 3.4: Helium-Neon Stream State Points

Stream	Temp.[K]	Press.[bar]	Flowrate[kg/s]	Vapour Quality
HENE-1	310	73	9.7	1
HENE-2	75	71.5	9.7	1
HENE-3	41.84	13.3	9.7	1
HENE-4	24.44	2.5	9.7	0.9807
HENE-5	68.94	2.4	9.7	1
HENE-6	310	2.4	9.7	1

Table 3.5: Pre-cooling Refrigerant Stream State Points

Stream	Temp.[K]	Press.[bar]	Flowrate[kg/s]	Vapour Quality
MR-1	301.35	1.1	35	1
MR-2	310	24.8	35	0.7197
MR-3	310	24.8	20.656	1
MR-4	255	24.4	20.656	0.716
MR-5	255	24.4	12.4278	1
MR-6	235	24	12.4278	0.9172
MR-7	145	23.6	12.4278	0.3718
MR-8	75	23.2	12.4278	0.0146
MR-9	72	1.2	12.4278	0.0943
MR-10	139.34	1.2	12.4278	0.6857
MR-11	255	24.4	8.2278	0
MR-12	235	24	8.2278	0
MR-13	145	23.6	8.2278	0
MR-14	144.44	1.2	8.2278	0.0301
MR-15	142	1.2	20.656	0.4969
MR-16	223.24	1.2	20.656	0.9402
MR-17	310	24.8	14.344	0
MR-18	255	24.4	14.344	0
MR-19	235	1.2	14.344	0.1904
MR-20	225.8	1.2	35	0.7397
MR-21	235.7	1.1	35	0.8034

3.3.1. Estimation of Fluid Properties

As Aspen HYSYS is capable of interfacing with the REFPROP databank of the National Institute of Standards and Technology (NIST), the thermodynamic properties of normal, ortho, and para-hydrogen can be accurately estimated using the state-of-the-art equation of state (EOS) developed by Leachman et al.[38]. The hydrogen feed stream that is cooled in the heat exchangers with continuous catalytic ortho- to para-hydrogen conversion can be simulated by assuming equilibrium-hydrogen [14]. For this purpose the pseudo-equilibrium-hydrogen heat capacity model is considered developed by Valenti et.al [13].

The operational characteristics of gaseous hydrogen entering the liquefaction plant at 21 bar and the properties of the resultant liquid product upon exiting are evaluated using a pseudo-equilibrium-hydrogen model. Additionally, the thermodynamic properties of the mixed-refrigerant fluids within the precooling and cryogenic liquefaction Brayton cycle are computed utilizing the Peng-Robinson cubic equation of state as implemented in Aspen HYSYS.

3.3.2. Calculation of Exergy Efficiency

The specific liquefaction power of the hydrogen-liquefaction plant is calculated using equation (3.2) for which the enthalpy and entropy of the inlet H-1 and outlet Liquid H₂ streams values have been considered from Aspen HYSYS and the ambient temperature that has been considered is 298.15 K. In this study, two distinct SEC values are under assessment:

- SEC with electric power recovery from turbine generators
- SEC without electric power recovery

This comparative analysis seeks to quantify the economic benefits and operational efficiencies associated with the integration of turbine power recovery systems, specifically turbo-generators, into the overarching liquefaction infrastructure. By evaluating key performance indicators and leveraging advanced techno-economic assessment methodologies, the study aims to elucidate the potential for cost savings and enhanced energy utilisation within the liquefaction process.

For analysis the main reference process in this study is the Large-scale hydrogen liquefier utilizing mixed-refrigerant pre-cooling developed by Berstad et al. [22] of 86 TPD. The specific liquefaction power of this plant calculates to 3.014 kWh/kg_{LH₂} and the SEC of the plant is 24.85 MW i.e. 6.9025 kWh/kg_{LH₂} considering the power recovery from turbine generators and without turbine power recovery the value is 7.3187 kWh/kg_{LH₂}. The exergy efficiency of the reported plant is 43.665% considering the electric power recovery using equation (3.3).

Equation to calculate Specific Liquefaction Power of the plant:

$$-\frac{\dot{W}_i}{\dot{m}_f} = T_0(s_1 - s_f) - (h_1 - h_f) \quad (3.2)$$

Table 3.6: Specific liquefaction power calculation parameters.

Symbol	Parameter	Unit
$\dot{W}_i$	Theoretical idea work required by the liquefier system	kW
$\dot{m}_f$	Mass flow rate of product Hydrogen	kg/s
h_1	Specific Enthalpy of input hydrogen at 21 bar and 310 K	kJ/kg
h_f	Specific Enthalpy of liquid hydrogen at 1 bar and 20 K	kJ/kg
s_1	Specific Entropy of input hydrogen at 21 bar and 310 K	kJ/kg-K
s_f	Specific Entropy of liquid hydrogen at 1 bar and 20 K	kJ/kg-K
T_0	Ambient Temperature (298.15)	K
$\dot{W}$	Actual work required by the liquefier system	kW

$$\text{FOM} = \frac{\frac{\dot{W}_i}{\dot{m}_f}}{\frac{\dot{W}}{\dot{m}_f}} \quad (3.3)$$

4

Equipment Preliminary Design

As indicated in the literature review, the majority of conceptual hydrogen liquefaction plants proposed have not delved into the granular aspects of technical feasibility and economic viability. This thesis aims to evaluate the technical aspects of conceptual large-scale hydrogen liquefaction systems. The turbine and compressor design procedures have been operationalized via a pre-developed Python program by et al. Panji [23], which is available in the corresponding GitHub repository [39]. For the heat exchanger design, the equipment from the plant model developed in Aspen HYSYS was utilized and subsequently imported into Aspen EDR to determine the appropriate sizing of the component.

The pre-developed codes on Python for compressor and turbine sizing were updated with REFPROP data for calculating the state properties using the Peng-Robinson equation of state. The sizing of the components mainly focuses on Compressors, Turbines and Heat Exchangers. This section aims to analyse the impact of technical limitations on the base process.

4.1. Plate-Fin Heat Exchanger sizing

Preliminary sizing and design of plate-fin heat exchangers used in the plant are performed on Aspen EDR design mode. The inputs for the design are imported directly from the Aspen HYSYS hydrogen liquefaction plant developed based on the Brayton cycle concept. In these designs, the catalytic conversion of ortho-para hydrogen was not considered because the code developed by O'Neil et al. [40] only supports single-component cold fluid streams. However, the heat exchangers simulated in this plant involve mixed refrigerants as the cold fluid stream. Additionally, the syntax for obtaining the latent heat of vaporization from REFPROP is not available. The catalytic conversion of hydrogen isomer spins from ortho to para is necessary to expedite the process; however, this conversion is exothermic and releases heat. Consequently, additional cooling duty would be required for the cooling streams in the plate-fin heat exchanger, impacting the overall design and sizing of the heat exchanger.

In Aspen EDR's design mode, comprehensive evaluations of geometric (mechanical), thermal, and hydraulic parameters are conducted. Further, it provides the estimated stream properties and wall temperature at every calculation node. These points are used to check the design constraints. Figure 4.1 illustrates the main outcomes of the preliminary designs of PFHX from Aspen EDR design mode, that fulfil the criteria described in Table 4.1.

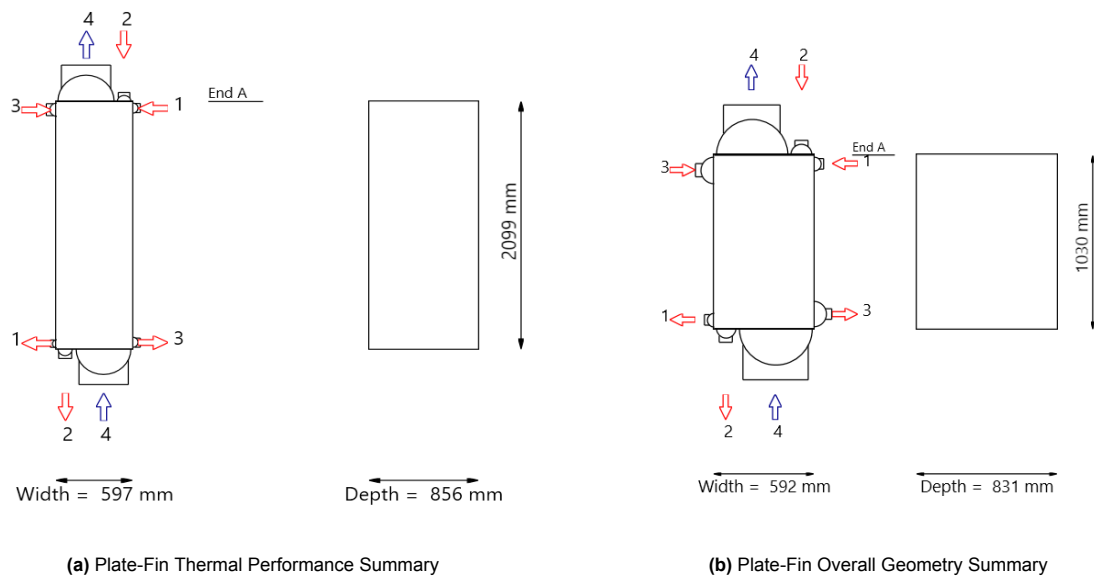
Table 4.1: Design Limitations of plate-fin heat exchangers [14]

Parameter	Value	Unit
Max. Length	8.2	m
Max. Width	1.5	m
Max. Height	3.0	m
Volume	15-30	m ³
Specific Surface	500-1,800	m ² /m ³
Max. Temperature Difference	25.0	K
Min. Temperature Difference	1.00	K

	Stream 1	Stream 2	Stream 3	Stream 4
Main stream number	H-2	MR-3	MR-17	MR-21
Stream name	H-2->H-3	MR-3->MR-4	MR-17->MR-18	MR-21->MR-1
Flow direction	End A to B (down)	End A to B (down)	End A to B (down)	End B to A (up)
Total mass flow rate	kg/s	1	20.6556	14.3445
Heat load	kW	-1711.7	-4694.5	-1858.2
Heat load per layer	kW	-42.8	-27.9	-25.8
Inlet temperature	°C	36.85	36.85	36.85
Outlet temperature	°C	-18.15	-18.15	-18.15
Bubble point	°C		34.74	
Dew point	°C		36.7	-10.65
Inlet quality(vapor mass fraction)		1	1	0
Outlet quality(vapor mass fraction)		1	0.6	0
Inlet specific enthalpy	kJ/kg	1711.2	228.6	129.5
Outlet specific enthalpy	kJ/kg	-0.5	1.3	0
Fouling resistance	m ² -K/W	0	0	0
Minimum [T-Twall]	°C	1.96	1.96	1.96
Mean [T-Twall]	°C	8.65	8.75	8.65
Mean heat transfer coefficient	W/(m ² -K)	794.9	1378.2	1425.4
Mean fin efficiency		0.96	0.89	0.89
Solution method	Design	Design	Design	Design
Heat load as fraction of maximum				
Theoretical maximum heat load	kW			

(a) Plate-Fin Thermal Performance Summary

Number of exchangers in parallel	8
Number of exchangers per unit	1
Number of layers per exchanger	101
Orientation	Vertical, end A at top
Core length	m
Core width	m
Core depth(stack height)	m
Number of X-flow passes	0
Number of layer groups	1
Distributor length - end A	mm
Main heat transfer length	mm
Distributor length - end B	mm
Internal (effective) width	mm
Side bar width	mm
Parting sheet thickness	mm
Cap sheet thickness	mm
Exchanger metal	Aluminum
Exchanger weight - empty	kg
Exchanger weight - full of water	kg
Exchanger weight - operating	kg

(b) Plate-Fin Overall Geometry Summary**Figure 4.1:** HEX1 Aspen EDR plate-fin heat exchanger design mode results**(a)** Plate-Fin Thermal Performance Summary**(b)** Plate-Fin Overall Geometry Summary**Figure 4.2:** HEX1 and HEX2 Aspen EDR Plate-Fin Heat Exchanger Diagram

4.2. Preliminary sizing of Compressor

From the process simulation in Aspen HYSYS, the inlet flow rates of the hydrogen feed compressor units, precooling refrigerant compressor units and cryogenic liquefaction cycle compressor units have a flow rate in the range of 2,300-45,000 m³/h with a maximum discharge pressure of 73 bar the type of compressors selected in the design were centrifugal compressors. In the sizing of this component, each centrifugal compressor is equipped with an aftercooler that cools outlet gas to 310 K utilizing cooling water.

