Process Simulation, Optimization and Techno-Economic Analysis of Ammonia Production from Natural Gas

By

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Process Modelling, Optimization and Cost Analysis of Ammonia Production from Natural Gas

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THESIS ACCEPTANCE CERTIFICATE

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Presented on: **05 Oct 2023** at: **1500 hrs in SCME (Seminar Hall)**

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Dedication

This thesis is dedicated to family, teachers and friends for their endless support, encouragement, love and honour.

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All praise and eminence are due to "ALLAH," the undisputed architect of this world, who gave us the capacity for comprehension and sparked our curiosity about the planet as a whole. Warmest welcomes to the supreme ruler of this world and the hereafter, "Prophet Mohammed (PBUH)," a source of knowledge and benefits for all of humanity as well as for Uma.

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Muhammad Umar Shahid

Abstract

The increasing global demand for ammonia, primarily used as a key raw material in the production of fertilizers and other chemical compounds, necessitates efficient and cost-effective production methods. This thesis aims to address this challenge by conducting a comprehensive study focused on process modelling, optimization, and cost analysis of ammonia production from natural gas. The first phase of the thesis involves process modelling, where a detailed investigation of the Haber-Bosch synthesis process is carried out. Various process parameters, such as temperature, pressure, and flow rates, are analysed using advanced simulation tools. A robust and accurate process flow diagram is developed using Aspen HYSYS, offering valuable insights into the complex kinetics and dynamics of ammonia synthesis. In the optimization phase, pinch analysis is carried out with the help of Aspen Energy Analyzer to enhance the efficiency and sustainability of the ammonia production process. Pinch analysis is used to determine the optimal operating conditions, maximizing ammonia yield while minimizing energy consumption, utilities required and greenhouse gas emissions. The final aspect of this thesis involves conducting a comprehensive cost analysis of ammonia production from natural gas. An economic evaluation is performed, taking into account various factors such as feedstock prices, energy costs, capital investments, and environmental compliance. This is done by activating Aspen Economic Analyzer in the HYSYS simulated model. The objective is to identify potential cost reduction strategies while ensuring the overall economic viability and competitiveness of ammonia production. The findings of this thesis contribute significantly to the field of ammonia production, providing valuable insights into process optimization and cost-efficient production methods. The developed process model and optimization strategies offer a reliable framework for industrial implementation, fostering sustainable ammonia production from natural gas. As the world seeks to address the challenges of population growth and food security, this research contributes to the global endeavour to achieve sustainable and responsible production of essential chemical commodities.

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Nomenclature

PFD	Process Flow Diagram
AEA	Aspen Energy Analyser
GHG	Greenhouse Gas Emissions
SMR	Steam Methane Reforming
VOC	Volatile Organic Compounds
LCA	Life Cycle Assessment
WGS	Water Gas Shift Reactor
HTS	High Temperature Shift Reactor
LTS	Low Temperature Shift Reactor
HPS	High Pressure Separator
LNG	Liquefied Natural Gas
CCU	Carbon Capture and Utilization
DEA	Diethanolamine
ECON	Economic Evaluation
NPV	Net Present Value
IRR	Internal Rate of Return
HAZOP	Hazard and Operability Analysis
HEN	Heat Exchanger Network
FCI	Fixed Capital Investment
WCI	Working Capital Investment
ROR	Rate of Return

Chapter 1

Introduction

1.1. Background

One of the most important petrochemical products used in the preparation of fertilizers (Urea, Di-ammonium phosphate, and ammonium nitrate), explosives, explosive materials, polymers, acids, fuel, pharmaceutical and cleaning products is ammonia [1-4]. The global production capacity was estimated to be over 175 million metric tons in 2016 and it is expected to increase by 23% from 2019 to 2030 [5]. The largest producer of ammonia is China taking charge of 31.4% of global production. Russia seconds China by producing 10% ammonia followed by United States (i.e. 8.9%) and lastly, India takes place in the top four producers by contributing 7.8% to the overall production [6]. Currently, ammonia gas is under limelight for being a potential energy carrier or hydrogen storage medium due to having three times higher volumetric energy density in comparison to hydrogen [7]. It is also gaining attention for its significant storage and transportation properties [8]. Despite all these benefits, the ammonia (above 80%) is still mainly used for the production of fertilizers [9].

There are different methodologies to synthesize ammonia, such as the Haber-Bosch process, electrochemical synthesis, photo-catalysis or chemical-looping [10-12]. However, the major industrial method is Haber-Bosch process, which was initially developed in 1905 by Fritz Haber and adapted for industry in 1910 by Carl Bosch and it solemnly accounts for greater than 90% of total ammonia production [13, 14]. The hydrogen required in the process is mostly produced from natural gas [15]. In the Haber-Bosch process, the reaction of nitrogen and hydrogen results in the production of ammonia under high pressure and temperature within the presence of iron catalyst. Currently, almost 150 million tonne of ammonia is produced annually by the Haber-Bosch process that is around five times more than the production in past years. For ammonia synthesis, hydrogen is produced by natural gas and ambient air is utilized as the source of nitrogen [16].

One of the major problems is the greenhouse gas (GHG) emissions despite the necessity of significant amount of ammonia production. The annual usage of fossil fuels accounts approximately 2% of worldwide energy consumption, resulting in CO_2 emissions of over 420 million metric tonne [17, 18]. The GHG emissions related to ammonia production will rise by the same order of magnitude to meet the rising demand for it. To advance towards sustainable ammonia plant operations, alternative environmentally friendly production pathways should be developed.

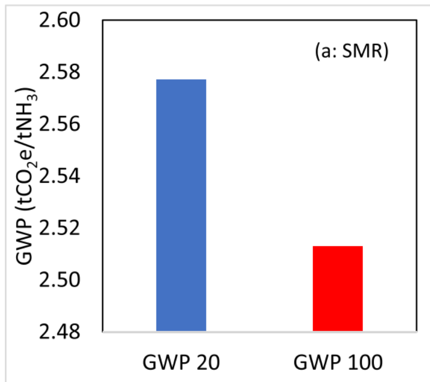

Figure 1: Figure shows the global warming potential estimates for SMR using 100-year and 20-year time-horizon[5].

Over the years, the demand of ammonia production has significantly enhanced due to increasing global population. The ammonia production plant is an energy intensive plant thus, it requires humongous amount of energy to process. The world is currently looking for a retrofit design that leads to net zero emissions. The emissions intensity of ammonia plants ranks higher than any other plant. Its major emissions include CO_2 and steam by mainly two sources that is electricity generated and the kinetic reactions taking place in the processing plant. In 2021, energy intensity of 46.2 GJ/ton and 2.4 t of CO_2/t was reported which is twice as emissions intensive as steel production and four times higher than cement industry while only accounting on the basis of direct CO_2 emission.

The production of hydrogen for the ammonia reaction is done either by steam reforming of hydrocarbons or gasification of carbon base compounds such as coal. Nitrogen is obtained from secondary reformer by introducing air or by air separation unit. The procedures based on hydrocarbons are widely used, particularly the steam reforming of natural gas (which accounts for around 72%). These procedures made up 78%, whereas coal gasification made up 22%. Steam reforming process uses between 28-33.8 gigajoules of natural gas for every metric tonne of ammonia, and each metric tonne of ammonia releases roughly 1.6 metric tonne of CO_2 into the atmosphere [5]. Similarly, for every metric tonne of ammonia, the life cycle greenhouse gas emission comprises of around 2.6 metric tonne of CO_2 [19]. In contrast, the energy consumption ranges from 51.3-77 gigajoules per tonne of ammonia, whereas the life cycle GHG emissions of the coal gasification process range from 5.1-7.8 tonne of CO_2 per tonne of ammonia [19, 20].

Nuclear, hydropower, municipal waste, biomass, solar, and wind energy are the technologies that are available to produce hydrogen and they frequently provide challenging obstacles. A few of these processes are expensive to implement. Zhang and co. evaluated the economic viability of green hydrogen-based ammonia generation methods [21]. For a large-scale ammonia production, they investigated water electrolysis and biomass gasification. According to their findings, the electrolysis-based method is not cost-effective whereas the biomass gasification method will have a longer payback period than the traditional steam-methane reforming method. As a result of some of these technologies being more complicated than the steam-methane reforming process, plant operations become more uncertain.

A prominent illustration is the multi-step thermochemical cycle used in the nuclear CuCl cycle to create ammonia [22]. A potential issue is the accessibility and pre-processing of feedstock, like biomass and municipal waste materials. Appropriate economic and environmental conditions are necessary for a high production of biomass [23]. Throughout the year, undesirable environmental conditions may have a negative effect on biomass yield [24]. Another difficulty arises from the significant variation in feedstock material. When municipal garbage and biomass are burned, dangerous air pollutants such as carbon monoxide, nitrogen oxides NO_x's, and volatile organic compounds (VOC's) are frequently released into the atmosphere [25]. As a result, the ammonia production industry is under immense pressure to transition towards greener and more cost-effective processes.

1.2. Problem statement

The production of ammonia from natural gas using the conventional Haber-Bosch process is a critical industrial process, accounting for a significant portion of global ammonia supply. However, the traditional method suffers from inefficiencies, high energy consumption, and substantial greenhouse gas emissions. As the world intensifies its focus shifts towards sustainability and climate change mitigation hence, there is an urgent need to address the environmental impact of ammonia production while ensuring economic viability.

The primary problem addressed in this thesis is the lack of comprehensive process modelling, optimization, and cost analysis studies for ammonia production from natural gas. Despite the widespread use of the Haber-Bosch process, there remains a limited understanding of the various technological and operational factors that affect the overall efficiency, environmental impact, and production costs. The specific challenges to be addressed are as follows:

- Inefficiencies in the Haber-Bosch Process:

The conventional ammonia synthesis process exhibits several inefficiencies, including low conversion rates, high energy consumption, and an overreliance on non-renewable fossil fuels.

- Environmental Impact:

Ammonia production is a significant contributor to greenhouse gas emissions, with the generation of carbon dioxide being a major concern. The emissions result from both the reaction itself and the energy-intensive nature of the process.

- Cost Competitiveness:

The economic viability of ammonia production is critical to sustain the industry. However, the current production methods, particularly those that rely on natural gas, face fluctuations in feedstock prices and uncertainties in energy costs, impacting the overall cost of ammonia production.

- Limited Process Optimization:

There is a lack of comprehensive studies that analyse the impact of process parameters, catalysts, and operating conditions on the efficiency, yield, and environmental performance of ammonia production from natural gas.

Addressing these challenges is crucial for advancing the state of ammonia production from natural gas, ensuring its sustainability, and aligning it with global climate goals. This thesis aims to provide a systematic analysis of the various factors influencing ammonia production, optimizing the process for enhanced efficiency, and conducting a comprehensive cost analysis to evaluate the economic feasibility of different production pathways. The findings will aid in identifying more sustainable and economically viable approaches to ammonia production from natural gas, contributing to a greener and more competitive ammonia industry.

Objectives

The objective of this thesis is to comprehensively investigate the process of ammonia production from natural gas, focusing on three fundamental aspects: process modelling, optimization, and cost analysis. By developing a detailed and accurate process model, the intricate kinetics and dynamics involved in ammonia synthesis can be better understood. This knowledge lays the foundation for subsequent optimization efforts, aiming to improve the process efficiency, reduce energy consumption, and minimize greenhouse gas emissions. Furthermore, an economic evaluation of the entire production process enables a thorough assessment of its viability, identifying potential cost reduction strategies and contributing to the overall competitiveness of ammonia production. The methodology followed in this thesis is shown in Figure 2.

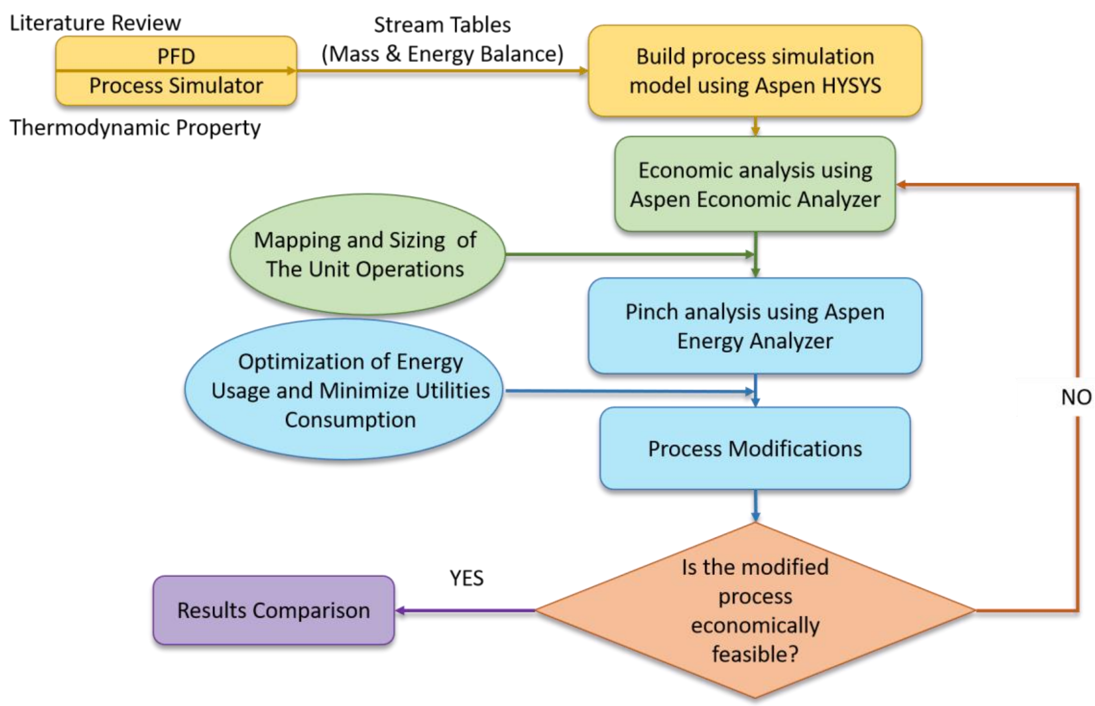

Figure 2: Schematic flowchart for methodology followed in this thesis

1.3. Scope and limitations

The scope of this research stems from its potential to revolutionize the ammonia production industry. By providing insights into novel and more sustainable methods for producing ammonia from natural gas, this study strives to contribute to global efforts in sustainable development and responsible resource management. The adoption of more efficient and eco-friendly ammonia production processes will not only bolster the fertilizer and chemical industries but also play a pivotal role in achieving global sustainability goals.

This thesis encompasses several key aspects such as process modelling, optimization, environmental impact assessment and cost analysis. The development of a rigorous process model for the ammonia synthesis unit assumes the chemical reactions, kinetics, and mass balances involved in the Haber Bosch process. A parametric study is then conducted on the developed model to optimize the operating conditions and process parameters to improve the overall efficiency, yield, and energy utilization of ammonia synthesis from natural gas. Using life cycle assessment (LCA) methods, carbon dioxide emissions and other pollutants are assessed. Lastly, a detailed economic analysis is done on the model considering the capital and operating costs associated with each production method. The presented modelling gives practical recommendations of enhancing sustainability and increased production rate along with economic viability of ammonia production from natural gas.

Despite the comprehensive scope, this thesis has certain limitations that should be considered. The availability of accurate and up-to-date techno-economic data for all ammonia production technologies, especially emerging ones, may be limited, potentially impacting the precision of cost analyses and feasibility assessments. Furthermore, the robustness and validity of data sources used for the environmental impact assessment and cost analysis might be subject to variations and uncertainties. While the thesis aims to cover a range of ammonia production technologies, it may not encompass all possible emerging methods or variations due to the vastness of the field. The study only focuses on the technical aspects of ammonia production and cost analysis but may not delve into detailed commercial aspects and market dynamics, which can also significantly influence the viability of specific production methods. Finally, the thesis will mainly focus on pilot-scale studies, and the results may not directly represent the challenges and complexities associated with large-scale industrial ammonia production.

Nonetheless, this research endeavours to provide an integrated and holistic approach to the sustainable production of ammonia from natural gas. By addressing the technical, environmental, and economic aspects of the process, it aspires to contribute to a more sustainable and resilient future for the ammonia production industry and the broader chemical sector.

Chapter 2

Literature Review

2.1. Ammonia Production process

The Haber-Bosch process is one of the most significant and revolutionary achievements in the field of industrial chemistry. It is a method for the large-scale synthesis of ammonia from nitrogen (N_2) and hydrogen (H_2) gases. This process was developed independently by two scientists, Fritz Haber and Carl Bosch, and it marked a critical milestone in the production of ammonia-based fertilizers and played a pivotal role in shaping the modern world.

The story of the Haber-Bosch process begins with the work of German chemist Fritz Haber in the early 20th century. In 1905, Fritz Haber succeeded in developing a method to combine nitrogen gas from the air with hydrogen gas to produce ammonia through a chemical reaction. This reaction is exothermic, meaning it releases heat, and it is favoured at high temperatures. However, achieving high conversion rates and yields proved challenging, and early attempts were not economically viable. The equation for this reaction is:

$$N_2 + 3H_2 \leftrightarrow 2NH_3 \qquad 2.1$$

Haber though, continued his struggle with high pressure route to produce ammonia and finally achieved 6% ammonia concentration in a reactor having osmium catalyst in 1906. This ground breaking work was marked as the significant contribution to the ammonia synthesis. Later, he proposed a recycle stream to increase the production rate of ammonia and patented his work [26].

The next critical phase in the development of the Haber-Bosch process involved the efforts of another German chemist and engineer Carl Bosch. Bosch, in collaboration with his team at BASF, faced the challenge of scaling up Haber's laboratory process to an industrial level. The main obstacle was the need for high pressure and temperature to achieve favourable reaction rates. Bosch and his team designed and built high-pressure reaction vessels that could withstand the conditions required for the ammonia synthesis reaction [27].

In 1910, after several years of intense research and development, Carl Bosch successfully demonstrated the industrial feasibility of the ammonia synthesis process. BASF constructed the first ammonia synthesis plant in Oppau, Germany, which went into production in 1913 with a production capacity of 30 million tons per day. This achievement revolutionized the production of ammonia and set the stage for the large-scale production of nitrogen-based fertilizers [28].

The ammonia production process consists of syngas compression train, the ammonia synthesis reactor, the heat recovery network, and the refrigeration process. These unit processes are interlinked such that they affect each other's operating conditions [29]. The ammonia production process involves several key steps, outlined below.

2.1.1. Feedstock Preparation

The two main feedstocks for the Haber-Bosch process are nitrogen and hydrogen gases. Nitrogen is sourced from the air, which is composed of approximately 78% nitrogen gas. Hydrogen, on the other hand, can be prepared from thermochemical, biochemical or electrical processes however, the process that moves the equilibrium rightest is preferred. Hence, finding the most feasible hydrogen producing process that is both commercially and economically feasible is the first problem faced for ammonia synthesis. Typically, hydrogen is obtained through steam methane reforming of natural gas (methane) due to its high efficiency and low water consumption. Both gases need to be purified to remove impurities that could interfere with the catalytic process and affect the efficiency of ammonia synthesis [8].

The nitrogen and hydrogen gases are then separately compressed to high pressures to promote the reaction's forward direction and achieve better conversion rates. Pressures in the range of 150 to 300 atmospheres are commonly used. The steam methane reforming (SMR) of natural gas solemnly responsible for 72% of global ammonia production capacity [18]. The process consists of two parts viz. syngas production via SMR and ammonia production via HB process. The SMR-HB pathway is shown in Figure 3 [5].

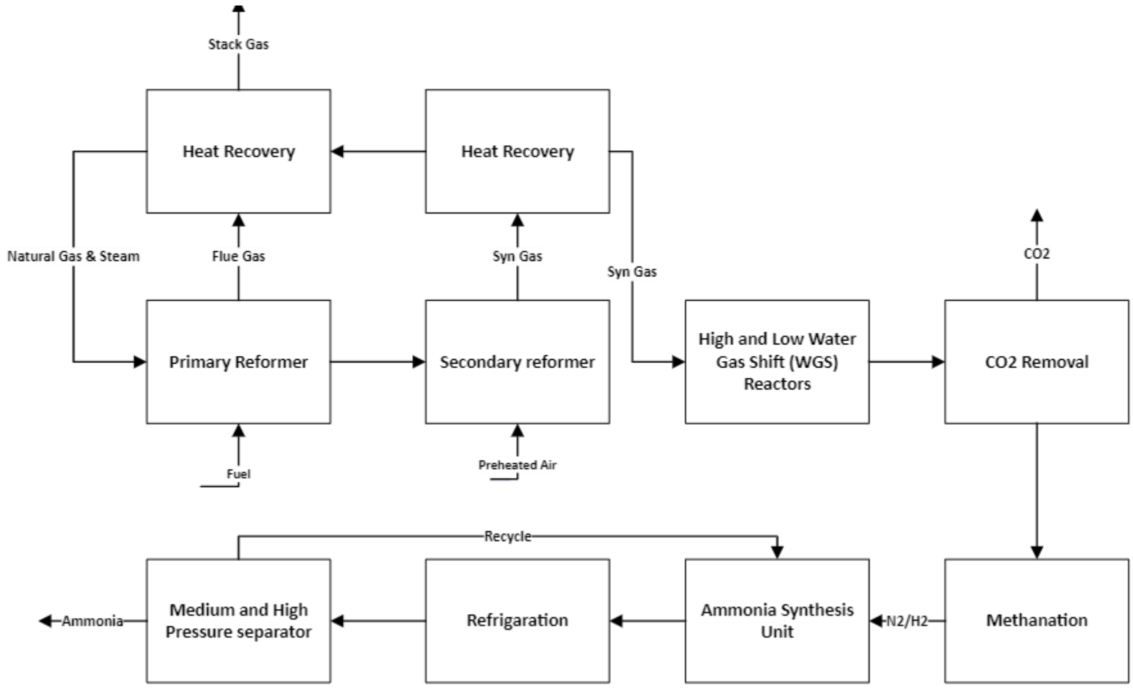

Figure 3: Steam methane reforming (SMR) pathway

2.1.2. Primary Reformer

The primary reformer is a sub-unit of SMR plant, in which a heated steam to carbon ratio is set at 3:1 by mole fraction. The primary reformer is a huge combustion chamber where reaction takes place in its tubes. Since the reactions involved in primary reformer are highly endothermic in nature, they require immense amount of energy to move towards completion. The reactions are shown in Equation 2.2 and 2.3. Natural gas is used to increase the temperature of the chamber depending on the steam to carbon ratio. The energy requirement is met by hydrogen and methane coming from ammonia synthesis purge and methane undergoing combustion on the outside of the vertical pipes supplied by radiation-heated channels. For the above reaction, nickel-based catalyst is used to produce hydrogen (H_2), carbon monoxide (CO) and carbon dioxide (CO_2) from around 66% of initial natural gas supplied [30]. A convection bank is utilized for recycling of produced waste heat for use in later operations. Optimization of fuel consumption is attained by varying steam to carbon ratio such that higher the ratio, lower the operating temperature required [31].

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \qquad 2.2$$

$$CH_4 + 2H_2O \leftrightarrow CO_2 + 4H_2 \qquad 2.3$$

The mixture of natural gas and steam enter the primary reformer at 530°C and the product stream, that is reformed gas leaves at 830°C. It should be ensured that no oxidants leave the primary reformer with reformed gas by regulating the volume of methane. Further, an excess of steam is added in primary reformer to prevent formation of free carbon. The process is made environmentally friendly by cooling down the flue gases to 200°C before releasing them in the atmosphere so they may not be harmful.