The preliminary sizing of this component was performed using the python code developed by Panji et al.[14]. The modification was done for calling the state properties for the fluids from REFPROP using the Peng-Robinson Equation of State to make the code compatible with the properties from Aspen HYSYS. The design limitations assumed for the preliminary design of centrifugal compressors are summarised in Table 4.2

Table 4.2: Design Limitations of Centrifugal Compressor [14]

Parameter	Value	Unit
Max. Number of Stages per Compressor	8	stages
Min. Volumetric Inlet Flowrates	1,000	m ³ /h
Max. Volumetric Inlet Flowrates	300,000	m ³ /h
Max. Compressor Power	37,000	kW
Max. Impeller Tip Velocity	500	m/s

4.2.1. Compressor Units in the Liquefaction Cycle

For selection of number of stages and rotational speed of turbo-compressor, usage of n-z (Rotational Speed - Number of Stages) diagrams becomes feasible. Figures 4.4, 4.5, and 4.7 represents the n-z diagrams modelled from the python code developed for all the three compressor units in the plant. For detailed analysis of the development of the code for compressor and turbine preliminary design selection procedure refer et al.[23].

Hydrogen Feed Compressor Unit

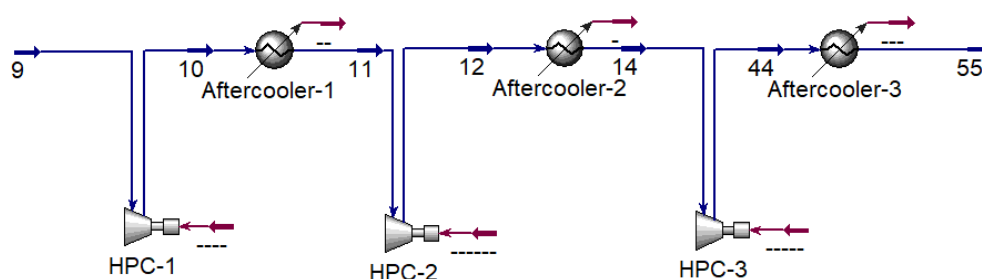


Figure 4.3: H₂ Feed compressor system modelling in Aspen HYSYS

The Hydrogen gas introduced into the liquefaction plant is compressed to 80 bar from 21 bar utilizing three compressor units of which the outputs are post-cooled using after coolers as shown in Figure 4.3. The pressure ratio of this system is about four and the minimum number of stages that can be selected for the centrifugal compressor system is restricted by the compressor's impeller tip velocity. The impeller or blade tip velocity in the base scenario is limited to 500 m/s. The number of stages selected for HPC-1 and HPC-2 are six from the python code and for HPC-3 is seven.

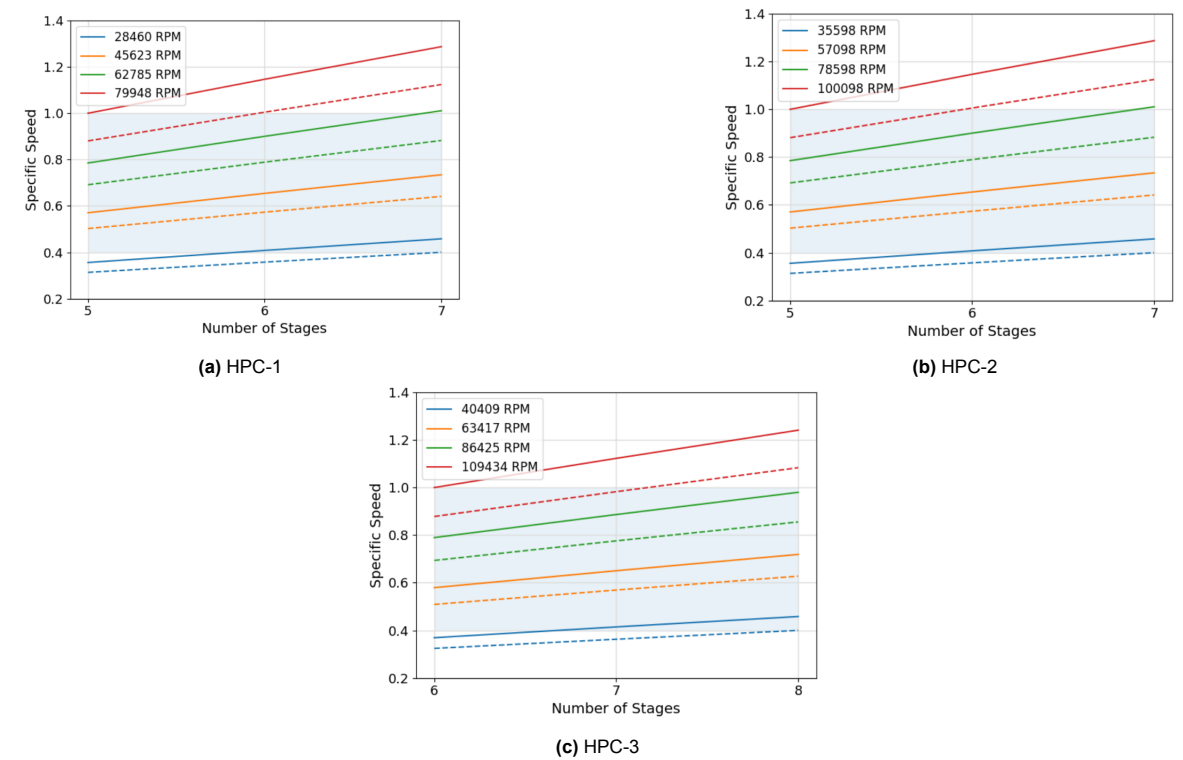


Figure 4.4: n-z selection diagram for feed hydrogen compressors

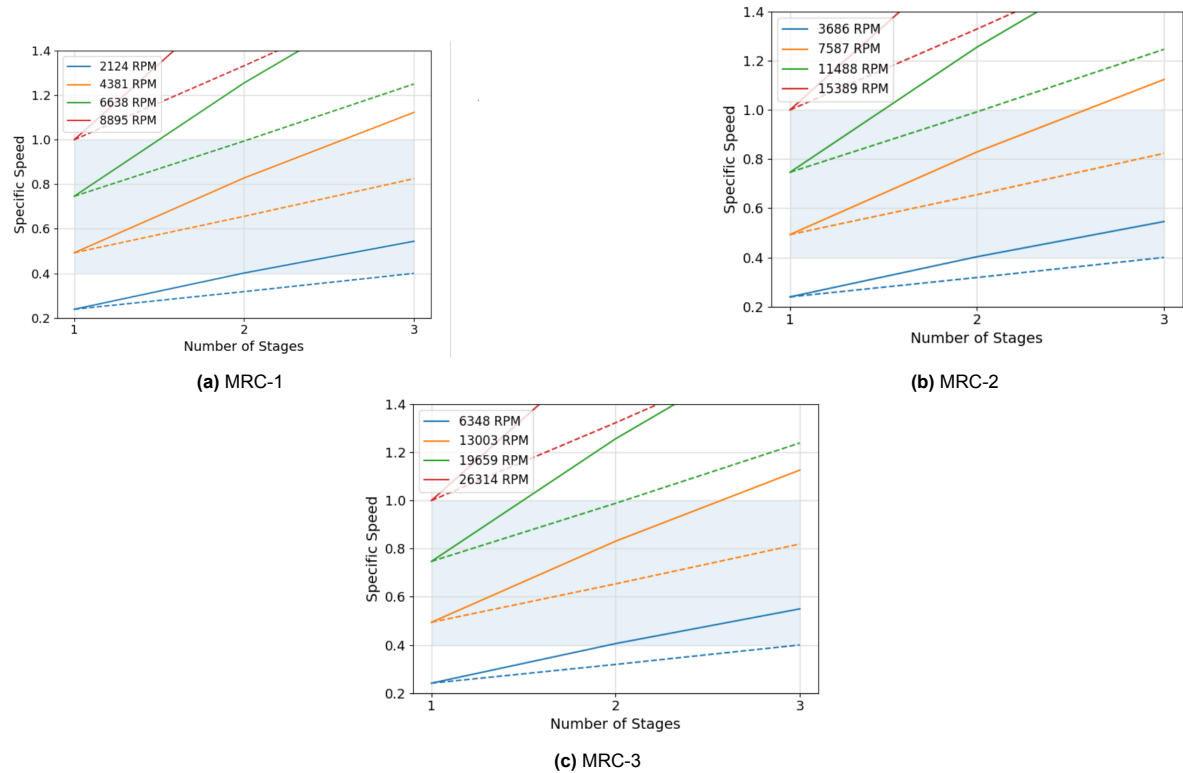


Figure 4.5: n-z selection diagram for mixed refrigerant compressors

Precooling mixed refrigerant cycle compression unit and flash compressor unit

The mixed refrigerant consisting of eight components is compressed from 1.1 bar to 24.8 bar using three compressor units. The number of stages selected for each is two and the n-z plot is shown in Figure 4.3. The flash H_2 gas in stream H-9 of Figure 3.1 is compressed from 1 bar to 11 bar using two compressor units with number of stages selected for FC-1 as two and for FC-2 as four and isentropic efficiencies of 81.61% and 79.44% each.

Nelium Cryogenic liquefaction cycle compression unit

In the reference plant from [22], the Nelium refrigerant was compressed from 2.4 bar to 73 bar using a 15-stage compression unit. This thesis has split the one compression unit into five compressors with each of three stages. Figure 4.6 depicts the 1st compressor with three stages operating at 9500 RPM. Each of these compressors have intercooling system which is modelled in Aspen HYSYS accordingly.

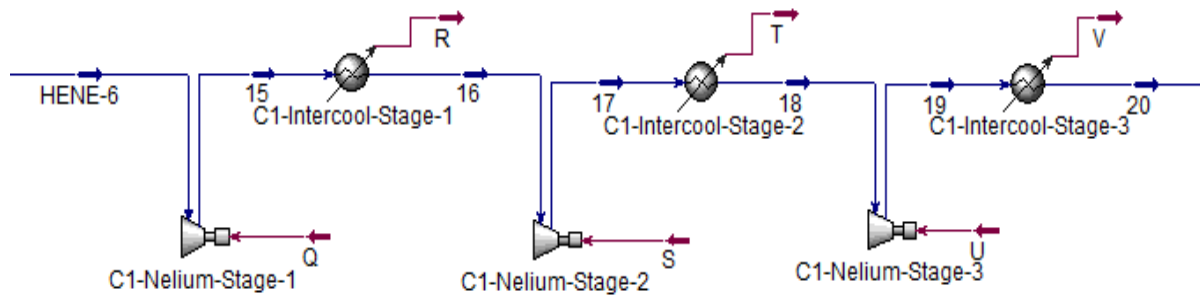
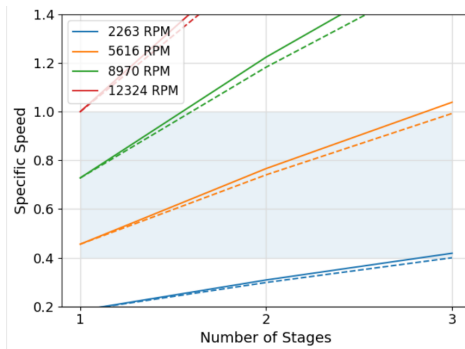
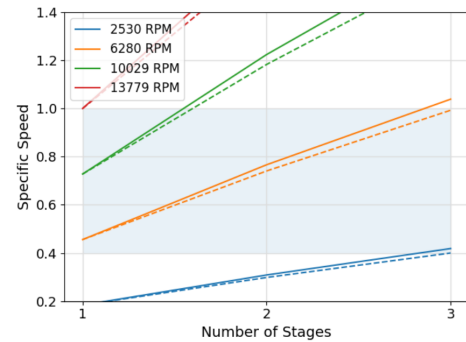


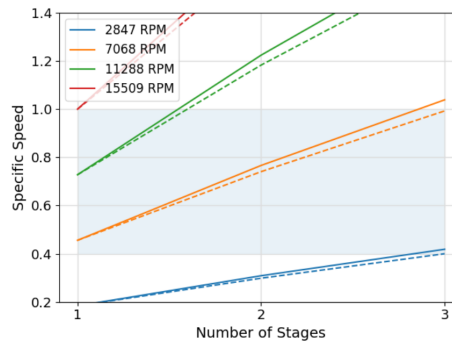
Figure 4.6: Nelium Compressor 1 Modelling with 3 stages and intercooling in Aspen HYSYS



(a) Nelium Compressor 1 Stage 1



(b) Nelium Compressor 1 Stage 2



(c) Nelium Compressor 1 Stage 3

Figure 4.7: n-z selection diagram for Nelium compressors

The preliminary design of centrifugal compressors is deemed acceptable when the chosen input parameters meet the design constraints throughout all stages of calculation. The parameter constraints assumed for the preliminary design of multistage centrifugal compressors are summarized in Table 4.3. While these constraints are not overly stringent, they represent recommended values aimed at optimizing efficiency. In cases where specified values are challenging to achieve, a 10% tolerance is allowed for certain parameters.