2.1.3. Secondary Reformer

The amount of air to be added is adjusted to attain H_2/N_2 ratio of 3:1 in the compressor. The air, being used as the nitrogen source is compressed from atmospheric pressure to the pressure of process gas. The compressor is assumed to be purely adiabatic having 75% efficiency. The air is then mixed with reformed gas from primary reformer and enters into the secondary reformer. The reactants in secondary reformer burns to produce an endothermic reaction. Almost all the methane in raw material is adiabatically converted passing through the catalytic reformers whereas, only low concentration of approximately 0.6% left unreacted. The process gas leaves the secondary reformer at high temperature thus, it is cooled before entering shift reactors [32]. The chemical reaction equations involved in secondary reformer are:

$$CH_4 + 0.5O_2 \leftrightarrow CO + 2H_2 \qquad 2.4$$

$$CH_4 + 2H_2O \leftrightarrow CO_2 + 4H_2 \qquad 2.5$$

2.1.4. Water Gas Shift Reactors

In water gas shift reactors (WGS), the CO produced back in primary secondary reformer reacts with steam to produce hydrogen over a catalyst. The reaction involved is exothermic. Conventionally, WGS reactors are primarily used to convert CO into a form that can be easily removed from atmosphere. The supply of adequate amount of water is essential to terminate Boudouard reaction with the help of Fischer-Tropsh catalysts. The WGS reactors are of two types comprising of high temperature shift (HTS) and low temperature shift (LTS) reactors. The reformers must meet the requirements of HTS that is at least S/C ratio of 3. The reaction occurring inside HTS reaction is:

$$CO + H_2O \leftrightarrow H_2 + CO_2 \qquad 2.6$$

Around 2% of less of CO_2 is obtained at the outlet stream of HTS reactor therefore, LTS reactor should convert the remaining CO to synthesis gas. The gas leaving the WGS reactor goes for purification where H_2O and CO_2 are separated [33]. The reaction inside LTS reactor is given by Equation:

$$CO + H_2O \leftrightarrow H_2 + CO_2 \qquad 2.7$$

2.1.5. Methanation Reaction

Methanation is commonly used for lowering carbon contents. The hydrogen-nitrogen-rich gas from WGS reactors is brought in to methanation reactor, where methane is produced over a nickel-alumina catalyst from traces of carbon oxides. The methanation reaction consumes the produced hydrogen but it is mandatory to prevent otherwise, poisoning of Haber-Bosch Catalyst for ammonia synthesis. The exothermic process taking place in methanation reactor is simultaneously used to recover energy and recycle it back into the system [34]. The chemical reaction equation is as follows:

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O \qquad 2.8$$

2.1.6. Ammonia Synthesis Reactor

The ammonia production only takes place in the last stage of the reactions. In order to create ammonia, the produced gas is compressed and transported to a three-bed quench reactor. Before the essential synthesis temperature is attained, preheating and elevating the synthesis gas pressure to 15–25 MPa needs to be carried out. The major component of the synthesis process is the reactor where NH_3 is produced. The performance of the converter as a whole is influenced by its operational settings and response rate. Owing to the positive equilibrium reaction and the reaction rate itself, the ammonia yield increases rapidly when the pressure is increased. In modern ammonia manufacturing plants, the synthesis pressure ranges from 15,000 to 25,000 kPa. Furthermore, keeping the required temperature is essential because the speed of synthesis process fluctuates significantly as the temperature shifts. Together with the above-mentioned elements, the feed stream speed and the H_2/N_2 ratio in the entering synthesis gas have an effect on the reactor's performance. The highest conversion rate is observed at high space velocity and by keeping the H_2/N_2 ratio at 2 [35, 36]. The famous Haber-Bosch ammonia synthesis reaction equation is:

$$N_2 + 3H_2 \leftrightarrow 2NH_3 \qquad 2.9$$

2.1.7. Refrigeration and Ammonia Separation

After the reaction takes place, the gas leaving the reactor contains ammonia, unreacted nitrogen and hydrogen, as well as other by-products and impurities. The gas stream, undergoes a series of separation and purification steps to isolate and concentrate the ammonia product. These steps involve multiple stages of cooling, condensation, and absorption to recover ammonia from the reaction mixture. Ammonia is then chilled in a refrigeration system to liquefy the ammonia by using high-pressure separator. At the same time, the unconverted gaseous feed is separated and recycled. Finally, the liquid product, which is high in ammonia, is flashed in a medium pressure separator to remove purge gases. The purified ammonia condensed to a liquid state, stored in appropriate containers, and then distributed for various applications.

2.2. Natural Gas as a Feedstock

2.2.1. Introduction

Natural gas, a versatile and abundant fossil fuel, plays a multifaceted role in the global energy landscape, serving not only as a primary source of clean-burning energy but also as a valuable feedstock for various industrial processes. With its diverse applications and contributions to economic growth and technological advancement, natural gas has emerged as a cornerstone of modern industrial development.

Natural gas primarily consists of methane (CH_4), a simple hydrocarbon compound composed of one carbon atom bonded to four hydrogen atoms. While methane is the predominant component, natural gas can also contain varying amounts of other hydrocarbons, such as ethane, propane, and butane, as well as trace amounts of nonhydrocarbon gases like nitrogen, carbon dioxide, and hydrogen sulfide. The composition can vary based on the source and geological conditions.

Natural gas is formed through the decomposition of organic matter over millions of years, typically in underground rock formations. It can be found alongside crude oil reserves or in dedicated natural gas fields. Technological advancements in exploration, drilling, and extraction techniques have greatly expanded our ability to locate and recover natural gas reserves, contributing to its status as a globally accessible resource [37, 38].

2.2.2. Energy Resource and Environmental Benefits

Natural gas is renowned for its clean-burning characteristics, emitting significantly fewer pollutants and greenhouse gases compared to other fossil fuels such as coal and oil. When combusted, natural gas releases primarily carbon dioxide (CO_2) and water vapor, minimizing the emission of particulates, sulfur dioxide (SO_2), and nitrogen oxides (NO_x) that contribute to air pollution and climate change.

In recent years, natural gas has played a pivotal role in transitioning toward a lower-carbon energy mix. It has been widely used to replace coal in electricity generation, reducing carbon emissions and improving air quality. Natural gas power plants offer flexibility, allowing for quick ramp-up and response to changing energy demand, making them an ideal complement to intermittent renewable energy sources like wind and solar [39].

2.2.3. As a Feedstock for SMR Process

Beyond its role in energy production, natural gas has gained prominence as a crucial feedstock for numerous industrial processes. One of the most significant applications is in the production of hydrogen, used in ammonia synthesis. About 70% of global ammonia production is dependent on SMR pathway using natural gas as its feedstock. Natural gas is considered as the best suitable raw material for the ammonia production plant especially due to its low energy consumption and minimal levels of CO_2 emissions in comparison to other energy sources available. China varies drastically in its choice of energy sources for ammonia plant with rest of the world as coal and fuel oil dominates as major feedstocks [40].

The comparison of all the energy sources for steam methane reforming and partial oxidation methods is shown in Table 1.

Table 1: Energy consumption and CO_2 emissions by various pathways

Energy Source	**Process**	**Energy Consumption (GJ/t NH_3)**	**CO_2 Emissions (Tonnes/t NH_3)**
Natural Gas	SMR	28	1.6
Naphtha	SMR	35	2.5
Heavy Fuel Oil	Partial Oxidation	38	3.0
Coal	Partial Oxidation	42	3.8

Natural gas is also knowns as a preferable feedstock owing to its low cost and wide availability. As most of the current plants operate on natural gas, it must be purified before utilisation in manufacturing plant. Hence, several patents have been issued on purification processes of raw natural gas setting the standard adsorption characteristics of gases occupying acceptable range of raw composition [32].

2.2.4. Economic Impacts and Future Prospects

The availability and affordability of natural gas have driven economic growth and industrial competitiveness in regions with abundant reserves. It has facilitated the expansion of energy-intensive industries, spurring innovation, job creation, and increased exports of value-added products. Additionally, natural gas liquefaction and transportation technologies have enabled the global trade of liquefied natural gas (LNG), enhancing energy security and diversification for importing countries.

Looking forward, natural gas is poised to play a role in the transition to more sustainable energy systems. As technologies for carbon capture and utilization (CCU) and hydrogen production continue to advance, natural gas can contribute to the development of greener fuels and materials, further reducing emissions and environmental impact.

In conclusion, natural gas stands as a versatile and indispensable feedstock that fuels industrial progress, energy security, and environmental responsibility. Its contributions to energy generation, chemical manufacturing, and innovative technologies underscore its significance in shaping a sustainable and prosperous future. As the world seeks to balance energy needs with environmental considerations, the responsible utilization of natural gas as a feedstock will continue to be a pivotal factor in achieving a cleaner and more resilient global economy [41].

2.3. Simulation and Optimization Techniques

Process simulation stands as the foundational pillar of this thesis, enabling the creation of a virtual replica of the ammonia production process. Advanced simulation software, such as Aspen HYSYS, provides a dynamic and steady-state platform to capture the myriad interactions, reactions, and transformations inherent in ammonia synthesis from natural gas. By integrating thermodynamics, kinetics, and transport phenomena, this simulation elucidates the process's behaviour under varying conditions. This virtual playground becomes a testing ground for experimentation, enabling the exploration of diverse scenarios and illuminating how changes impact ammonia yield, energy consumption, and other critical factors.

The complete process flow diagram using steam methane reforming (SMR) was created on Aspen HYSYS V11. Aspen HYSYS is typically used for processes in the energy sector, but it has been developed to simulate a variety of industries, including oil refineries, the sweetening of acid gases with DEA, heavy chemical and petrochemical plants, the treatment of natural gas, the oil and gas sector etc.

Exact thermodynamic and physical property forecasts for chemical fluids, petrochemicals, non-hydrocarbons, and hydrocarbons can be seen in the HYSYS property package. The HYSYS database has a large number of components exactly more than 1500 components and over 16000 fitted binary coefficients and when the database is empty, hypothetical components are generated [16].

Ammonia synthesis is an extremely energy-intensive process; the steam reforming process uses roughly 28–35 GJ of energy per tonne of ammonia. Theoretical, actual, and operational energy efficiencies for processes following steam reforming pathway for ammonia plants are shown in Figure 4. Due to feedstock, energy prices, and utility restrictions, ammonia plants that are currently in operation have a wide range of energy efficiency. The majority of plants consume far more energy than it is necessary, with the top performances averaging to 37 GJ/tonne of ammonia. or falling between a range of 28-33 GJ/tonne of ammonia. Energy usage could decline by 20–25% if all plants in the world were to operate at the optimum levels of efficiency. Currently, focus has been brought to regular assessments for improvements, and then revamp ideas that increase efficiency can be put into practice [42].

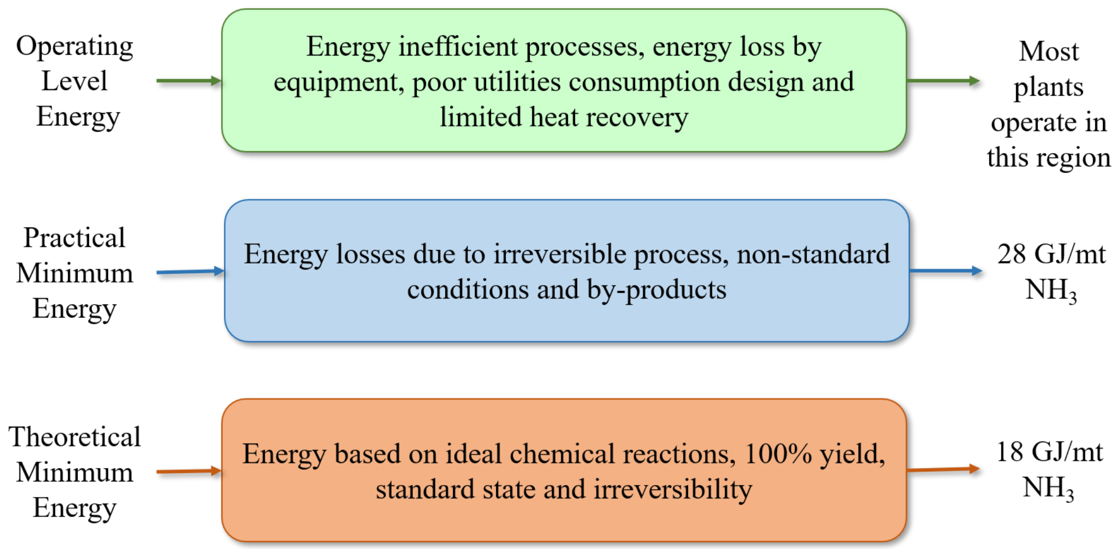

Figure 4: Energy efficiencies of process plants

Hence, this thesis firstly simulates ammonia production from steam methane reforming method on Aspen HYSYS. Then, to optimize the process pinch technology is applied to reduce the cost and energy consumption. The economic analysis of the modelled plant was done by Aspen Economic Analyzer whereas the cost of the fired heater was obtained from the vendor due to aspen limitations and pinch was applied on the Aspen Energy Analyzer which shows optimal use of the utilities to reduce the cost of the plant annually [43].

By utilizing Aspen Energy Analyzer, an understanding of the complex interplay of heat exchange, unveiling the optimal orchestration of temperature differentials among process streams is developed. Pinch Analysis not only delineates the vital boundary known as the

"Pinch Point," where heat integration is maximized, but also unveils the intricate ballet of heat recovery and distribution. This optimization paradigm resonates deeply with the goals of resource conservation and sustainability, resulting in minimized utility requirements, elevated energy efficiency, and reduced environmental impact. Ultimately, Pinch Analysis shines as a pivotal technique, imbued with the power to transform the ammonia production process into a symphony of energy conservation and operational excellence, aligning seamlessly with the thesis's core objectives.

2.4. Cost Analysis of Ammonia Production

Cost analysis is a critical facet of the ammonia production process, exerting a profound influence on industrial decision-making and economic viability. The meticulous assessment of costs encompasses a multitude of intricacies, ranging from raw material procurement and energy consumption to capital investments and operational expenditures. An exhaustive cost analysis not only provides a comprehensive understanding of the financial implications of ammonia production but also provides strategic choices for optimizing resource allocation, process efficiency, and profitability. Through the lens of cost analysis, the interplay of economic factors becomes discernible, allowing stakeholders to weigh the trade-offs between various operational parameters, technological advancements, and environmental considerations. This evaluative framework empowers industry leaders and policymakers to make informed decisions that balance the imperatives of sustainable production, competitive pricing, and financial resilience, fostering a dynamic synergy between economic prudence and technological innovation.

In the contemporary landscape of evolving energy markets, stringent environmental regulations, and shifting consumer demands, the significance of cost analysis within ammonia production is magnified. The judicious application of advanced tools and methodologies, such as Aspen Economic Analyzer, enables a granular examination of cost structures, unravelling the intricate web of fixed and variable expenses associated with the entire production lifecycle. Aspen economic analyser is coupled with Microsoft Excel to obtain total production cost, total income, net profit and many other desirable cost variables briefly discussed in Chapter 3.

Furthermore, cost analysis extends beyond immediate financial considerations, enabling the anticipation of future trends, market dynamics, and investment risks. This forward-looking perspective empowers stakeholders to proactively adapt to changing economic landscapes, seize emerging opportunities, and fortify their competitive edge. Ultimately, cost analysis serves as a compass that navigates the journey of ammonia production, guiding the trajectory towards optimal resource allocation, operational excellence, and sustainable growth in a dynamic and ever-evolving industrial panorama.

Chapter 3

Methodology

3.1. Simulation Model Development

3.1.1. Selection of Simulation Software

Aspen HYSYS is a powerful process simulation software widely used in the engineering and chemical industries to model, optimize, and analyse various processes. It provides engineers and researchers with a comprehensive platform to design, simulate, and troubleshoot complex systems in the oil, gas, petrochemical, pharmaceutical, and other process-related sectors.

With Aspen HYSYS, users can create detailed process models that replicate real-world operations, allowing them to evaluate the behaviour of diverse processes under different conditions. The software facilitates the simulation of unit operations, mass and energy balances, fluid flow, heat transfer, and chemical reactions, among other critical aspects of process engineering. Aspen HYSYS's user-friendly interface and robust capabilities enable engineers to improve process efficiency, optimize resource utilization, and minimize environmental impact, contributing to safer and more sustainable industrial practices. Its extensive library of components and thermodynamic models allows for accurate representation of a wide range of substances and operating conditions.

In Aspen HYSYS, economic evaluation is an essential step in the process design and optimization workflow. Economic evaluations help engineers and decision-makers assess the financial viability of a process and make informed choices about equipment selection, operating conditions, and overall plant design. This evaluation is typically done using the Economic Evaluation (ECON) feature in Aspen HYSYS.

The economic evaluation in Aspen HYSYS involves the following key components:

- Cost Estimation: Aspen HYSYS allows users to input equipment costs, raw material costs, labour costs, utilities costs, and other expenses associated with the process.

These costs can be estimated based on industry-standard data or specific vendor quotations.

- Profitability Analysis: By integrating process simulation results with economic data, Aspen HYSYS can calculate the profitability of the process. This includes estimating revenue from product sales, taking into account product prices and production rates.
- Sensitivity Analysis: Engineers can perform sensitivity analyses to evaluate how changes in key variables (e.g., feedstock prices, product prices, energy costs) impact the overall economic performance of the process.
- Cost Optimization: Aspen HYSYS can be used to optimize the process design by finding the most economical operating conditions and equipment configurations while still meeting the desired process objectives.
- Net Present Value (NPV) and Internal Rate of Return (IRR): Aspen HYSYS can calculate financial metrics such as NPV and IRR, which are critical indicators of a project's economic viability and potential profitability over time.
- Energy Integration: Aspen HYSYS allows for the integration of process streams and utility systems, enabling engineers to explore opportunities for energy optimization and energy cost reduction.
- Feasibility Studies: Engineers can use Aspen HYSYS to compare multiple process configurations or technologies, enabling them to select the most economically attractive option.

By conducting economic evaluations in Aspen HYSYS, engineers can make well-informed decisions, identify potential bottlenecks or cost-saving opportunities, and optimize their process designs to achieve the best balance between technical feasibility and economic viability. This approach ensures that projects are economically sound and align with the overall strategic goals of the organization.

3.1.2. Assumption and Data Inputs

The assumptions considered in this thesis as follows:

- Pure methane (43920 Kg/hr) was the feed stock for the ammonia synthesis
- Natural gas for a feed stream is sulphur free hence sulphur removal is neglected.

- Ionization and filtration of water is neglected for steam production.
- Air for secondary reformer contains 78% nitrogen and 21% oxygen.
- All the reactors are modelled as Plug flow reactor.
- Both the steam reformer and secondary reformer were considered to contain all linearly independent reactions discovered in the atom-species matrix of the current reactants and the products carbon monoxide, carbon dioxide, and hydrogen.
- The production of ammonia and by products like methanol were neglected in the water-gas shift reactors since it was thought that the water-gas shift reaction was the only actual reaction that took place.
- The methanation of carbon monoxide and carbon dioxide was considered to be among the only reactions included in the reaction set in the methanation reactor.
- It was supposed that the only reaction occurring in the synthesis reactor is the generation of ammonia from hydrogen and nitrogen.
- Although the method of carbon dioxide absorption is not specified, splitters are used to completely separate carbon dioxide.
- All heat exchangers were modelled as heaters and coolers.
- Simulation is done on steady state mode of the HYSYS.
- All compressors efficiencies were assumed 75%
- All the condition (temperature, pressure and flow rates) are taken from the literature.
- Cost of the fired heater was taken from the literature due to HYSYS limitation. Whereas rest of the equipment cost were taken from Aspen economics analyser.
- The heaters and coolers were assumed to be U-tube shell and tube exchangers.

The inlet stream data and conditions were taken from literature as shown in Table 2. The data input is kept close to real world production plant to simulate the model on real-design basis. The details of all other streams involved in the process flow diagram are shown in appendix.

Table 2: Thermodynamic details of inlet streams

Stream name	Temperature (°C)	Pressure (bar-g)	Flow rate (Kg/hr)
Natural Gas	6	70	43920
Water	30	1	140400
Air	25	1	100080.

The reaction kinetics involved in the reactors for all the reactions involved in the process flow diagram are given below in the Table 3.

Table 3: Reaction kinetics of all reactions involved in ammonia synthesis process

Reactor	Configuration	Reaction	A	E (kJ/kmol)	Ref
Primary Reformer	PFR-100	$CH_4 + H_2O \leftrightarrow CO + 3H_2$	5.75×10^{12}	67130	[44]
		$CH_4 + 2H_2O \leftrightarrow CO_2 + 4H_2$	7.24×10^{10}	204000	
Secondary reformer	PFR-101	$CH_4 + 2H_2O \leftrightarrow CO_2 + 4H_2$	7.24×10^{10}	204000	[44]
		$CH_4 + 0.5O_2 \leftrightarrow CO + 2H_2$	8.11×10^{5}	86000	[45]
High temperature shift converter	PFR-102	$CO + H_2O \leftrightarrow H_2 + CO_2$	1.26×10^{-2}	4639	[44]
Low temperature shift converter	PFR-103	$CO + H_2O \leftrightarrow H_2 + CO_2$	1.26×10^{-2}	4639	[44]
Methanation Reactor	PFR-104	$CO + 3H_2 \leftrightarrow CH_4 + H_2O$	10266.76	26830	[46]
Ammonia synthesis	PFR-105	$N_2 + 3H_2 \leftrightarrow 2NH_3$	8.849×10^{14}	40765	[47]

3.1.3. Process Flow Diagram

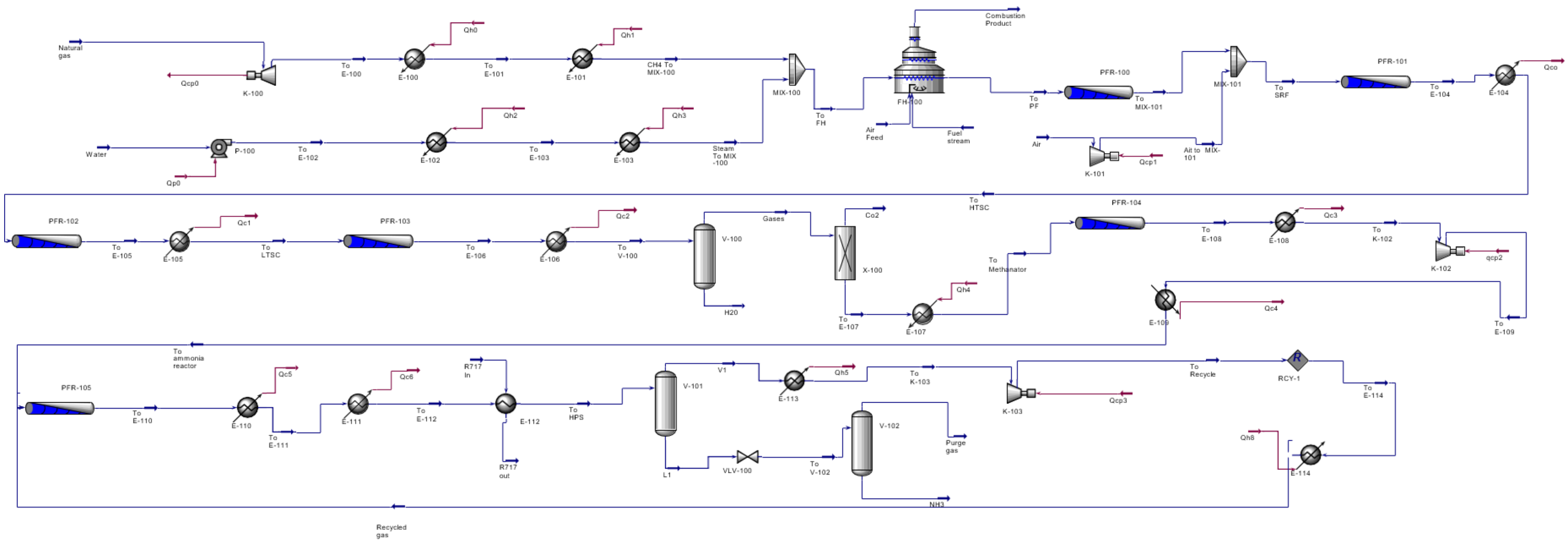

Figure 5: Process flow diagram (PFD) of ammonia production plant

3.2. Optimization Techniques

3.2.3. Selection of Optimization Algorithm:

The ammonia synthesis process is an energy intensive process hence, even small heat recovery results in significant amount of energy savings. Lately, some major developments have been done that would impact the way ammonia was conventionally produced. These methods are in trial mood for now and yet to be fully developed to implement on commercial scale. The improvements involve reformer combustion air preheat, control of steam to carbon ratio, hydrogen to be recovered from purge gas, improved system for removal of CO_2 [48, 49]. Further researches have been conducted on process optimization, HAZOP and safety, enhanced control, efficient catalysts and heat integration [50-55]. Pinch technology is an energy efficient method that point potential solution to a process plant by properly understanding the complex relation between process streams and utility streams. It is a technique that maximizes utilization of internal utilities and reduces consumption of external utilities thus, lowering energy consumption of the overall process plant and optimizing it [56]. Figure 6 shows the steps involved in pinch analysis.