Table 4.3: Parameter constraints of centrifugal compressors [41]

Parameter	Range	Remark
Specific Speed, ω_s	0.4 - 1.0	
Flow coefficient, φ	0.2 - 0.3	
Work coefficient, ψ	0.5 - 0.6	
Degree of Reaction, R	0.6 - 0.7	10% tolerance
Rotor tip diameter ratio, δ_t	0.5 - 0.75	
δ_t/δ_h	0.2 - 0.7	
Rotor outlet absolute flow angle, α_2	60° - 70°	10% tolerance
Rotor outlet relative flow angle, β_2	0° - 60°	10% tolerance
Impeller tip speed velocity, u_2	< 500 m/s	

4.3. Preliminary sizing of Turbine

In this thesis only radial in-flow turbines, also called centrifugal turbines, are considered for the design of turbo-expanders that are required in the hydrogen liquefaction process. In most present air separation and petrochemical process specifications, turbo expanders are generally radial reaction turbine because this geometry is often the most efficient [42]. Compared to axial flow expanders, they experience lower stresses at a given tip speed, allowing them to operate at a higher rotational speed, resulting in higher efficiencies [43]. Axial turbines may have higher efficiency at high Reynolds number ($Re > 10^6$), but they require a higher capital cost [2]. Radial in-flow turbines, also termed centrifugal turbines, are highly reliable and require low maintenance.

Table 4.4: Design Limitations of radial-inflow turbines [14]

Parameter	Value	Unit
Max. Number of Stages per Turbine	1	stages
Min. Volumetric Inlet Flowrates	8.5	m ³ /h
Max. Volumetric Inlet Flowrates	339,800	m ³ /h
Max. Rotational Speed	100,000	rpm
Max. Turbine Power	1,500	kW
Max. Impeller Tip Velocity	500	m/s

The preliminary design of turbo-expanders, similar to compressors, adheres to the design limitations established in this thesis. These limitations are detailed in Table 4.4. Turbines T-1 and T-2, as depicted in Figure 3.1, achieve isentropic efficiencies of 77.16% and 88.32%, respectively. Based on the n-z diagram shown in Figure 4.8, both turbines were designed with two stages. The parameter constraints used in this preliminary design are summarized in Table 4.5. While these constraints are not rigid, they serve as recommended values intended to maximize performance. Tolerance percentages are applied to certain parameters when the specified values are difficult to achieve.

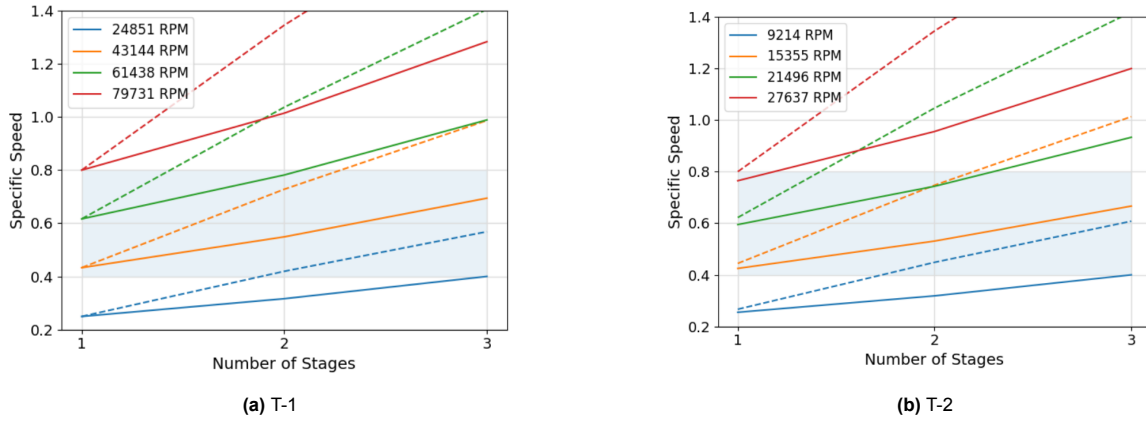


Figure 4.8: n-z selection diagram for Helium Turbines

Table 4.5: Parameter constraints of radial in-flow turbines [41]

Parameter	Range	Remark
Specific Speed, ω_s	0.4 - 0.8	
Flow coefficient, φ	0.2 - 0.3	25 % tolerance
Work coefficient, ψ	0.8 - 1.0	20 % tolerance
Degree of Reaction, R	0.45 - 0.65	15 % tolerance
Rotor meridional velocity ratio, ζ	0.65 - 1.0	
Rotor tip diameter ratio, δ_t	< 0.7	10% tolerance
δ_t/δ_h	> 0.4	45% tolerance
Rotor inlet absolute flow angle, α_1	66° - 78°	
Rotor inlet relative flow angle, β_1	22° - 40°	
Impeller tip speed velocity, u_2	< 500 m/s	

The H-7 line, containing highly pressurized hydrogen at 73 bar, undergoes a two-stage expansion process. First, the hydrogen is expanded in an isentropic turbine with a calculated efficiency of 85%. Following this, it is further expanded using an isenthalpic (Joule-Thomson) valve. This dual-stage expansion approach is adopted because a purely isentropic expansion caused work coefficient, degree of reaction, rotor tip diameter ratio, rotor inlet absolute flow angle and rotor hub/tip ratio to exceed acceptable limits.

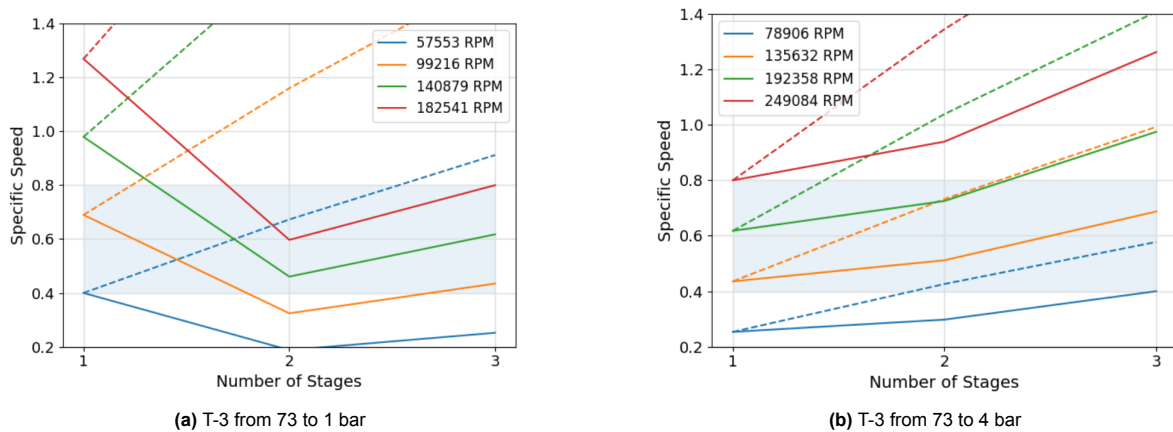


Figure 4.9: n-z Diagrams for H2 Turbine

When the pressure of H-7 hydrogen stream from Figure 3.1, was reduced from 73 bar to 4 bar, instead of the target of 1 bar, there is an observed reduction in the work coefficient by 11.2%. Although this reduction lies outside the defined range, it remains within the specified control limits. Additionally, the degree of reaction increased by 33.34%, and the rotor hub-to-tip ratio increased by 78%. Despite this increase, the rotor hub-to-tip ratio remains below the defined limit. The rotor tip diameter ratio and rotor inlet absolute flow angle were maintained within the specified limits when the pressure was reduced to 4 bar. Considering these factors, it is decided to first reduce the pressure using isentropic expansion in a turbine, followed by further expansion in an isenthalpic valve. In this thesis the following components were not designed and considered for CAPEX and OPEX calculations: 1) coldboxes, 2) vapour -liquid separators, 3) valves, 4) control units, 5) cryogenic adsorbers.

5

Techno-Economic Analysis

Techno-economic analysis (TEA) is a robust methodology for evaluating the economic performance of technological systems. In this thesis, a TEA is conducted to determine the specific levelized cost (SLC) of a large-scale hydrogen Brayton liquefaction plant. This analysis aims to quantify the overall value of liquid hydrogen (H_2) by balancing the benefits against the costs associated with its liquefaction, utilizing the Brayton-cycle concept detailed in Chapter 3.

For conducting the techno-economic analysis, the Aspen Process Economic Analyzer, a software package from Aspen, was utilized. APEA is chosen due to its capability to project equipment expenses based on fairly current cost data gathered from actual EPC projects and equipment manufacturers [14]. In addition to estimating equipment purchase costs, the Aspen Process Economic Analyzer (APEA) also assesses total installed costs, which encompass both direct and indirect field costs. It should be noted that ASPEN HYSYS simulations can be integrated with the Aspen Process Economic Analyzer (APEA) to estimate the total project capital cost, total operating cost, and the cost of utilities utilized in the plant.

The following sections delineate the workflow developed for conducting the techno-economic analysis of hydrogen liquefiers in this thesis. They include a detailed description of the general specifications, equipment input parameters, and process assumptions that underpin the techno-economic analysis of the hydrogen liquefiers.

5.1. APEA Workflow and Project Basis

The Aspen Process Economic Analyzer is designed to automate the preparation of comprehensive designs, cost estimates, investment analyses, and time likes from minimal project scope definitions [44]. The APEA project work flow has been discussed in the following sections of this chapter and some adjustments have been made to the APEA workflow. Figure 5.1 illustrates the TEA workflow tailored for the cost Analysis in this study.

5.1.1. Project Basis

The project basis defines specifications relevant to the overall project scenario. These specifications exert influence over the design and cost estimation processes by establishing system defaults and environmental variables. Within APEA, these specifications encompass various components, including **Project Properties, General Project Data, Basis for Capital Costs, Investment Analysis, Process Designs, and Streams** [14].

In project properties and general project data, user can specify the base unit measure, the base country and the base currency for the evaluation of project costs. In this thesis, European Union (EU) and Euro (EUR) are selected as the project country and currency base, respectively. The ASPEN HYSYS process simulation file developed in Chapter 3 and refined by the preliminary design results in Chapter 4 is loaded into APEA Process Design. The utilities used in the process for heating and cooling are outlined within the Utility Specifications. For both the process simulation and the Techno-Economic