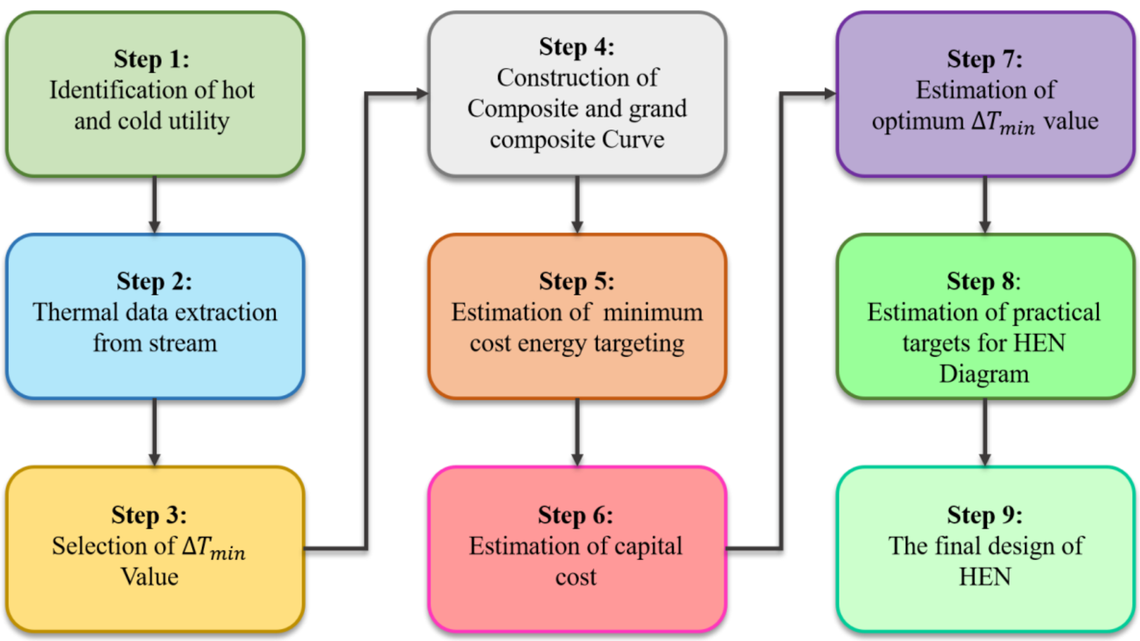

Figure 6: Steps involved in pinch analysis

The first step is identification of hot and cold streams to find the number of hot and cold utilities required. Once, the streams are identified, then their heat duty can be found from thermal data of the concerning stream. The next step is the selection of ΔT_{min} which is followed by construction of composite curves and grand composite curves. Then, the energy cost, capital cost of heat exchangers and utility cost of the overall process is determined. Finally, the optimum ΔT_{min} is calculated and heat exchanger network (HEN) diagram is drawn from where, a retrofit deign is obtained.

3.2.4. Design of Experiment

The design of experiment offers a systematic framework to uncover optimal energy integration strategies and heat exchange networks, enhancing efficiency and resource utilization. It consists of several tailored steps:

3.2.4.1.Factors and Levels Identification

Identify key factors that influence energy utilization and heat exchange within the ammonia production process. These may encompass parameters such as process stream temperatures, flow rates, and heat transfer surfaces. Define levels for each factor, capturing the feasible range of values that warrant investigation. For instance, temperatures may span from minimum to maximum allowable limits.

3.2.4.2.Experimental Matrix Design

Construct an experimental matrix aligning with the principles of Pinch Analysis. Employ techniques like systematic sampling or factorial design to explore diverse combinations of factors and levels while adhering to the constraints imposed by the Pinch Point. The matrix guides the execution of experiments, which involve adjustments to process variables to explore energy integration possibilities.

3.2.4.3.Data Collection and Analysis

Execute the designed experiments within the established Pinch Analysis framework. Collect data on energy consumption, heat transfer, and heat exchanger performance for each trial. Employ statistical tools and specialized software to analyse the data, unravelling trends, and relationships between process variables and energy utilization. This analysis provides insights into the optimal configuration of heat exchange networks and energy flows.

3.2.4.4.Model Development and Optimization

Develop predictive models that capture the intricate interactions between process variables and energy utilization. These models aid in forecasting optimal energy integration strategies within the constraints of the Pinch Point. Utilize optimization techniques compatible with Pinch Analysis, such as Composite Curves and Grand Composite Curves, to identify the point of optimal energy recovery and minimum utility requirements.

3.2.4.5.Validation of The Model

Validate the optimized energy integration strategies by applying them within the actual ammonia production process. Assess the robustness of the results by subjecting the system to variations and perturbations.

The integration of these methodologies empowers the exploration of innovative energy integration strategies that enhance process efficiency, mitigate energy wastage, and contribute to the overarching objectives of the thesis.

3.3. Optimization of Ammonia Process

For optimization of ammonia production process from natural gas, pinch analysis is applied. The first step in pinch analysis is to identify process streams hence the details of heat exchangers involved in process flow diagram along with its inlet and outlet conditions to cover step 2 that is thermal data extraction are given in Table 4.

Table 4: Details of heat exchangers in simulation model of ammonia synthesis

Heat Exchanger	**Type**	**Duty kJ/hr**	**Hot Side Temperatures (^{0}C)**		**Cold Side Temperatures (^{0}C)**	
			Inlet	**Outlet**	**Inlet**	**Outlet**
E-100	Heater	2.62×10^7	250	249	-33.6	194.4
E-101	Heater	2.26×10^7	1000	400	194.4	360
E-102	Heater	8.28×10^7	175	174	30.3	163.7
E-103	Heater	3.42×10^8	1000	400	163.7	360
E-107	Heater	1.11×10^8	1000	400	40	300
E-112	Heater	5.31×10^8	30.1	-5	-33	-18.5
E-113	Heater	3.05×10^8	125	124	-5	20
E-114	Heater	2.86×10^9	280	250	32	270
FH-100	Cooler	8.60×10^8	2000	900	355.3	1746.5
E-104	Cooler	2.74×10^8	775.4	355	249	250
E-105	Cooler	1.94×10^8	505.5	205	174	175
E-106	Cooler	2.06×10^8	213.4	40	20	25
E-108	Cooler	1.12×10^8	320	55	30	35
E-109	Cooler	4.59×10^7	375.5	270	249	250
E-110	Cooler	2.19×10^9	293	115.1	30	35
E-111	Cooler	1.05×10^9	115.1	30.1	20	25

A constant ΔT_{min} of 10°C was opted for this model. The composite curves are then, drawn to understand multiple streams, all the streams over various temperature intervals are added together on the basis of their heat loads. This results in a single composite curve for hot streams and another for cold streams. The composite curves are drawn as temperature-enthalpy (T/H) diagram. These curves help in complete understanding of total energy available and amount of energy that can be recovered in the process. The overlap between the composite curves represents maximum heat recovery. Whereas, the overshoot describes the minimum amount of external utility required either hot or cold in cold and hot composite curves respectively [57]. The composite curve of ammonia synthesis unit modelled in HYSYS is shown in Figure 7. In the following figure, red line shows hot composite curve and blue represents cold composite curve.

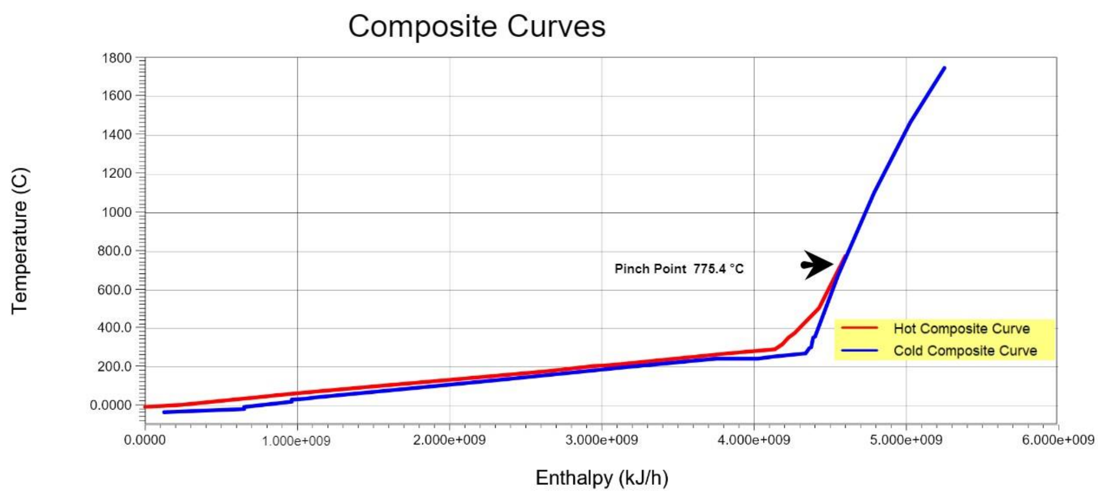

Figure 7: Hot and cold composite curves of ammonia simulation model

The grand composite curve (GCC) is a graphical plot of heat cascade table. It is drawn between net heat flow and shifted temperatures. It builds a relation that shows the amount of heat available due to hot streams and required amount from cold streams relative to the pinch at given shifted temperatures in the process flow diagram [57]. The grand composite curve is shown in Figure 8.

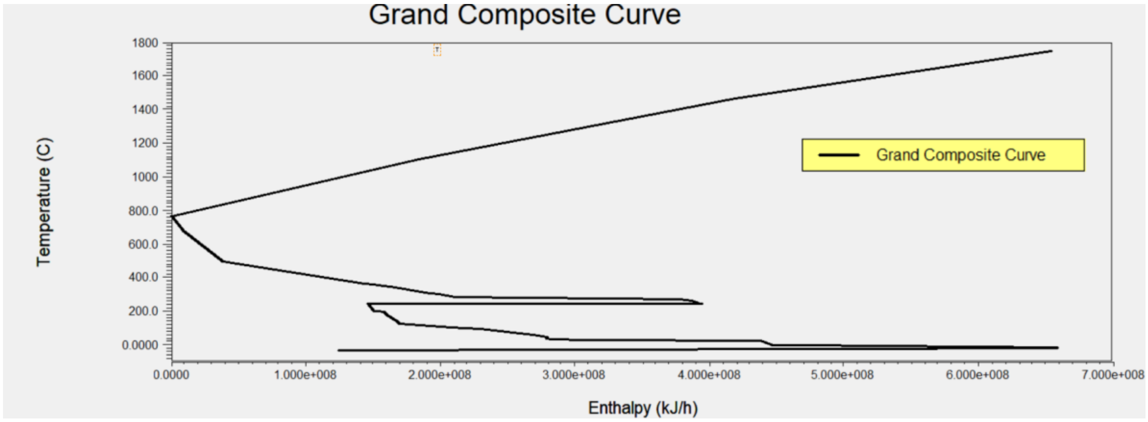

Figure 8: Grand composite curve (GCC) of ammonia simulation model

Hence, concluding the pinch analysis applied by Aspen Energy Analyzer. The heat exchanger network (HEN) diagram of the simulated ammonia model is shown in Figure 9. The analyser calculates pinch temperature for hot and cold streams as 775.4°C and 765.4°C respectively. Table 5 shows the summary of utilities used for pinch analysis with thermal data.

Table 5: Details of utilities involved in overall process plant

Utility stream	**Temperature (°C)**		**Heat Load Designed (kJ/hr**
	Inlet	**Outlet**	
LP Steam	125	124	3.05×10^8
Fired Heat (2000)	2000	900	8.60×10^8
HP Steam	250	249	2.62×10^7
Fired Heat (1000)	1000	400	4.75×10^8
MP Steam	175	174	8.28×10^7
Hot Oil	280	250	2.86×10^9
Total Hot Utilities			$\mathbf{4.60 \times 10^9}$
MP Steam Generation	174	175	1.94×10^8
Cooling Water	20	25	1.26×10^9
HP Steam Generation	249	250	3.20×10^8
Air	30	35	2.30×10^9
Total Cold Utilities			$\mathbf{4.07 \times 10^9}$

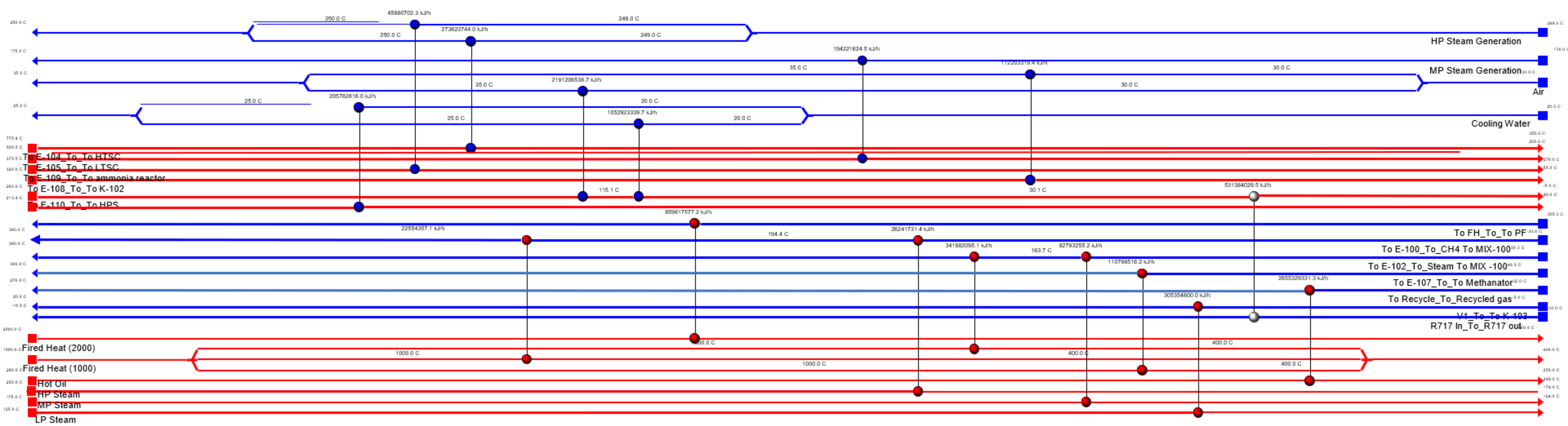

Figure 9: Pinch analysis by AEA on simulation model of ammonia synthesis (base case)

The Process and utilities streams used in HEN diagram for the ammonia process are depicted below in Table 6. It briefly explains the heat load requirements of process stream and the corresponding utilities stream that satisfies it demand.

Table 6: Process streams data for pinch analysis (base case)

Sr No.	Process Stream Name	Stream Type	Temperature (°C)		Heat Load Required (kJ/hr)
			Inlet	Outlet	
1	To E-104_to_To HTSC	Hot	775.4	355	2.74×10^8
2	To E-105_to_To LTSC	Hot	505.4	205	1.94×10^8
3	To E-109_to_To ammonia reactor	Hot	375.5	270	4.59×10^7
4	To E-108_to_To K-102	Hot	320	55	1.12×10^8
5	To E-110_to_To HPS	Hot	293	-5	3.78×10^9
6	To E-106_to_To V-100	Hot	213.4	40	2.06×10^8
7	To FH_to_ To PF	Cold	355.3	1746.5	8.60×10^8
8	To E-100_to_CH4 To Mix-100	Cold	-33.6	360	4.88×10^7
9	To E-102_to_Steam To Mix-100	Cold	30.3	360	4.25×10^8
10	To E-107_to_To Methanator	Cold	40	300	1.11×10^8
11	To Recycle_to_Recycle Gas	Cold	32	270	2.86×10^9
12	V1_to_K-103	Cold	-5	20	3.05×10^8
13	R717 In_to_R717 Out	Cold	-33	-18.5	5.31×10^8

Table 7 shows the utilities meeting the demands of heat exchanger for proper design leading to negligible heat losses to mimic theoretical energy efficiency as far as possible.

Table 7:Details of heat load exchange between process and utility streams for pinch analysis (base case)

Sr No.	Stream Name	Utility Streams	Satisfied Heat Load
1	To E-104_to_To HTSC	HP Steam Generation	2.74×10^8
2	To E-105_to_To LTSC	MP Steam Generation	1.94×10^8
3	To E-109_to_To ammonia reactor	HP Steam Generation	4.58×10^7
4	To E-108_to_To K-102	Air	1.12×10^8
5	To E-110_to_To HPS	Air	2.19×10^9
		Cooling Water	1.05×10^9
		R717 In_to_R717 Out	5.31×10^8
		Total	$\mathbf{3.78 \times 10^9}$
6	To E-106_to_To V-100	Cooling Water	2.05×10^8
7	To FH_to_ To PF	Fired Heat (2000)	8.59×10^8
8	To E-100_to_CH4 To Mix-100	Fired Heat (1000)	2.25×10^7
		HP Steam	2.62×10^7
		Total	$\mathbf{4.87 \times 10^7}$
9	To E-102_to_Steam To Mix-100	MP Steam	8.27×10^7
		Fired Heat (1000)	3.41×10^8

		Total	$\mathbf{4.25 \times 10^8}$
10	To E-107_to_To Methanator	Fired Heat (1000)	1.10×10^8
11	To Recycle_to_Recycle Gas	Hot Oil	2.85×10^9
12	V1_to_K-103	LP Steam	3.05×10^8
13	R717 In_to_R717 Out	To E-114_to_To HPS	5.31×10^8

3.4. Design of the Optimized Model

The above discussion gave detailed insights of pinch analysis hence, making it feasible to enter retrofit design. Aspen Energy Analyzer not only give the HEN diagram for the base case that is the simulated case but it also gives some improvements to make in the plant for a retrofit design. It suggests weather to add, modify or relocate a heat exchanger so that energy savings can be increased. In our case, we can save 1.91% more energy by adding another heat exchanger of cost 4,90,184 USD which reduces the cost of utilities by 1,753,784 USD/year and the payback period to 0.2797 years. The suggested scenario is shown in Figure 10.

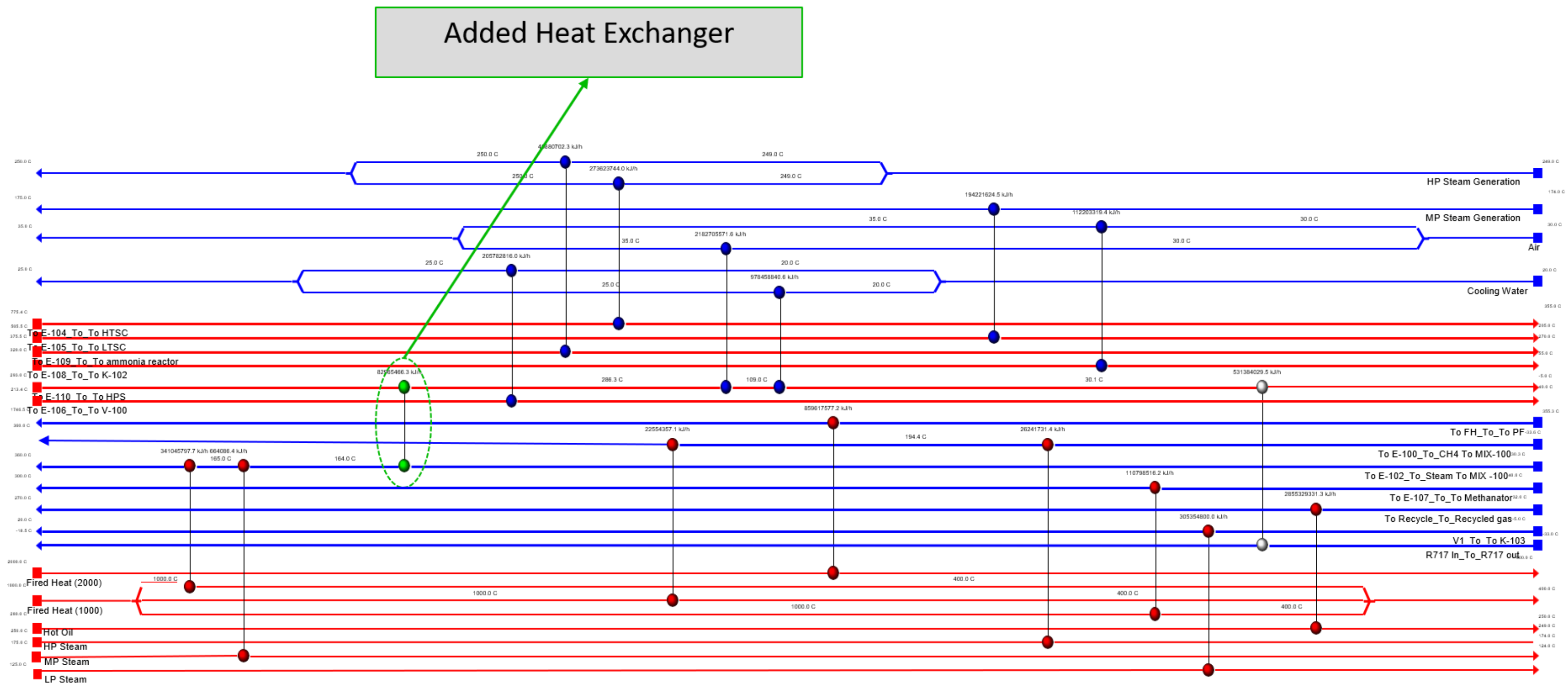

Figure 10: Pinch analysis by AEA on proposed retrofit design for ammonia simulation model (proposed scenario)

The proposed retrofit design reduces utilities consumption by 1.5% owning to addition of another heat exchanger thus, minimizing external utility demand and satisfying the heat load with already present energy source in the plant otherwise eliminating as waste heat. The heat exchanger is added between two process streams viz. To E-110_to_To HPS and To E-102_to_Steam To Mix-100. The utility details of the proposed scenario are given below in Table 8 and its process stream data is listed in Table 9. Table 10 explains energy exchange between process and utility streams.

Table 8: Details of utilities involved in proposed scenario

Utility stream	**Temperature (°C)**		Heat Load
	Inlet	**Outlet**	**Designed (kJ/hr**
LP Steam	125	124	3.05×10^8
Fired Heat (2000)	2000	900	8.60×10^8
HP Steam	250	249	2.62×10^7
Fired Heat (1000)	1000	400	4.75×10^8
MP Steam	175	174	6.64×10^5
Hot Oil	280	250	2.86×10^9
Total Hot Utilities			$\mathbf{4.52 \times 10^9}$
MP Steam Generation	174	175	1.94×10^8
Cooling Water	20	25	1.18×10^9
HP Steam Generation	249	250	3.20×10^8
Air	30	35	2.29×10^9
Total Cold Utilities			$\mathbf{3.99 \times 10^9}$

Table 9: Process stream data for proposed scenario

Sr No.	Stream Name	Stream Type	Temperature (°C)		Heat Load Required (kJ/hr)
			Inlet	Outlet	
1	To E-104_to_To HTSC	Hot	775.4	355	2.74×10^8
2	To E-105_to_To LTSC	Hot	505.4	205	1.94×10^8
3	To E-109_to_To ammonia reactor	Hot	375.5	270	4.59×10^7
4	To E-108_to_To K-102	Hot	320	55	1.12×10^8
5	To E-110_to_To HPS	Hot	293	-5	3.78×10^9
6	To E-106_to_To V-100	Hot	213.4	40	2.06×10^8
7	To FH_to_ To PF	Cold	355.3	1746.5	8.60×10^8
8	To E-100_to_CH4 To Mix-100	Cold	-33.6	360	4.88×10^7
9	To E-102_to_Steam To Mix-100	Cold	30.3	360	4.25×10^8
10	To E-107_to_To Methanator	Cold	40	300	1.11×10^8
11	To Recycle_to_Recycle Gas	Cold	32	270	2.86×10^9
12	V1_to_K-103	Cold	-5	20	3.05×10^8
13	R717 In_to_R717 Out	Cold	-33	-18.5	5.31×10^8

Table 10: Energy exchange between process and utility streams in proposed scenario

Sr No.	Stream Name	Utility Streams	Satisfied Heat Load
1	To E-104_to_To HTSC	HP Steam Generation	2.74×10^8
2	To E-105_to_To LTSC	MP Steam Generation	1.94×10^8
3	To E-109_to_To ammonia reactor	HP Steam Generation	4.58×10^7
4	To E-108_to_To K-102	Air	1.12×10^8
5	To E-110_to_To HPS	Air	2.18×10^9
		Cooling Water	9.78×10^8
		R717 In_to_R717 Out	5.31×10^8
		To E-102_to_Steam to Mix-100	8.29×10^7
		Total	$\mathbf{3.78 \times 10^9}$
6	To E-108_to_To V-100	Cooling Water	2.05×10^8
7	To E-104_to_PF	Fired Heat (2000)	8.59×10^8
8	To E-100_to_CH4 to Mix-100	Fired Heat (1000)	2.25×10^7
		HP Steam	2.62×10^7
		Total	$\mathbf{4.87 \times 10^7}$
9	To E-102_to_Steam to Mix-100	MP Steam	6.65×10^5
		Fired Heat (1000)	3.41×10^8

		To E-114_to_To HPS	8.29×10^{7}
		Total	$\mathbf{4.25 \times 10^{8}}$
10	To E-109_to_To Methanator	Fired Heat (1000)	1.10×10^{8}
11	To Recycle_to_Recycle Gas	Hot Oil	2.86×10^{9}
12	V1_to_K-106	LP Steam	3.05×10^{8}
13	R717 In_to_R717 Out	To E-114_to_To HPS	5.31×10^{8}

3.5. Cost Analysis

The economic analysis is done to estimate the total annual cost, capital cost, utility cost and operating cost of the process. The cost analysis also figures out the total product cost/kg of ammonia. For this analysis, total 365 operation days are taken as basis for a plant in a year that makes 7200 hours of total working period. For cost estimation, Aspen Economic Analyzer was enabled in Aspen HYSYS process simulation model and hence, the cost of utilities and equipment were obtained. The utilities cost was estimated to be 118,571,000 USD/year. Whereas, the total equipment cost sums to 88,393,300 USD/year however, this estimate does not include fired heater due to aspen's limitations of economic analysis. The cost of fired heater was obtained by literature to be added because of being a major unit operation [58]. Hence, the equipment cost adds up to 88,983,300 USD/year. Hence, the equipment cost adds up to 88,983,300 USD/year. The cost summary for equipment is shown in Table 11.