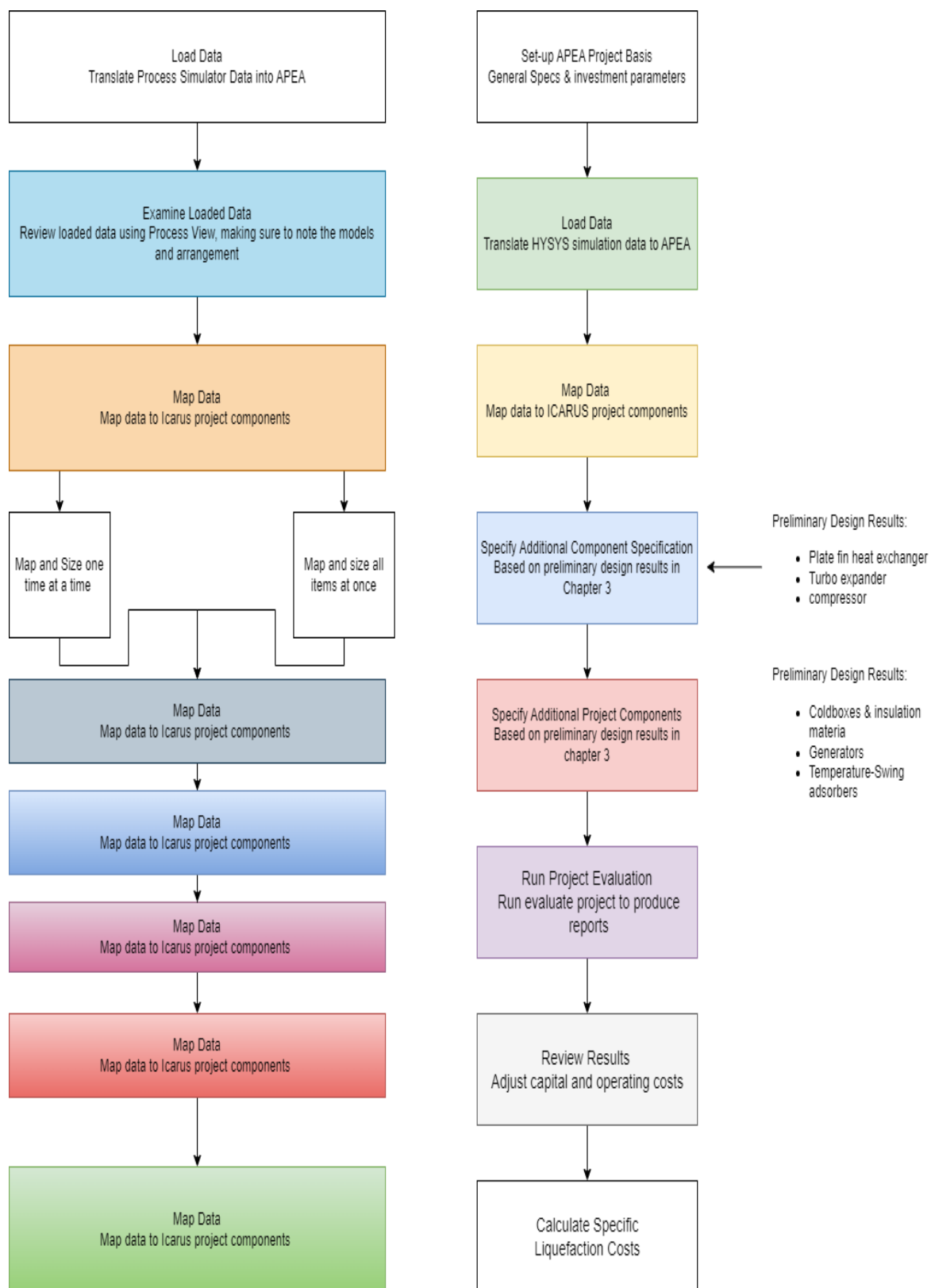


Figure 5.1: Techno-Economic Analysis workflow using APEA

Analysis (TEA) model, the cooling water used for the aftercoolers is assumed to operate at a pressure of 3.45 bar. The inlet temperature of the cooling water is set at 20°C, while the outlet temperature is 35°C. In 2019, € 0.343 per m³ of tap water was charged in The Netherlands. Hence, this corresponds to around 38 cents per m³, including VAT. Hence, the unit cost of cooling water is set as 0.38€/m³ [45]

Name	Item 1
Process Description	New process
Process Complexity	Typical
Process Control	Digital
PROJECT INFORMATION	
Project Location	Rotterdam
Project Type	Grass roots/Clear field
Contingency Percent	30
Estimated Start Day of Basic Engineering	1
Estimated Start Month of Basic Engineering	APR
Estimated Start Year of Basic Engineering	19
Soil Condition Around Site	SOFT CLAY
EQUIPMENT SPECIFICATION	
Pressure Vessel Design Code	ASME
Vessel Diameter Specification	ID
P and I Design Level	FULL

Figure 5.2: General Specifications

In general specs, includes the inputs about Process Description, Process Complexity, and Process Control. The project information section in general specs include project location, project type, contingency percentage, start date, and soil conditions. The project location was selected is Rotterdam and the soil condition around the site is soft clay as shown in figure 5.2.

Name	Units	Item 1
Period Description		Year
Number of Weeks per Period	Weeks/period	52
Number of Periods for Analysis		20
Tax Rate	Percent/period	40
Interest Rate/Desired Rate of Return	Percent/period	20
Economic Life of Project	Period	10
Salvage Value (Percent of Initial Capital Cost)	Percent	20
Depreciation Method		Straight Line
ESCALATION PARAMETERS		
Project Capital Escalation	Percent/period	5
Products Escalation	Percent/period	5
Raw Material Escalation	Percent/period	3.5
Operating and Maintenance Labor Escalation	Percent/period	3
Utilities Escalation	Percent/period	3
PROJECT CAPITAL PARAMETERS		
Working Capital Percentage	Percent/period	5
OPERATING COSTS PARAMETERS		
Operating Supplies	Cost/period	25
Laboratory Charges	Cost/period	25
Operating Charges	Percent/period	25
Plant Overhead	Percent/period	50
G and A Expenses	Percent/period	8
FACILITY OPERATION PARAMETERS		
Facility Type		Chemical Processing Facility
Operating Mode		Continuous Processing - 24 Hou
Length of Start-up Period	Weeks	20
Operating Hours per Period	Hours/period	8,000
Process Fluids		Liquids and Gases

Figure 5.3: Investment Analysis Parameters

Investment Analysis Parameters consists of Escalation Parameters, Project Capital Parameters, Operating Cost Parameters, Facility Operating Parameters. Figure 5.3, depicts the input parameters that are considered in the project to calculate the CAPEX and OPEX. The Process fluids selected is Liquid and Gases as the input in the plant is gas Hydrogen and output is liquid hydrogen.

5.2. Equipment Mapping and Specifications

5.2.1. Compressors

To execute the files using the Aspen Process Economic Analyzer, it is imperative to map the components with the ICARUS project. The compressor utilized in this project is of the centrifugal type. Consequently, the compression systems modelled in the HYSYS process simulations are correspondingly mapped to ICARUS's Gas Centrifugal Compressor - Horizontal (GC CENTRIF) model.

Name	Units	Item 1
Remarks 1		Equipment mapped from 'H2-COMP
Remarks 2		
Item description		H2-COMPRESSOR-1
User tag number		H2-COMPRESSOR-1
Drawing reference number		
Structure tag		
Component WBS		
Quoted cost per item	EUR	
Currency unit for matl cost		
Source of quote		
Number of identical items		1
Installation option		
Code of account		
Icarus/User COA option		
Casing material		SS304
Actual gas flow rate Inlet	M3/H	2,439.867816
Design gauge pressure Inlet	KPAG	1,998.67108
Design temperature Inlet	DEG C	36.85
Design gauge pressure Outlet	KPAG	3,178.437076
Design temperature Outlet	DEG C	57.277983
Number of impellers		6
Compressor speed	RPM	45,550
Driver power	KW	719.658194
Molecular weight		2.01588
Specific heat ratio		1.343503
Compressibility factor Inlet		1.012084
Compressibility factor Outlet		1.018116
Intercooler required		NO
Intercooler type		WATER
Aftercooler required		YES
Aftercooler type		WATER
Inter/Aftercooler excess area	PERCENT	0
Maximum interstage temperature	DEG C	175
Intercooler outlet temperature	DEG C	37
Interstage pressure drop	KPAG	35
Driver type		MOTOR
Turbine gauge pressure	KPAG	2,050
Gear reducer type		
Lube oil system		YES
Allow resizing		

(a) HPC-1 APEA Inputs

Name	Units	Item 1
Item Reference Number		2
Remarks 1		Equipment mapped from 'H2-COMP
Remarks 2		
Item description		H2-COMPRESSOR-2
User tag number		H2-COMPRESSOR-2
Drawing reference number		
Structure tag		
Component WBS		
Quoted cost per item	EUR	
Currency unit for matl cost		
Source of quote		
Number of identical items		1
Installation option		
Code of account		
Icarus/User COA option		
Casing material		SS304
Actual gas flow rate Inlet	M3/H	1,572.750614
Design gauge pressure Inlet	KPAG	3,178.437076
Design temperature Inlet	DEG C	36.85
Design gauge pressure Outlet	KPAG	5,021.353206
Design temperature Outlet	DEG C	57.328674
Number of impellers		6
Compressor speed	RPM	57,000
Driver power	KW	725.632928
Molecular weight		2.01588
Specific heat ratio		1.342688
Compressibility factor Inlet		1.018905
Compressibility factor Outlet		1.02836
Intercooler required		NO
Intercooler type		WATER
Aftercooler required		YES
Aftercooler type		WATER
Inter/Aftercooler excess area	PERCENT	0
Maximum interstage temperature	DEG C	175
Intercooler outlet temperature	DEG C	30
Interstage pressure drop	KPAG	35
Driver type		MOTOR
Turbine gauge pressure	KPAG	2,050
Gear reducer type		
Lube oil system		YES
Allow resizing		

(b) HPC-2 APEA Inputs

Figure 5.4: Centrifugal compressor component specification form in APEA

To estimate the capital cost of this compressor model, the essential inputs required include the actual gas flow rate at the inlet, along with the design gauge pressures at the inlet and outlet. These parameters are crucial for accurate cost estimation and system design evaluation. The Python code developed for the preliminary compressor design estimates the necessary number of impellers and the compressor's rotational speed. Figure 5.4 presents the input parameters for HPC-1 and HPC-2 used to determine the direct cost of the compressor component.

In APEA analysis, each compressor design is equipped with an aftercooler to bring the gas outlet temperature back to 310 K. Hence these aftercoolers are mapped to ICARUS's TEMA Shell and Tube Heat Exchanger - Fixed tube, float. head, u-tube exchnager (HE TEMA EXCH) model. Since compressor aftercoolers were not included in the equipment preliminary design in this thesis, the default sizing and design results from APEA mapping are used as the basis of the aftercoolers capital estimate.

5.2.2. Turbines

The simulation models of expansion turbines from Aspen HYSYS simulations are mapped to the ICARUS project's Turbine Turbo-expander (TUR TURBOEXP) component model. Certain initial specifications of the turbine are automatically populated within the turbo-expander specification based on the process data imported from Aspen HYSYS, similar to how the compressor's mapping functions. These specifications include the turbine's actual gas flow rate at the inlet and the design gauge pressure at the inlet and outlet of the turbine, which are the mandatory input parameters required for APEA to compute turbine capital costs. Figure 5.5 presents the input parameters for T-1 and T-2 used to determine the direct cost of the turbine component.

Name	Units	Item 1
Item Reference Number		16
Remarks 1		Equipment mapped from TURBINE-1
Remarks 2		
Item description		TURBINE-1
User tag number		TURBINE-1
Drawing reference number		
Structure tag		
Component WBS		
Quoted cost per item	EUR	
Currency unit for matl cost		
Source of quote		
Number of identical items		1
Installation option		
Code of account		
Icarus/User COA option		
Actual gas flow rate Inlet	M3/H	441.345076
Design gauge pressure Inlet	KPAG	7,046.67108
Design temperature Inlet	DEG C	21
Design gauge pressure Outlet	KPAG	1,228.67108
Power output	KW	831.019033
Molecular weight		7.238984
Specific heat ratio		1.579372
Compressibility factor Inlet		0.953799
Isentropic efficiency	PERCENT	87.819271
Number of spare cartridges		0
Allow resizing		

(a) Turbo-expander T-1 component specification form in APEA

Name	Units	Item 1
Item Reference Number		17
Remarks 1		Equipment mapped from TURBINE-2
Remarks 2		
Item description		TURBINE-2
User tag number		TURBINE-2
Drawing reference number		
Structure tag		
Component WBS		
Quoted cost per item	EUR	
Currency unit for matl cost		
Source of quote		
Number of identical items		1
Installation option		
Code of account		
Icarus/User COA option		
Actual gas flow rate Inlet	M3/H	1,290.764969
Design gauge pressure Inlet	KPAG	1,228.67108
Design temperature Inlet	DEG C	21
Design gauge pressure Outlet	KPAG	148.67108
Power output	KW	480.595628
Molecular weight		7.238984
Specific heat ratio		1.591373
Compressibility factor Inlet		0.929105
Isentropic efficiency	PERCENT	90
Number of spare cartridges		0
Allow resizing		

(b) Turbo-expander T-2 component specification form in APEA

Figure 5.5: Turbo-Expander component specification form in APEA

5.2.3. Plate-Fin Heat Exchanger

The LNG multi-flow heat exchanger model from Aspen HYSYS simulations are mapped to ICARUS project's Heat Exchanger - Multi-stream, plate fin heat exchanger (HE PLATE FIN) component model [14]. In Aspen Process Economic Analyzer, the minimum input information required to get the estimated direct cost are the dimensions and the core weight of the heat exchanger.

In Figure 5.6, an example is illustrated for mapping the plate fin heat exchanger into the project. The input values are taken from the preliminary design chapter (Chapter 4) for the number of heat exchanger in parallel, the core weight and the dimensions of the HEX. More details about conducting techno-economic Analysis can be found in Aspen Process Economic Analyzer user guide [46].