Table 11: Equipment cost summary given by aspen economic analyse

Equipment Name	Cost (USD)	Equipment Name	Cost (USD)
Fired Heater		**Vessels**	
FH-100	590000	V-100	64500
Heat Exchanger		V-101	311600
E-100	36700	V-102	65900
E-101	96300	**Pump**	
E-102	93900	P-100	104400
E-103	1177000	**Reactors**	
E-104	69300	P-100	547300
E-105	297800	P-101	329700
E-106	180900	P-102	3139000
E-107	555300	P-103	629800
E-108	161200	P-104	134900
E-109	139300	P-105	241800
E-110	7776700	**Compressors**	
E-111	14604700	K-100	360200
E-112	4476600	K-101	9899100
E-113	831500	K-102	8250900
E-114	22922100	K-103	1089490
Total		**88983300**	

Total capital investment of the processing plant is the sum of fixed capital investment (FCI) and working capital investment (WCI). The FCI is the sum of Direct and indirect cost which compromises of different operations that are carrying out in the plant. Table 12 shows the operation that are involved in estimating the direct cost which are percentages of purchased equipment cost whereas, Table 13 shows the calculation of indirect cost which are the percentages of total direct cost. FCI is estimated to be **335,182,294.4 $** and WCI that is 15% of FCI calculates to be **50,277,344** $. Hence the total capital investment that is calculated after adding FCI and WCI is **385,459,638$.**

Table 12: Total Direct Cost Estimation

Cost Type	**Value**	**Cost**
Direct Cost		
Purchased equipment	100%	88983300
Installation	40%	35593320
Instrument & Control	15%	13347495
Piping	50%	44491650
Electricity	10%	8898330
Building	15%	13347495
Land	4%	3559332
Service facility	40%	35593320
Yard Improvement	10%	8898330
Insulation cost	8%	7118664
Total Direct Cost	**259,831,236 $/yr**	

Table 13: Total indirect cost estimation

Cost Type	**Value**	**Cost**
Engineering & Supervision	8%	20786498.9
Contractor Fee	3%	7794937.08
Construction Expenses	10%	25983123.6
Contingencies	8%	20786498.9
Total Indirect Cost	**75,351,058.4 $/yr**	

After calculating the FCI the total production cost will be calculated which is the sum of Variable cost, fixed charges and overhead charges. The utility cost of the plant is taken from the Aspen HYSYS that is 118571000 $/yr. Table 14 shows the raw material cost and product selling cost.

Table 14: Cost of raw material and product

Material	**Cost**	**Ref**
Water	0.067 $/tonne	[59]
Natural gas	0.007 $/ft3	[60]
Ammonia	593.94 $/tonne	[61]

Miscellaneous material

Maintenance cost = 7% of FCI Maintenance cost

Maintenance cost = 23462760.61$

Miscellaneous Material = 2346276.061$ (It is 10% of maintenance cost)

3.5.3. Raw Material Cost:

Flow rate of natural gas = 65470 m^3/hr

For 365 days of operating time = 114204.2045 $/yr

Flow rate of water = 140400 Kg/hr

For 365 days of operating time = 82403.568 $/yr

Total cost of raw material = 82403.568 $/yr

Variable Cost

Variable cost = raw material cost + miscellaneous cost + utilities cost

Variable cost = 121113883.8 $

3.5.4. Fixed Operating Cost:

3.5.4.1.Direct production cost = variable cost + fixed cost

Fixed cost is compromises of different operations that are operating on the plant Table 15 show the calculation of fixed cost [59].

Table 15: Direct and annual production cost

Cost Type	Typical values	Calculated Values
Variable Costs		
1.Raw materials	From table	82403.568
Miscellaneous Materials	10 per cent of item 5	2346276.061
Utilities	From Aspen	118571000
Shipping and packaging	Usually negligible	-
Sub Total A		
Fixed Costs		
Maintenance	5-10 percent of FCI	23462760.6
Operating labour	From manning estimates	33518229.4
Laboratory cost	20-23 percent of 6	6703645.89
Supervision	20 per cent of item 6	5027734.42

Plant overhead	50 per cent of item 6	16759114.7
Capital charges	10 per cent of FCI	33518229.4
Insurance	1 per cent of FCI	3351822.94
Local taxes	2 per cent of FCI	6703645.89
Royalties	1 per cent of FCI	3351822.94
Sub Total B		
Direct production Cost = A+B		**253510890.1**
Sales expenses	20-30 per cent of Direct production cost	76053267.04
General overheads		
Research and Development		
Sub-total C		
Annual production Cost = A+B+C		**329564157.2**
Production Cost = $\frac{Annual\ production\ cost}{Annual\ production\ rate}$		

Direct production cost = 8835760+2325223

Direct production cost = 11160983 $

Direct production cost = 8835760+2325223

Direct production cost = 11160983 $

3.5.4.2.Overhead Charges:

30% of direct production cost

Overhead charges = 0.3 *253510890.1= 76053267.04 $

Annual production cost = 329564157.2 $/year

3.5.4.3.Production Cost:

Production cost = Annual production cost / Annual production rate

Annual Production rate = 93807kg/hr

Total Production Cost = 329564157.2 $/yr

Ammonia Production Rate = 93807 * 8760 = 821749320 kg/yr

Production Cost = Total Production Rate / Ammonia Production Rate

Production cost =0.4010 $/kg

3.5.5. Profitability Analysis:

3.5.5.1.Selling Price:

Selling price of product = 0.59394 $/kg

3.5.5.2.Profit:

Profit = Selling price - production cost

Profit = 0.13834 $/Kg

Profit = 138.3480622 $/ton

Total Production per year = 821749320 kg/year

Profit per year = 113687426 $/year

3.5.5.3.Total Income:

Selling Price = 0.5394 $/kg

Total Production per year = 821749320 kg/year

Total Income = 443251583.2 $/year

3.5.5.4.Gross Profit:

Gross Profit = Total Income - Total Production Cost

Gross Profit = 443251583.2 - 329564157.2

Gross Profit = 113687426 $/year

3.5.5.5.Net Profit:

Let the tax rate is 30%

Taxes = 0.3*Gross Profit =34106227.81 $/year

3.5.6. Depreciation:

Assume that the Fixed Capital Investment depreciate by straight line method for 20 years. Assuming 1 % Salvage value at the end of plant life

Depreciation = (V-Vs)/n

V = F.C.I =335182294.4 $

VS = 0.05 × F.C. I = 16759114.72$

N = Number of Years = 20 Years

Depreciation = $\frac{V-Vs}{n}$ = 15921158.99

Net profit = gross profit – depreciation

Net profit = 97766267.04$/year

3.5.6.1.Rate of Return

ROR = $\frac{\text{net profit}}{\text{total income}}$= 0.220566087

Rate of return = 22%

3.5.6.2.Payback Period:

Payback Period = 1/rate of return Payback period = 4.53 year

Chapter 4

Results and Discussions

4.1. Simulation Results

Through the utilization of Aspen HYSYS, a powerful process simulation tool, the thesis unravels a wealth of insights. The simulation outcomes elucidate the temporal evolution of key process variables, such as temperature, pressure, and reactant concentrations, offering a profound understanding of the chemical reactions and energy transformations that underpin ammonia synthesis. Furthermore, these results serve as a canvas for the exploration of diverse scenarios, allowing for the systematic evaluation of the effects of varying operating conditions on ammonia yield, energy consumption, and other critical parameters. By translating theoretical concepts into dynamic digital simulations, the study not only enhances our comprehension of the ammonia production process but also sets the stage for subsequent optimization endeavours and economic analyses, elevating the research to a pivotal juncture where scientific inquiry converges with practical application.

The results of simulation and its comparison to data obtained by literature is shown in Table 16. The difference in results is due to the fact that our model is based upon kinetic reactors whereas, the equilibrium reactors were used in literature [5]. The equilibrium reactors are used in simulation world as a basis because of their ease to converge and providing higher conversion rates however, kinetic reactors i.e. plug flow reactors give more realistic and reliable results.

Table 16: Comparison of simulation and literature results [5]

	Simulation Result		**Literature Results**	
Stream name	Ammonia	Purge gases	Ammonia	Purge gases
Temperature (^{0}C)	-2.5	-2.5	-2	-2
Pressure (bar-g)	25	25	25	25
Flow rate (tonnes/day)	2481.7	42.5	2215	19.0

4.2. Optimization Results

Through the meticulous application of optimization techniques, including the integration of Pinch Analysis through Aspen Energy Analyzer, the study navigates the intricate landscape of parameters, variables, and constraints inherent to ammonia synthesis as mentioned in earlier chapters. The optimization outcomes unveil a harmonious convergence of factors, delineating optimal temperature profiles, heat exchange networks, and energy integration strategies. These results not only unlock enhanced energy utilization and reduced utilities consumption but also offer a profound resonance with the overarching goals of sustainability and cost-effectiveness. Furthermore, the elucidation of optimal process conditions translates into a quantifiable economic framework, where direct production costs, net profit margins, return rates, and payback periods are meticulously calculated. Collectively, the optimization results exemplify a synthesis of theoretical acumen and pragmatic application, paving the way for a refined and optimized ammonia production process that resonates with efficiency, economic prudence, and environmental consciousness.

The proposed scenario of Aspen HYSYS reduce the cost of heating utilities to 4.52×10^9 from 4.60×10^9 and cooling utilities to 3.99×10^9 from 4.07×10^9 as explained below in the Table 17 owing to the optimization results of the process using the pinch technology. Around 1.99% utilities consumption were saved with optimizing the ammonia process.

Table 17: Comparison table for utilities consumption between base case and proposed scenario

Sr No.	Utility Name	Base Case (kJ/hr)	Scenario (kJ/hr)	Savings (kJ/hr)	Savings %
1	HP Steam Generation	3.20×10^8	3.20×10^8	0	0
2	MP Steam Generation	1.94×10^8	1.94×10^9	0	
3	Air	2.30×10^9	2.29×10^9	8.50×10^6	3.5993

4	Cooling Water	1.25×10^9	1.18×10^9	7.44×10^8	1.3837
	Total Cooling Load	$\mathbf{4.07 \times 10^9}$	$\mathbf{3.99 \times 10^9}$	$\mathbf{8.29 \times 10^7}$	**2.03**
5	Fired Heat (2000)	8.60×10^8	8.60×10^8	0	0
6	Fired Heat (1000)	4.75×10^8	4.74×10^8	8.36×10^5	0.1759
7	Hot Oil	2.86×10^9	2.25×10^9	0	0
8	HP Steam	2.62×10^9	2.62×10^7	0	0
9	MP Steam	8.28×10^7	6.65×10^5	8.21×10^7	99.1967
10	LP Steam	3.05×10^8	2.41×10^8	0	0
	Total Heating Load	$\mathbf{4.60 \times 10^9}$	$\mathbf{4.52 \times 10^9}$	$\mathbf{8.29 \times 10^7}$	**1.80**

4.3. Cost Analysis Results

The comprehensive cost analysis conducted as part of this study yields a profound understanding of the economic landscape of ammonia production from natural gas. The total equipment cost, encompassing investments in reactors, heat exchangers, compressors, and other essential components, offers a tangible glimpse into the capital-intensive nature of the process. This dovetails into the total capital investment, which not only considers equipment but also includes expenses related to engineering, construction, and project management. Utility costs, a pivotal facet of operational expenditure, underscore the significance of energy consumption in the production process. The meticulous calculation of direct production costs, encompassing raw materials, labour, maintenance, and overheads, sheds light on the financial implications of day-to-day operations. Furthermore, the determination of net profit offers a compelling insight into the financial viability of ammonia production, weighing revenues against total costs. In conjunction with this, the rate of return becomes a critical yardstick, quantifying the profitability and attractiveness of the venture to potential investors. Finally, the calculated payback period synthesizes the economic narrative, signifying the time required for the initial capital investment to be recouped through net profits, rendering a pragmatic perspective on the project's financial sustainability and resilience. Collectively, these cost analysis results offer a panoramic view of the economic viability of ammonia production, arming stakeholders with the insights required for informed decision-making and strategic planning [59, 62]. Moreover, a comparison is drawn between before and after optimization of ammonia process to conclude the importance of pinch analysis. The percentages optimized are also shown in Table 18 to quantify the effect of optimization and its feasibility for real-time improvements in ammonia production plants.