Name	Units	Item 1
Item Reference Number		32
Remarks 1		Equipment mapped from 'HX1'.
Remarks 2		
Item description		HX1
User tag number		HX1
Drawing reference number		
Structure tag		
Component WBS		
Quoted cost per item	EUR	
Currency unit for matl cost		
Source of quote		
Number of identical items		8
Installation option		
Code of account		
Icarus/User COA option		
Material		A3003
Core length	M	2.0988
Core width	M	0.5971
Core height	M	0.8564
Number of streams		4
Parting sheet thickness	MM	1.5
Cap sheet thickness	MM	5
End bar width	MM	38
Side bar width	MM	38
Core weight	KG	1,625.5375
Pipe material		AL
Layer data		
Stream data		
Allow resizing		

(a) HEX1

Name	Units	Item 1
Item Reference Number		34
Remarks 1		Equipment mapped from 'HX3'.
Remarks 2		
Item description		HX3
User tag number		HX3
Drawing reference number		
Structure tag		
Component WBS		
Quoted cost per item	EUR	
Currency unit for matl cost		
Source of quote		
Number of identical items		7
Installation option		
Code of account		
Icarus/User COA option		
Material		A3003
Core length	M	5.4174
Core width	M	0.5954
Core height	M	0.8816
Number of streams		4
Parting sheet thickness	MM	2
Cap sheet thickness	MM	5
End bar width	MM	38
Side bar width	MM	38
Core weight	KG	4,176.55714
Pipe material		AL
Layer data		
Stream data		
Allow resizing		

(b) HEX2

Figure 5.6: Plate-Fin Heat Exchanger components specification form in APEA

5.3. Results and SLC Calculation

The total project capital and operating costs are the APEA executive summary report's main findings. These parameters are important for calculating the specific liquefaction cost (SLC) of the hydrogen liquefaction plant based on Brayton cycle concept.

To calculate the SLC, adjustments are necessary for the total capital cost and operating cost provided by APEA. Specifically, the total capital cost needs to be modified to include the plant's working capital. Figure 5.8 and 5.7, highlights the Summary of SLC based of APEA analysis and executive summary report generated from APEA.

The Aspen Process Economic Analyzer software used in this thesis has been configured to estimate the plant's expenses based on 2019 pricing data. However, to accurately apply the adjustment using CEPCI, the calculation must be performed in US\$. The following equation is used to adapt the capital costs to 2022 pricing in € using CEPCI and the average currency exchange rates in the base year of the capital costs pricing (in this case 2019) and the year of 2022:[47]

$$f(C)_{\text{€},2023} = f(C)_{\text{€},\text{base}} \cdot \left(\frac{\text{US\$}}{\text{€}} \right)_{\text{base}} \cdot \frac{\text{CEPCI}_{2022}}{\text{CEPCI}_{\text{base}}} \cdot \left(\frac{\text{€}}{\text{US\$}} \right)_{2023} \quad (5.1)$$

The subsequent formula for the capital recovery factor is utilized to determine the CAPEX annual cost contribution [23].

$$\text{CAPEX}_a = \text{CAPEX}_{\text{tot}} \cdot \frac{I_{\text{fix}} \cdot (1 + I_{\text{fix}})^{t_p}}{(1 + I_{\text{fix}})^{t_p} - 1} \quad (5.2)$$

The fixed annual interest rate, denoted as I_{fix} , is commonly assumed within the range of 0.07 to 0.11, as stated by Syed [35]. For the purpose of this thesis, a value of 0.1 is adopted. The specified payment duration in this analysis spans 20 years.

$$\dot{m}_{\text{LH}_2, a} = U_a \cdot 8760 \frac{\text{hours}}{\text{year}} \cdot 3600 \frac{\text{second}}{\text{hour}} \cdot \dot{m}_{\text{LH}_2} \quad (5.3)$$

	Project Capital Cost		Plant Operating Cost
Values Obtained from APEA:	€ 11,16,98,834.30		€ 2,98,99,707.99
Parameter	Value		Remarks
Working Capital (10 %):	€ 1,11,69,883.43		
Total CAPEX (2019)	€ 12,28,68,717.73		
CEPCI 2019	€ 607.50		CEPCI Composite Index
CEPCI 2023	€ 797.90		CEPCI Composite Index
Total CAPEX (2023)	€ 13,68,55,800.95		Equation 5.1
Payment Period	20		in years
Fixed Annual Interest	0.095		
Annual CAPEX of 2023	€ 1,55,29,944.02		Equation
Total Annual OPEX	€ 2,98,99,707.99		
Hydrogen Leaks	1.50%		of Plant Capacity
Refrigerant Leaks	1.5		kg/h
Total Annual OPEX with fluid loss	€ 3,15,47,682.99		
Total annual CAPEX + OPEX	€ 4,70,77,627.01		
Liquefier Capacity	86		tonnes per day
Utilization rate	0.95		
SLC	€ 1.57		per kg of LH2
Specific Cost Details			Remarks
Specific H2 Cost	€ 3.50	per kg of H2	Assumption
Specific MR Cost	€ 5.00	per kg of MR	Assumption
Electricity Price	€ 0.1000	per kWh	2019 Electricity Avg. Price
Cooling Water Price	€ 0.380000	per meter cube	2019 Price of Tap water

Figure 5.7: Summary of SLC calculations based on cost estimates from APEA

	A	B	C
1	EXECUTIVE SUMMARY		
2	=====		
3			
4	PROJECT NAME:	For feed pressure Analysis	
5			
6	CAPACITY:	ERR	
7			
8	PLANT LOCATION:	Rotterdam	
9			
10	BRIEF DESCRIPTION:	For feed pressure Analysis	
13			
14	SCHEDULE:	-----	
15	Start Date for Engineering	1APR19	
16	Duration of EPC Phase	60.00	Weeks
17	Completion Date for Construction	Thursday, May 28, 2020	
18	Length of Start-up Period	20.00	Weeks
19			
20			
21	INVESTMENT:	-----	
22	Currency Conversion Rate	1.00	EUR/EUROPEAN EURO
23	Total Project Capital Cost	111,698,834.30	EUR
24	Total Operating Cost	31,135,113.27	EUR/Year
25	Total Raw Materials Cost	0.00	EUR/Year
26	Total Utilities Cost	24,930,784.08	EUR/Year
27	Total Product Sales	0.00	EUR/Year
28	Desired Rate of Return	20.00	Percent/Year
29	P.O. Period	0.00	Year
30			
31	PROJECT INFORMATION:	-----	
32	Simulator Type	Aspen HYSYS	
33	Version		
34	Report File	c:\Users\Sharven\Desktop\Thesis\Models\Final Plant L	
35	Report Date		
36			
37	Economic Analysis Type	IPE	
38	Version	40.0.0	
39	System Cost Base Date	1Q 19	
40	Project Directory	C:\Users\Public\Documents\AspenTech\Shared Econo	
41	Analysis Date	Thu Aug 15 11:27:21 2024	
42	Country Base	EU	
43	Project Type	Grass roots/Clear field	
44	Design code	ASME	
45	Prepared By		
46			
47	NOTES:	-----	

Figure 5.8: APEA executive summary report

6

Results and Discussions

This chapter presents the final configuration and stream data for the large-scale hydrogen liquefaction process plant developed on Aspen HYSYS based on the Brayton cycle concept. The layout is developed using a reference process discussed in Chapter 3 and the preliminary equipment design and techno-economic analysis of the plant is discussed in Chapter 4 and 5. This thesis discusses about the exergy efficiency of the plant, efficiency of the equipment designed and specific liquefaction cost of the plant.

This chapter discusses the various parameters on which the plant's CAPEX and OPEX are dependent. These include the dependency of CAPEX and Specific Liquefaction Cost (SLC) on the fixed annual interest rate and payment period, as well as the dependency of CAPEX and OPEX on electricity price and feed pressure.

6.1. Baseline Scenario

Figure 6.1 and tables 6.1, 6.2, and 6.3 depict the refined flow diagram based on the reference used to develop it. The capacity of the plant is 86 TPD and the exergy efficiency with electricity recovery is 43.51%. The process flow diagram in Figure 6.1 includes compressor units with aftercoolers, heat exchangers, expander/turbine units, isenthalpic expansion valves, separator units, mixers and a recuperator. In the reference process plant Figure 2.15, there is a fifteen-stage Nelium compressor unit which has been refined to 5 compressors with 3 stages in each and inter cooling to the required temperature to pass it to the recuperator and then to the turbines T-1 and T-2 for utilizing its cooling duty for cryogenic liquefaction of hydrogen.

The initial design for the hydrogen gas compression system necessitates the deployment of three high-pressure compressors (HPCs) to achieve the desired pressure increase from 20 bar to 80 bar. The isentropic efficiencies of these compressors are as follows:

- HPC-1: 81.93%
- HPC-2: 81.95%
- HPC-3: 81.75%

Similarly, the compression system for the multi-component refrigerant mixture, consisting of eight distinct components, requires three compressor units to elevate the pressure from 1.1 bar to 24.8 bar. The respective isentropic efficiencies of the mixed refrigerant compressors (MRCs) are:

- MRC-1: 84.00%
- MRC-2: 84.51%
- MRC-3: 83.95%

To achieve the liquefaction of hydrogen, the temperature of the hydrogen gas must be reduced from 78 K to 33 K. For this cryogenic liquefaction process, a Nelium refrigerant is utilized. The Nelium refrigerant

is compressed from 2.4 bar to 73 bar using five compressor units, designated as C-1, C-2, C-3, C-4, and C-5. Each of these compressors is equipped with intercoolers after each stage of compression, and each compressor unit operates with three stages of compression. The flash hydrogen gas in stream (H-9) is compressed from 1 bar to 11 bar using two compressor units i.e. FC-1 and FC-2 having an isentropic efficiencies of 81.61 % and 80% each.

Table 6.1: Process Stream Data Points of Hydrogen

Stream	Temp.[K]	Press.[bar]	Vapour Quality
H-1	310	20	1
H-2	310	80	1
H-3	255	78.7	1
H-4	235	77.5	1
H-5	145	76.2	1
H-6	78	75	1
H-7	33	73.8	1
H-78	26	4	0.1551
H-8	20.2	1	0.3085
H-9	20.2	1	1
H-10	45.6	11	1
H-11	26.44	10.5	0
H-12	20.2	1	0.196
Liquid-H2	20.2	1	0

Table 6.2: Process Stream Data Points of Helium-Neon (Helium) mixed refrigerant

Stream	Temp.[K]	Press.[bar]	Vapour Quality
HENE-1	310	73	1
HENE-2	75	71.5	1
HENE-3	41.84	13.3	1
HENE-4	24.44	2.5	0.9807
HENE-5	68.94	2.4	1
HENE-6	310	2.4	1

Table 6.3: Process Stream Data Points of eight component Mixed Refrigerant

Stream	Temp.[K]	Press.[bar]	Vapour Quality
MR-1	301.35	1.1	1
MR-2	310	24.8	0.7197
MR-3	310	24.8	1
MR-4	255	24.4	0.716
MR-5	255	24.4	1
MR-6	235	24	0.9172
MR-7	145	23.6	0.3718
MR-8	75	23.2	0.0146
MR-9	72	1.2	0.0943
MR-10	139.34	1.2	0.6857
MR-11	255	24.4	0
MR-12	235	24	0
MR-13	145	23.6	0
MR-14	144.44	1.2	0.0301
MR-15	142	1.2	0.4969
MR-16	223.24	1.2	0.9402
MR-17	310	24.8	0
MR-18	255	24.4	0
MR-19	235	1.2	0.1904
MR-20	225.8	1.2	0.7397
MR-21	235.7	1.1	0.8034

As illustrated in Figure 6.1, the Brayton cycle used for cryogenic liquefaction employs two turbines T-1 and T-2. For respective Turbo-Expander, namely T-1 and T-2, the calculated isentropic efficiency values stands at 77.16% and 88.32%.

The plant's overall specific energy consumption (SEC) with recovery is 6.927 kWh/kg_{LH2} and without recovery is 7.3187 kWh/kg_{LH2}. Largest energy consumption is contributed by the Helium compression units accounting for 4.113 kWh/kg_{LH2}. The ideal specific work required for the liquefaction process is 3.0146 kWh/kg considering the conversion of ortho- to para-H₂. Based on these two results of specific

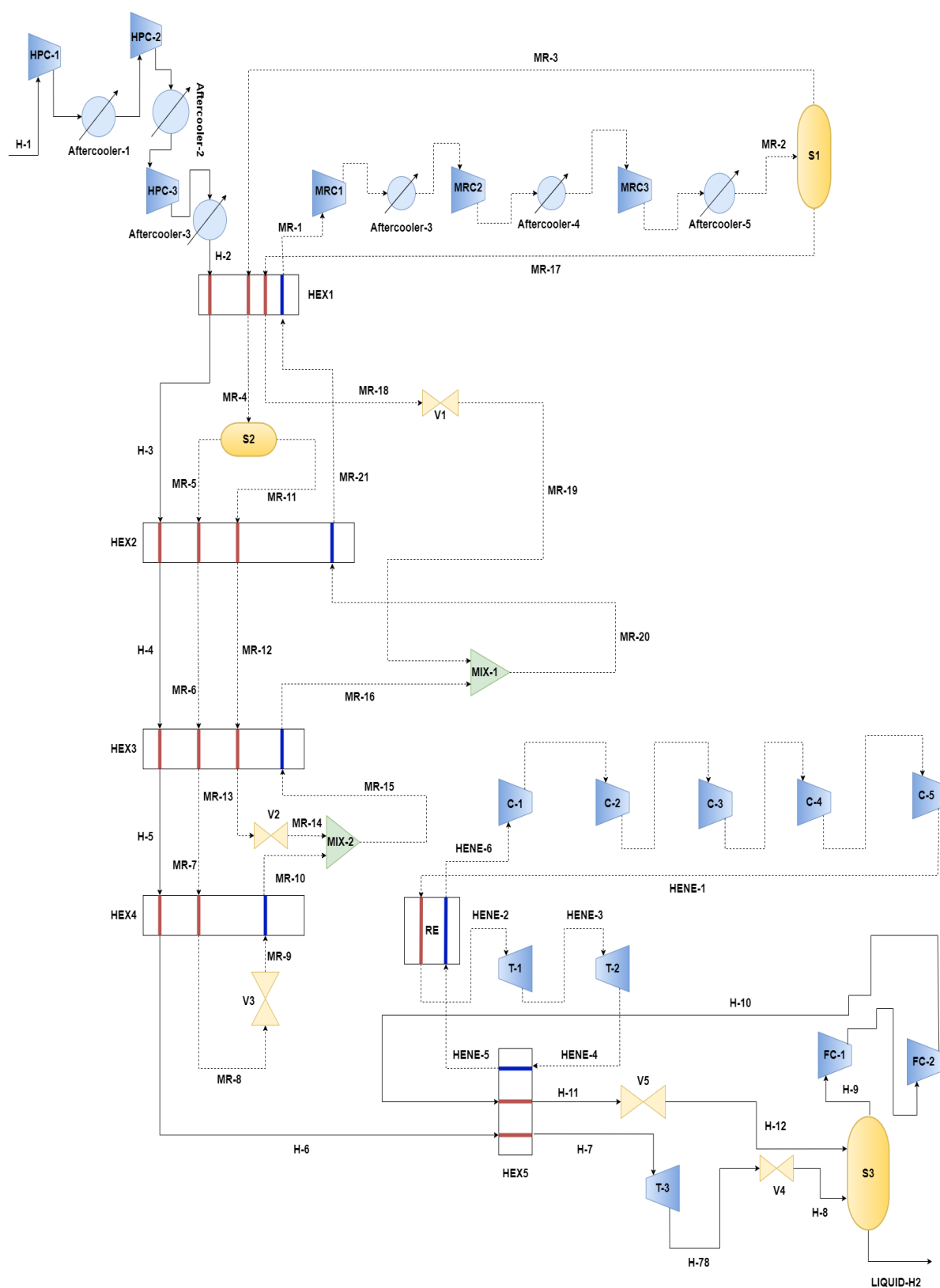


Figure 6.1: High-Pressure H₂ Brayton Cycle Liquefier Process Flow Diagram.

energy consumption and ideal specific work requirement the calculated exergy efficiency of the plant is 43.51%. In case power recovery is not considered, then the exergy efficiency reduces to 41.2%

The plant's CAPEX and OPEX evaluation follows the techno-economic methodology described in Chapter 5. The cost estimation of the plant, considering the power recovery is 1.57€/kg_{LH2}. The annual CAPEX of the liquefaction plant is 15.5 million € in 2023 and the OPEX considering the hydrogen leaks and Refrigerant leaks and power recovery from turbine shafts sums up to 31.5 million €. The total project cost is 111 million € (based on 2019 pricing) and when equation 5.2 was used to scale up the price to get value in 2023 it went up to 137 million €.

Table 6.4: Compressor Units main cost parameters and direct costs for 86 TPD

Compressors	Items in Parallel	Inlet flowrate [kg/s]	Power Input [kW]	Total direct costs €
HPC-1	1	1	719	1,855,600.00
HPC-2	1	1	725.6	1,874,200.00
HPC-3	1	1	736.6	1,907,100.00
MRC1	1	35	3102	8,397,400.00
MRC2	1	35	3103	4,002,300.00
MRC3	1	35	3024	2,515,800.00
C-1	1	9.7	2927	8,074,700.00
C-2	1	9.7	2975	5,375,200.00
C-3	1	9.7	2971	3,275,000.00
C-4	1	9.7	2978	2,674,800.00
C-5	1	9.7	2956	2,742,100.00
FC-1	1	0.3834	50.65	1,249,300.00
FC-2	1	0.3834	75.78	1,406,300.00

Table 6.5: Turbine units main cost parameters and direct costs for 86 TPD

Turbines	Items in Parallel	Inlet flowrate [kg/s]	Power Output [kW]	Total direct costs €
T-1	1	9.7	831.0	752,700.00
T-2	1	9.7	480.6	623,100.00
T-3	1	1	98.68	324,800.00

Table 6.6: Heat Exchanger units main cost parameters and direct costs for 86 TPD

Heat Exchangers	Items in Parallel	Dimensions [m]	Core Weight per HEX [kg]	Total direct costs €
HEX1	8	2.0988 x 0.5971 x 0.8564	1,625.5375	4,218,000.00
HEX2	5	1.0301 x 0.592 x 0.8312	776.6	2,226,600.00
HEX3	7	5.4174 x 0.5954 x 0.8816	4,176.557	5,874,900.00
HEX4	3	3.1818 x 0.5945 x 0.6884	1,929.3667	1,621,100.00
HEX5	1	3.9375 x 0.5988 x 0.7511	2,528.3	576,700.00

Tables 6.4, 6.5, and 6.6 indicate the total direct cost of compressor, turbine and heat exchangers based on the main cost-parameters. Among these compressors have the highest cost estimation of 45 million €. Figure 6.2, indicates the distribution of the total direct equipment costs of the project among the four systems of the liquefier, i.e. H₂ feed and flash compression system, precooling compression system, the cryogenic compression and expansion system and the heat exchanging system (5 heat exchangers of the plant). Among these four systems the most expensive one is the cryogenic liquefaction with an estimated value of 22.14 million €. The most expensive system of the plant is MRC1, with estimated direct cost of 8.39 million €.

Figure 6.3 indicates the distribution percentage of base scenario annual OPEX considering the pricing of 2019 in APEA simulation. Within this 31.5 million €/ year of operating expenses, the utility expenses accounts to 23.7 million € which is 75.11 % of the entire OPEX. In this particular scenario, the annual CAPEX and OPEX percentage are found to be approximately 33% and 67 % wrt the total annual OPEX and CAPEX.

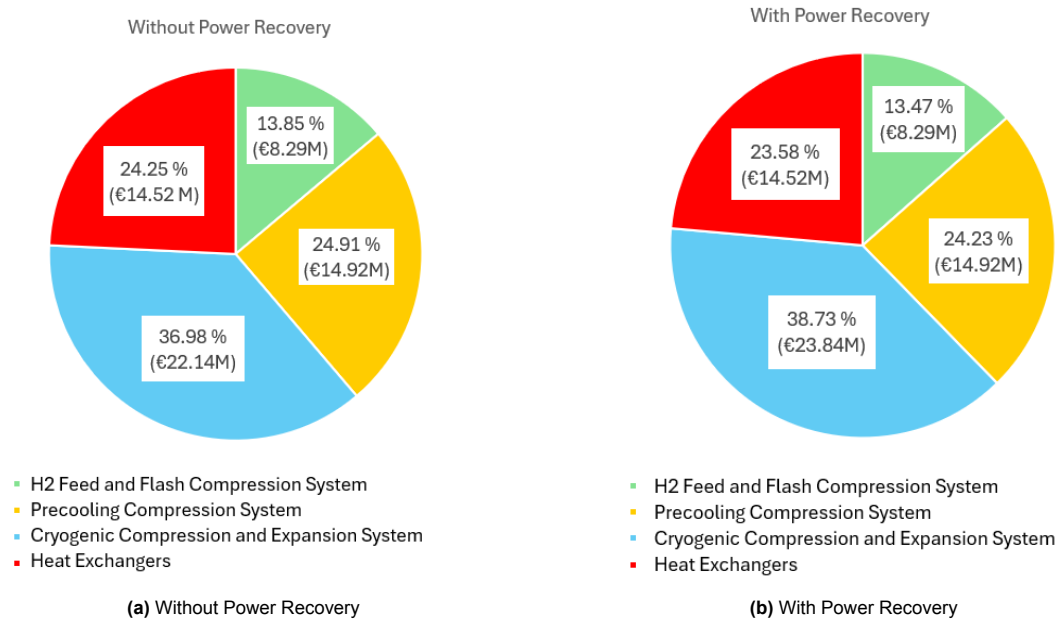


Figure 6.2: Proportion of System's Equipment Direct Costs (Estimated using APEA's 2019 pricing basis)

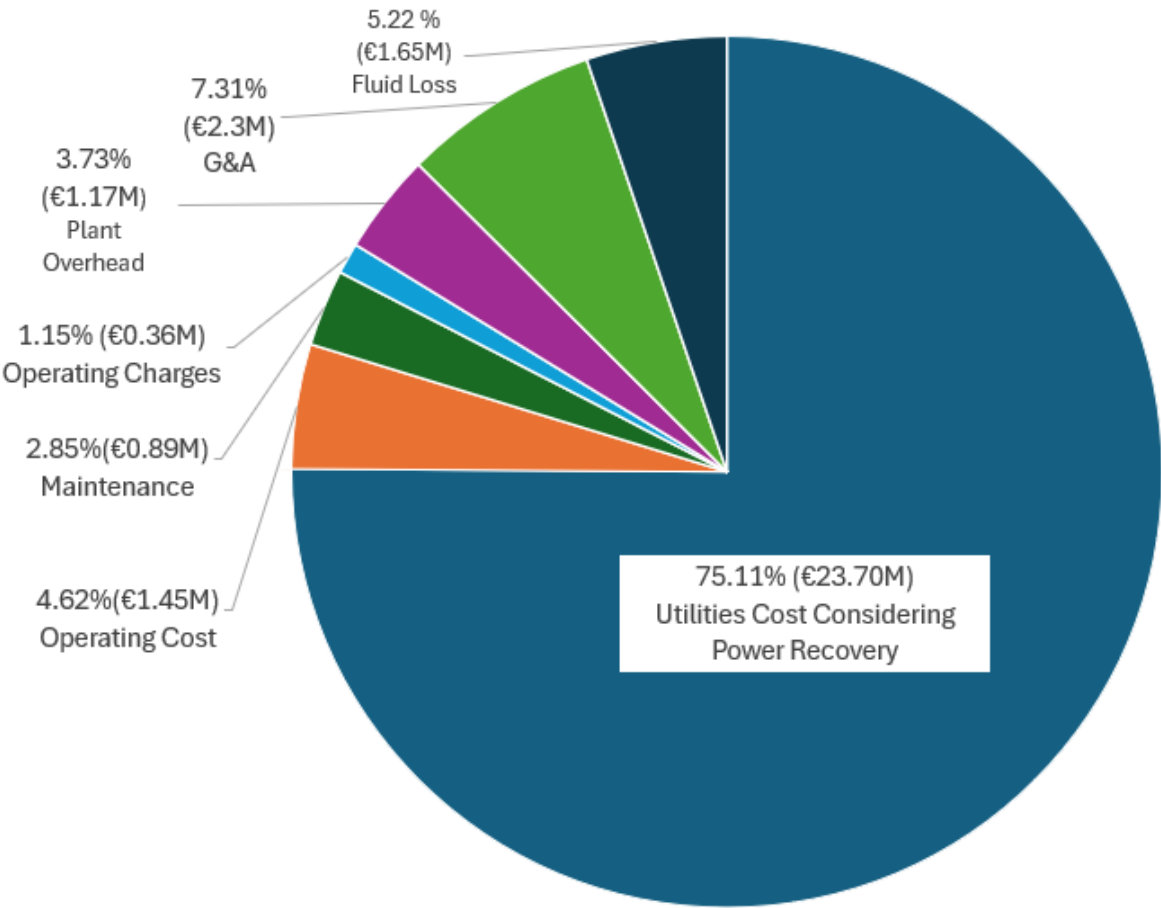


Figure 6.3: Distribution percentage of base scenario annual OPEX

6.2. Baseline Analysis

In the reference plant 2.15 of Berstad [22], the resulting exergy efficiency is 44.7% and the calculated exergy efficiency for Figure 6.1 plant is 43.5% which is 2.7% less than the reference case. The minimum theoretical specific liquefaction power calculates to approximately $2.90 \text{ kWh/kg}_{\text{LH}_2}$ in the reference plant and in Figure 6.1 plant is $3.0146 \text{ kWh/kg}_{\text{LH}_2}$ which is 7% more than the reference case. The SEC value of the large-scale liquefaction process presented in this thesis are significantly lower than those of state-of-the-art hydrogen liquefiers, typically falling within the range of $10 - 12 \text{ kWh/kg}_{\text{LH}_2}$. The calculated value with recovery is $6.927 \text{ kWh/kg}_{\text{LH}_2}$ and without recovery is $7.3187 \text{ kWh/kg}_{\text{LH}_2}$. These values are 35% less than the state-of-the-art values.