Table 18: A comparative analysis based on economics between base case and proposed scenario [59]

Economic Data	**Formulas**	**Before Optimization**	**After Optimization**	**Percentage Optimized**
Total Equipment Cost	Aspen	88,983,300	89,473,484	-
Fixed Capital Investment (FCI)	Direct Cost + Indirect Cost	335,182,294	337,028,719	-
Working Capital Investment (WCI)	15% of FCI	50,277,344	337,028,719	-
Total Capital Investment (TCI)	FCI + WCI	385,459,638	387,583,027	-
Utility Cost	Aspen	118,571,000	116,817,216	1.501
Variable Cost	Raw Material + Utility Cost + Miscellaneous	121,113,883	119,373,024	1.458

Fixed Operating Cost (FOC)	Table	132,397,006	133,126,344	0.547
Direct Production Cost (DPC)	Variable Cost + FOC	253,510,890	252,499,369	0.400
Overhead Charges	30% of DPC	76,053,267	75,749,810	0.400
Total Production Cost (TPC)	DPC + Overhead Charges	329,564,157	328,249,179	0.400
Gross Profit	Total Income - TPC	113,687,426	115,002,403	1.143
Net Profit	Gross Profit - Depreciation	97,766,267	98,993,539	1.239
Rate of Return (ROR)	Net Profit/Total Income	0.2205	0.223	1.091
Payback Period	1/ROR	4.53	4.47	1.427

Conclusion and Recommendations

Summary of Findings

This thesis accessed the sustainability and economic feasibility of ammonia production plant by using steam methane reforming (SMR) pathway. The three main objectives of the study involve modelling of the plant, optimization, and cost analysis. The first objective was achieved by a detailed process simulation on aspen HYSYS. This simulation gave data to perform other tasks such as energy and techno-economic analysis. The simulation results were also validated by literature. Based on the material and energy balances, the whole plant was analysed in order to reduce energy consumption, reduce energy losses, increase production rate while considering economic feasibility. The pinch analysis brought around 2.2% more savings except that some energy losses still remain due to the necessity to cool streams before transitioning in to other units in the process flow diagram hence, optimized it to only possible extent. To achieve the last objective, economic analysis on both the simulated and optimized plant was done. The results of which showed a decrease in utilities cost by 1.4% and increase in net profit of the overall plant by 2%. For a commercial scale plant, the above percentages play a significant role as the production cost also decreases whereas keeping the production rate constant at 22481.7 tones/day of purified ammonia gas which is around 10% more than the production in comparison to literature. In a nut shell, with a small modification, the plant can be optimized and profit can be improved.

Implications of Results

This thesis works on the integration of Aspen HYSYS for simulation modelling, Aspen Energy Analyzer for Pinch Analysis, and Aspen Economic Analyzer for cost analysis. Firstly, the substantial utilities savings of 1.99% signify enhanced operational efficiency and cost savings, positioning the ammonia synthesis process for improved economic competitiveness. The application of Pinch Analysis through Aspen Energy Analyzer facilitates optimal energy utilization, exemplifying the plant's commitment to resource efficiency and environmental responsibility. Furthermore, the use of Aspen Economic Analyzer empowers strategic decision-making, allowing stakeholders to make informed choices based on comprehensive economic evaluations. This integration of advanced simulation and analysis tools not only enhances process robustness and reliability but also showcases technological proficiency and innovation, positioning the research at the forefront of industry leadership. Overall, the implications of this thesis underscore its pivotal role in advancing sustainable and economically viable ammonia production, with ramifications that resonate across industrial practices and underscore its contribution to the broader landscape of process optimization and cost analysis.

Recommendations for Future Studies

In light of the insightful findings in this thesis, several compelling avenues for future studies emerge. Firstly, further exploration of alternative feedstock compositions, beyond natural gas, could provide valuable insights into the adaptability and robustness of the developed models and optimization strategies. Additionally, delving into the integration of emerging technologies, such as carbon capture and utilization, within the ammonia synthesis process could offer a comprehensive understanding of their potential synergies for enhancing both environmental and economic performance. Furthermore, a detailed investigation into the long-term operational dynamics and stability of the optimized process under varying conditions would contribute to a more holistic assessment of its real-world viability. Finally, extending the cost analysis framework to encompass a broader spectrum of economic variables, including market dynamics and price fluctuations, would enhance the accuracy and applicability of the economic evaluations. These recommended areas of future inquiry hold the promise of advancing the field of ammonia synthesis and its optimization while paving the way for sustainable and innovative industrial practices.

Appendices

A.1. Process Data Tables

Table 19: Aspen generated process stream data table involved in PFD

Name	Vapour Fraction	Temperature [C]	Pressure [bar_g]	Mass Flow [kg/h]	Name	Vapour Fraction	Temperature [C]	Pressure [bar_g]	Mass Flow [kg/h]
Natural gas		6	70	43920	To E-110	1	293.01	150	3420418.8
To E-100	1	-33.64	35	43920	To E-111	1	115	150	3420418.8
To E-101	1	196	35	43920	To E-112	0.99	30	150	3420418.8
Water	0	30	1	140400	TO HPS	0.98	-5	135	3420418.8
To E-102	0	30.30	35	140400	R717 In	0	-33	1.1	478200
To E-103	0	164	35	140400	R717 out	0.77	-18.48	1	478200
Steam to MIX - 100	1	360	35	140400	V1	1	-5	135	3325003.7
CH4 To MIX-100	1	360	35	43920	L1	0	-5	135	95415.08
To FH	1	355.28	35	184320	To K-103	1	20	135	3325003.7
To PF	1	1746.51	35	184320	To Recycle	1	31.95	150	3325003.7
Air	1	25	1	100080	To E-114	1	31.95	150	3296010.7
To SRF	1	775.44	35	284404.84	Recycled gas	1	270	150	3296010.7
To E-104	1	775.44	35	284405.27	To V-102	1.71E-02	-2.52	25	95415.086
To HTSC	1	355	34	284405.27	NH3	0	-2.52	25	93807.25
To E-105	1	505.49	34	284404.5	Purge gas	1	-2.52	25	1607.8359
To LTSC	1	205	21	284404.5	Fuel stream	1	50	35	17136
To E-106	1	213.43719	21	284404.46	Air Feed	1	1925	35	322834.52

To V-100	0.88223 63	40	21	284404.46	Combustion Product	1	1756.62	35	339970.52
Gases	1	40	21	243018.37	to mix 101	1	830.506	35	184324.83
H20	0	40	21	41386.092	To E-109	1	375.5	150	124410.76
Co2	1	56.153649	21	118607.57	To E-108	1	320.2	21	124410.76
To Methanator	1	300	21	124410.8	To ammonia reactor	1	270	150	124410.76
To K-102	1	55	21	124410.77	Ait to MIX-101	1	504.24	35	100080

Table 20: Component mole fraction distribution in process streams in PFD generated by Aspen

Component mole fraction										
Name	CH4	(CO)	(CO2)	(H2O)	N2	(Oxygen)	AR	NH3	H2	Refrig-717
Natural gas	1	0	0	0	0	0	0	0	0	0
To E-100	1	0	0	0	0	0	0	0	0	0
To E-101	1	0	0	0	0	0	0	0	0	0
Water	0	0	0	1	0	0	0	0	0	0
To E-102	0	0	0	1	0	0	0	0	0	0
To E-103	0	0	0	1	0	0	0	0	0	0
Steam To MIX-100	0	0	0	1	0	0	0	0	0	0
CH4 To MIX-100	1	0	0	0	0	0	0	0	0	0
To FH	0.25	0	0	0.740	0	0	0	0	0	0
To PF	0.25	0	0	0.740	0	0	0	0	0	0
Air	0	0	0	0	0.79	0.21	0	0	0	0
To SRF	3.96E-07	0.14	0	0.25	0.14	3.74E-02	0	0	0.42	0
To E-104	1.00E-40	0.14	5.44E-07	0.25	0.14	3.74E-02	0	0	0.42	0
To HTSC	1.00E-40	0.14	5.44E-07	0.25	0.14	3.74E-02	0	0	0.42	0
To E-105	0	8.70E-03	0.13	0.12	0.14	3.74E-02	0	0	0.55	0
To LTSC	0	8.70E-03	0.13	0.12	0.14	3.74E-02	0	0	0.55	0
To E-106	0	2.06E-03	0.13	0.12	0.14	3.74E-02	0	0	0.56	0

To V-100	0	2.06E-03	0.13	0.12	0.14	3.74E-02	0	0	0.56	0
Gases	0	2.34E-03	0.15	3.91E-03	0.15	4.24E-02	0	0	0.63	0
H20	0	1.05E-07	1.13E-03	0.99	3.53E-05	3.85E-06	0	0	2.36E-05	0
Co2	0	0	1	0	0	0	0	0	0	0
To E-107	0	2.77E-03	0	4.64E-03	0.189	5.03E-02	0	0	0.75	0
To Methanator	0	2.77E-03	0	4.64E-03	0.189	5.03E-02	0	0	0.75	0
To K-102	2.74E-03	4.51E-05	1.00E-40	7.41E-03	0.1901965	5.06E-02	0	0	0.7490446	0
To E-110	9.30E-03	1.65E-04	0	2.69E-04	1.04E-03	0.1849503	0	5.95E-02	0.7447641	0
To E-111	9.30E-03	1.65E-04	0	2.69E-04	1.04E-03	0.18	0	5.95E-02	0.74	0
To E-112	9.30E-03	1.65E-04	0	2.69E-04	1.04E-03	0.18	0	5.95E-02	0.74	0
TO HPS	9.30E-03	1.65E-04	0	2.69E-04	1.04E-03	0.18	0	5.95E-02	0.74	0
R717 In	0	0	0	0	0	0	0	0	0	1
R717 out	0	0	0	0	0	0	0	0	0	1
V1	9.42E-03	1.68E-04	0	3.40E-07	1.06E-03	0.18	0	4.67E-02	0.75	0
L1	8.70E-04	3.06E-06	0	1.92E-02	7.59E-06	1.33E-02	0	0.9588045	7.83E-03	0
To K-103	9.42E-03	1.68E-04	0	3.40E-07	1.06E-03	0.18	0	4.67E-02	0.75	0

To Recycle	9.42E-03	1.68E-04	0	3.40E-07	1.06E-03	0.18	0	4.67E-02	0.75	0
To E-114	9.41E-03	1.68E-04	0	3.62E-07	1.12E-03	0.18	0	4.66E-02	0.75	0
Recycled gas	9.41E-03	1.68E-04	0	3.62E-07	1.12E-03	0.18	0	4.66E-02	0.75	0
To V-102	8.70E-04	3.06E-06	0	1.92E-02	7.59E-06	1.33E-02	0	0.95	7.83E-03	0
NH3	4.96E-04	6.04E-07	0	1.95E-02	6.79E-07	6.59E-03	0	0.97	8.87E-04	0
Purge gas	2.24E-02	1.44E-04	0	1.04E-06	4.05E-04	0.40	0	0.16	0.40	0
Fuel stream	1	0	0	0	0	0	0	0	0	0
Air Feed	0	0	0	0	0.79	0.21	0	0	0	0
Combustion Product	0	0	4.56E-02	9.11E-02	0.75	0.10	0	0	0	0
to mix 101	4.82E-07	0.17	0	0.31	0	0	0	0	0.51	0
To E-109	2.74E-03	4.51E-05	1.00E-40	7.41E-03	0.19	5.06E-02	0	0	0.74	0
To E-108	2.74E-03	4.51E-05	1.00E-40	7.41E-03	0.19	5.06E-02	0	0	0.74	0
To ammonia reactor	2.74E-03	4.51E-05	1.00E-40	7.41E-03	0.19	5.06E-02	0	0	0.74	0
Ait to MIX-100	0	0	0	0	0.79	0.21	0	0	0	0

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