6.3. Sensitivity Analysis

6.3.1. Annual Interest Rate and Payment Period impact on SLC of the plant and CAPEX of the plant

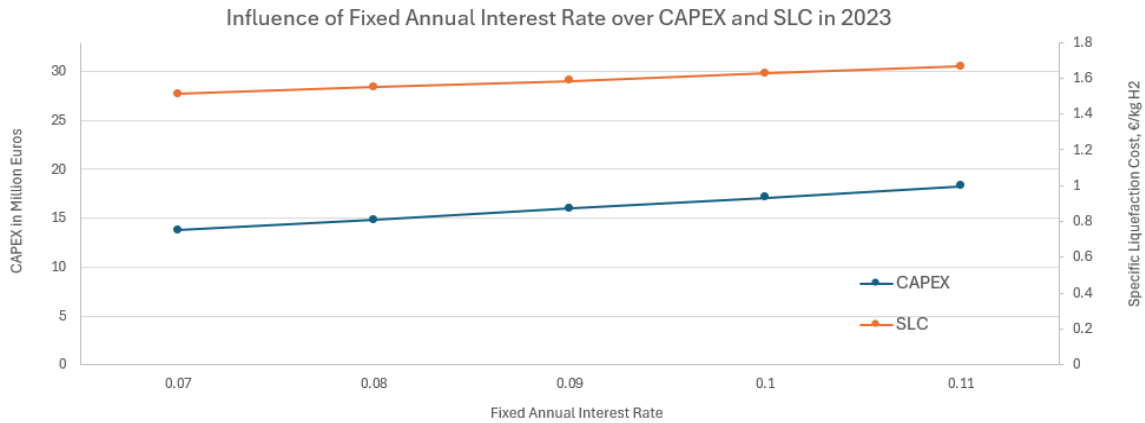


Figure 6.4: Influence of Fixed Annual Interest Rate over CAPEX and SLC in 2023

Figure 6.4 explains the trends of influence of fixed interest rate over CAPEX and specific liquefaction cost (SLC) of the plant in 2023 utilizing equation 5.2. It can be concluded that when the fixed annual interest rate increases from 0.07 to 0.11 there is an increase in CAPEX by 33% and increase in SLC by 10 %. When conducting this analysis, a payment period of 20 years and electricity price of 0.1 kWh was considered in APEA simulation.

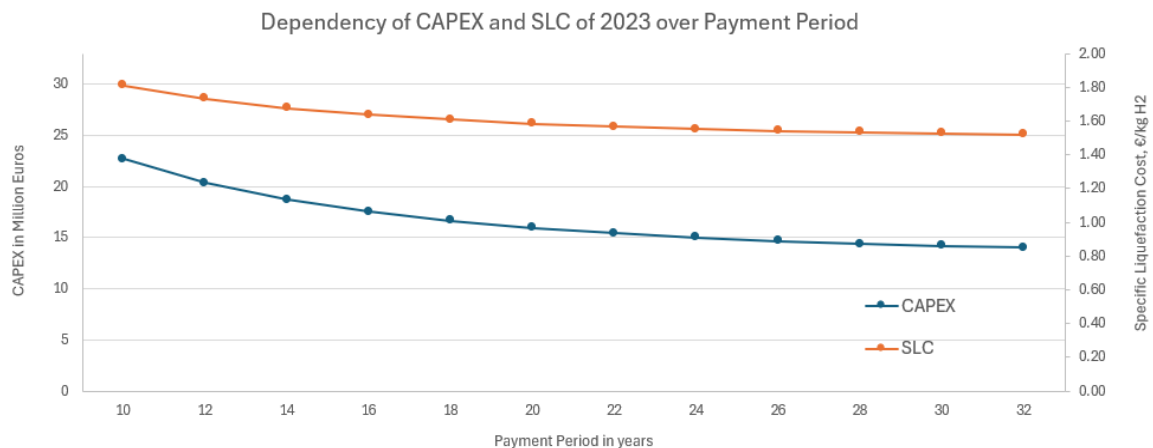


Figure 6.5: Dependency of CAPEX and SLC of 2023 on Payment Period

Figure 6.5 explains the trends of dependency of CAPEX and SLC of 2023 over Payment Period utilizing equation 5.2. It can be concluded that when the Payment Period increases from 10 to 32 years there is a decrease in CAPEX by 40% and decrease in SLC by 19%. When conducting this analysis, a fixed Annual Interest Rate of 0.09 and electricity price of 0.1 kWh was considered in APEA simulation.

6.3.2. Electricity Cost Analysis

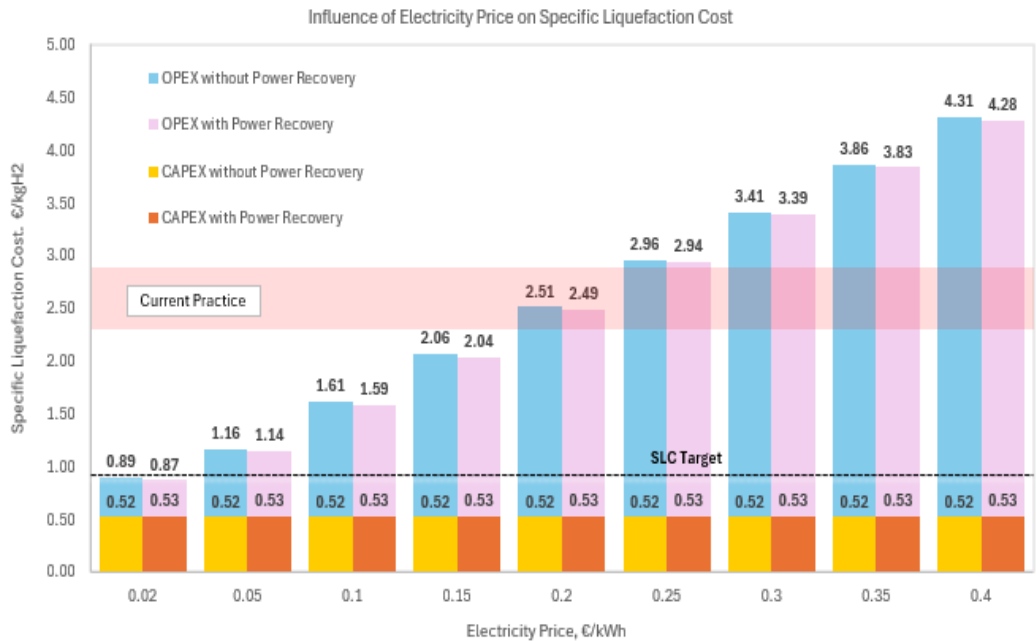


Figure 6.6: SLC of the 86 TPD hydrogen liquefier concept as a function of electricity price

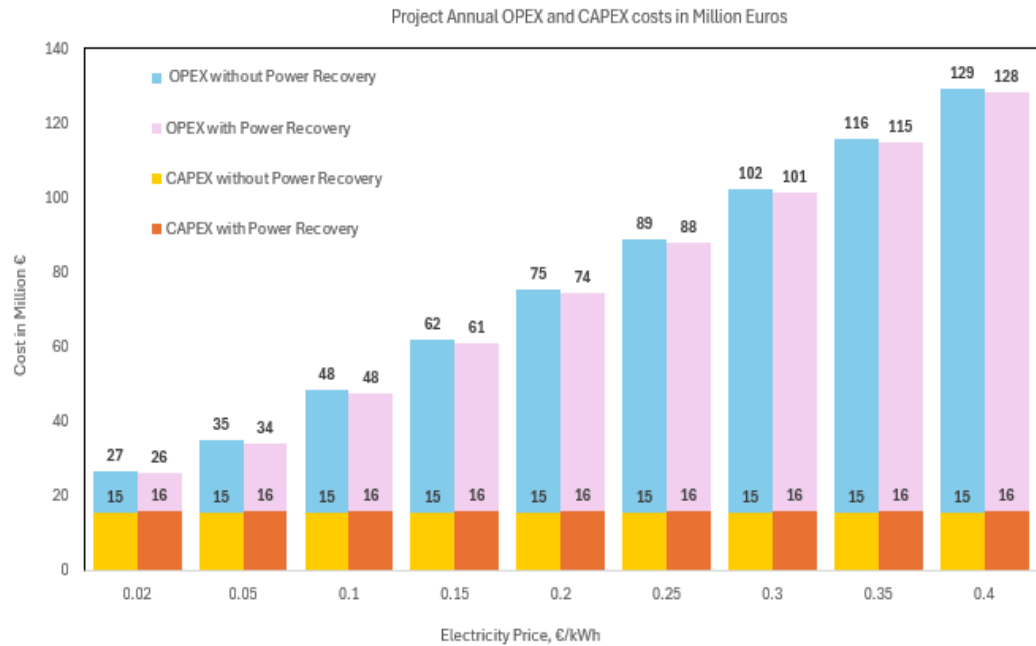


Figure 6.7: Project Annual OPEX and CAPEX costs as a function of electricity price for 86 TPD

In the baseline scenario, the specific liquefaction costs are calculated with specific electricity costs of 0.1€/kWh. In this sensitivity analysis, the 86 TPD conceptual plant's annual total costs and specific liquefaction costs are computed by varying electricity costs between 0.02 and 0.4€/kWh. Figures 6.6 and 6.7 presents these outcomes. The graphs reveal that the SLC of hydrogen liquefier are considerably influenced by the electricity costs. The SLC values of the large-scale plant increase to the current industrial value of 2.37 to 2.85€/kgLH₂ when the electricity is priced relatively high at 0.2-0.25 €/kWh. It is important to note that the range of electricity prices used in this analysis has been deliberately set to exceed the typical variation in electricity costs across the EU. This approach is intentional, aiming to assess the potential impact of a sudden surge in energy prices—similar to those experienced in the EU in recent years—on the overall costs of the hydrogen supply chain. When the electricity price is between 0.02-0.05 €/kWh, the SLC value drops down close to the target value i.e. 0.95€/kgLH₂. It is also noted that the OPEX values are dominated at higher prices of electricity.

6.3.3. Feed Pressure Analysis

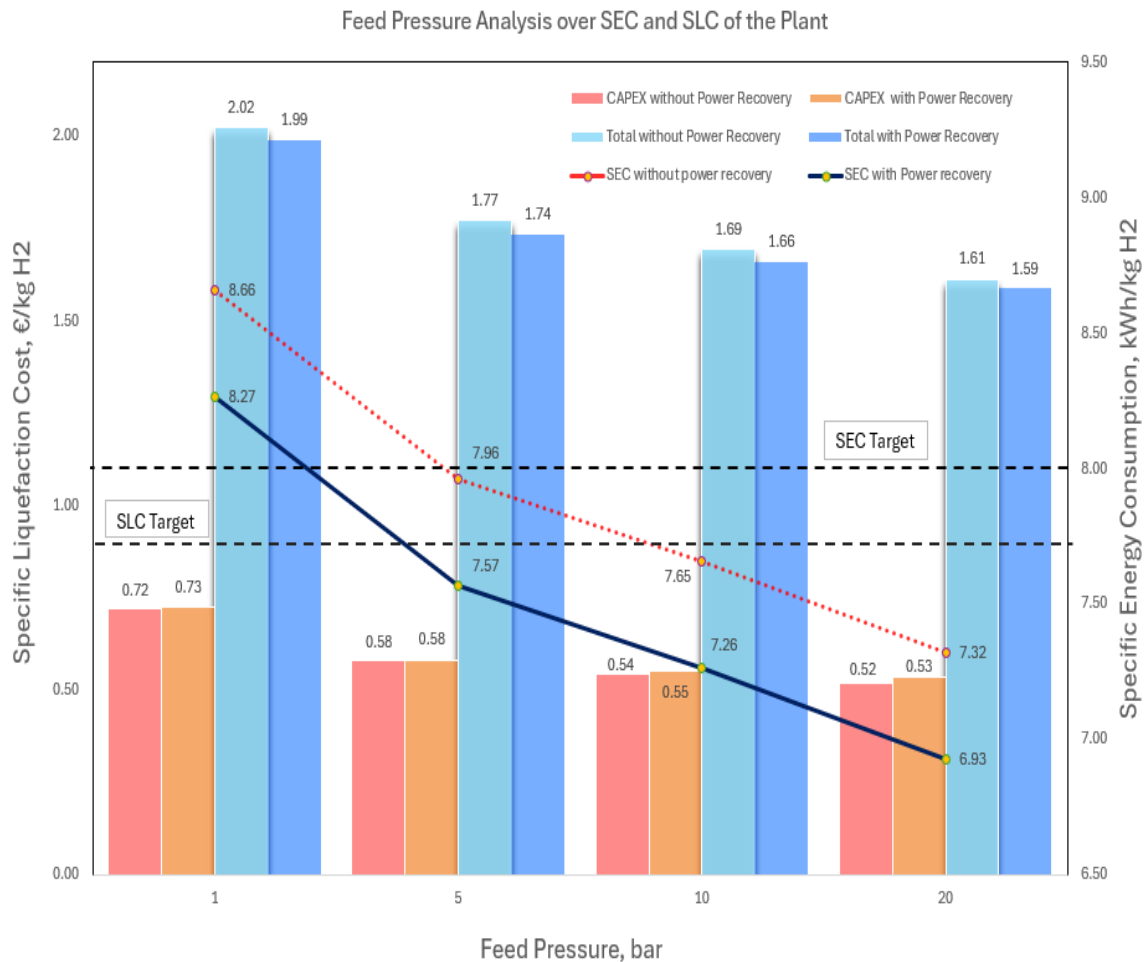


Figure 6.8: SEC and SLC of the 86 TPD Hydrogen Liquefier concept as a functions of feed pressure

In this thesis, a feed pressure of 20 bar is considered for the hydrogen liquefaction process. The literature review indicates that increasing the hydrogen feed pressure can reduce the energy input required for the liquefaction process. To evaluate this observation, the feed pressure was systematically varied, reducing it to 1 bar, 5 bar, and 10 bar. In each case, the hydrogen was subsequently pressurized to the required inlet pressure of 80 bar before being introduced into HEX1. This approach allows for a comparative analysis of the impact of feed pressure on the specific energy consumption (SEC) and specific liquefaction cost (SLC) during the liquefaction process.

In this work, the precompression system is assumed to be constructed using one or multiple centrifugal compressors equipped with aftercoolers. These compressors are designed following the same guidelines and limitations outlined in Section 4.2. As seen in Figure 6.8, The SEC and SLC of the plant increase drastically when the feed pressure is lowered to 1 bar. This is because the pressure ratio requirement increases drastically from 4 to 80 when the feed pressure is reduced from 20 bar to 1 bar. The CAPEX has increased by 24% and OPEX has increased by 9.2% when feed pressure is decreased from 5 to 1 bar. From this analysis, it can be concluded that the efficiency and economic performance of the plant design are fairly sensitive to decreasing feed hydrogen pressure.

Table 6.7: Compressor Units Data

Feed Pressure (bar)	Compression Ratio	Number of feed compressors	Number of stages
1	80	9	6 in each compressor
5	16	6	6 in each compressor
10	8	4	6 in each and 7 in last compressor
20	4	3	6 in each and 7 in last compressor

Conclusion and Recommendation

In this chapter, the sub-research questions outlined in the introduction are addressed by drawing on the key insights and implications uncovered throughout the research.

7.1. Conclusions

How can a conceptual high-capacity H_2 liquefaction plant be accurately modelled based on the Brayton Cycle concept using a commercial process simulation tool?

In this thesis, a modified version of the high-pressure H_2 Brayton-cycle large-scale hydrogen liquefaction concept presented by Berstad [22], is selected for evaluation. The process modeling was carried out using Aspen HYSYS process simulation software, utilizing its built-in unit operation models to simulate the performance of various components, including heat exchangers, compressors, and expanders. Specifically, for the calculation of the multi-stream counter-current PFHX unit operation, the 'LNG Exchanger' model available in Aspen HYSYS was employed.

The eight-component mixed refrigerant used in the precooling cycle was modeled using the Peng-Robinson cubic equation of state (EOS) available in Aspen HYSYS. This EOS was employed to input the thermodynamic properties at each state point necessary for the plant's development. Similarly, the thermodynamic state properties of Nelium (80% He and 20% Ne) refrigerant used in the cryogenic liquefaction Brayton cycle are derived from Peng-Robinson cubic equation of state (EOS) available in Aspen HYSYS.

For the purpose of simulating the hydrogen feed stream, which undergoes continuous catalytic ortho-to para-hydrogen conversion within the heat exchangers, the assumption of equilibrium hydrogen is applied. For this purpose, the pseudo-equilibrium-hydrogen heat-capacity model developed by Valenti et al. [13] is employed. The implementation of the pseudo-e- H_2 model by Valenti et al. [13] involves modifying the REFPROP [48] fluid file (.FLD file) for parahydrogen and subsequently calling REFPROP's parahydrogen model from Aspen HYSYS.

Before initiating the preliminary equipment designs, the isentropic efficiency values for the pressure-changing components and the pressure drops in the PFHXs have been adopted from the reference work of Berstad [22]. These initial assumptions will be refined in subsequent equipment design iterations as necessary. The SEC of the plant considering the recovery of power from turbine shafts is as 6.9025 kWh/kg $_{LH_2}$. The exergy efficiency of the plant is calculated as 43.665% and the specific liquefaction power of this plant calculates to 3.014 kWh/kg $_{LH_2}$.

What is the technical evaluation procedure for the preliminary designs of the main equipment in a large-scale hydrogen liquefaction process, and how can the findings from these preliminary designs be incorporated into the overall plant design?

This thesis primarily evaluates the preliminary design of major process equipment for large-scale liquefaction systems, including compressors, turbines, and heat exchangers. Due to time constraints, the sizing of cryogenic adsorbers and coldboxes is not included in this work and will be addressed in future studies. Compatibility with existing technology constrains is ensured.

All five heat exchangers were sized using Aspen EDR's PFHX design mode, with input data directly imported from the Aspen HYSYS simulation file. The resulting calculations, especially the pressure drop estimates, were used to refine the pressure values in the Aspen HYSYS simulation.

Centrifugal compressors are suitable for the compression process required in the liquefaction plant under evaluation, with flow rates ranging from 2,300–45,000 m³/h and max discharge pressure of 80 bar. Therefore, only radial-flow turbo-compressors are considered in this thesis. The H₂ compressors and mixed-refrigerant compressor units are equipped with after-coolers that cool the outlet gas to 310 K using cooling water. Similarly, the Neon refrigerant compressors are fitted with intercoolers that cool the outlet of each compression stage to 310 K.

The preliminary designs for the centrifugal compressors estimate the isentropic efficiencies for each compression stage and determine the number of modules, stages, and rotational speeds for each compressor. The isentropic efficiency values obtained are then used to refine the initial assumptions in the process simulation. Additionally, the determined number of units, stages, and rotational speeds are utilized to improve the accuracy of the cost estimation. The procedure is a simplification of the preliminary design procedure given by Gambini and Vellini. [41]

Radial in-flow turbines, or centrifugal turbines, are considered for the turboexpanders. The design process for these turbines follows a similar approach to that of compressors but involves different input and output parameters. The design outcomes include estimations of isentropic efficiencies, the number of turbine modules, and the acceptable rotational speeds for the turboexpander system. These results are then used to refine the process simulation and provide additional input for cost estimation.

How to effectively estimate the capital and operating costs of a conceptual hydrogen liquefier based on the process simulation model and equipment preliminary designs, and what are the key factors influencing the plant's economic feasibility?

In chapter 5 of this report, the CAPEX and OPEX associated with the large-scale high-pressure hydrogen Brayton cycle concept is estimated and the specific liquefaction cost is determined to understand the hydrogen economy in the European market. To determine these capital expenditures (CAPEX) and operating expenditures (OPEX) of the plant, the Aspen Process Economic Analyzer (APEA) software is utilized for its ability to estimate equipment expenses using up-to-date cost data obtained from real engineering, procurement, and construction (EPC) projects and equipment manufacturers.

In addition to estimating equipment purchase costs, APEA also evaluates the total installed costs, including both direct and indirect field expenses. A key advantage of using APEA over other cost estimation methods is its integration with Aspen HYSYS simulation software, which is employed for process modeling in this thesis. The estimation of primary process equipment costs is based on design parameters established during the preliminary equipment design and sizing. Additionally, APEA enables the calculation of the plant's operating costs, encompassing both variable and fixed operational expenditures.

In the baseline scenario, the electricity price was estimated to be 0.1 €/kWh. The specific liquefaction cost (SLC) for the 86 TPD plant was calculated to be 1.57 €/kgLH₂, which is lower than the current industrial hydrogen liquefaction costs, ranging from 2.37 to 2.85 €/kgLH₂. During the calculation of OPEX and CAPEX, the costs associated with hydrogen leakage, refrigerant leakage, and power recovery from turbine generator shafts were considered. The total annual CAPEX was calculated to be 15.5 million €, while the total OPEX, including fluid loss and power recovery, amounted to 30 million €. This indicates that the OPEX is the dominant factor over CAPEX for this hydrogen liquefaction plant. In this scenario, the annual CAPEX and OPEX contributions were found to be approximately 33% and 67%, respectively, with respect to the total annual expenditure.

Aspen Process Economic Analyser (APEA) gave the detailed direct costs of each and every component and the compressors had the largest impact on the CAPEX of the plant. A sensitivity analysis was conducted to identify the parameters that influence the specific liquefaction cost (SLC) of the plant. The analysis focused on two key parameters: 1) electricity price and 2) feed pressure. The results reveal that fluctuations in electricity prices have a substantial impact on the plant's economic performance. Additionally, the analysis indicates that the plant's efficiency and economic viability are significantly sensitive to decreases in feed hydrogen pressure. The CAPEX has increased by 24% and OPEX has increased by 9.2% when feed pressure is decreased from 5 to 1 bar refer to figure 6.8 for more details.

7.2. Recommendation and Future Scope

This thesis focuses on the development of a large-scale hydrogen liquefaction plant utilizing the Brayton Cycle concept with an initial capacity of 86 tons per day (TPD). The study can be further explored in the potential for scaling up the plant's capacity to 125 TPD. The performance and results of this scaled-up plant can then be compared with those of a hydrogen liquefaction plant previously developed by [23].

The cooling capacity of the flash hydrogen (H₂) gas in the H-9 stream, as shown in Figure 6.1, can be effectively utilized to cool the hydrogen gas streams in all five heat exchangers. This optimization will lead to a reduction in the flow rates required for the cryogenic liquefaction and precooling cycle compressor units, thereby increasing the exergy efficiency of the plant. Additionally, the cooled H-9 stream can be recycled into the feed hydrogen gas stream (H-1), further enhancing overall system efficiency.

For the preliminary design of plate-fin heat exchangers, the refrigerant used in the precooling cycle is mixture composed of eight components. Due to incompatibility in the pseudo-homogeneous continuum reactor model developed by O'Neil et al. [40] for mixed refrigerants utilized for cooling the hot hydrogen gas stream, all design calculations were performed using the Aspen EDR software package to accurately determine the dimensions of the heat exchanger. A new code can be developed for the preliminary design of plate-fin heat exchangers by utilizing the necessary properties of the mixed refrigerant obtained from REFPROP. Additionally, the existing codes for compressors and turbines can be further enhanced by incorporating intercoolers and aftercoolers into the design.

Optimizing liquefaction costs within the framework of this thesis may present significant challenges, as capital and operating costs are estimated using the Aspen Process Economic Analyzer (APEA). While previously conducted liquefaction cost optimization by integrating Honeywell UniSim Process Simulation with MATLAB [Ref], the cost estimation method used in their study was self-developed and based on adapted cost correlations that have not been fully published. Study of et al.[49] introduces a robust systematic approach by integrating a thermodynamic framework, ML methods, and metaheuristic techniques to optimize the operational variables of the H₂ liquefaction cycle.

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