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Theme:

Conceptual design for green hydrogen and ammonia production plant

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Dédicace

I want to give a shoutout to everyone who had my back during this whole process. Seriously, I couldn't have done it without you.

First off, to my parents—thanks for always being there, no matter what. Your love and support mean everything.

To my professors, I really appreciate all the time you took to guide me and share what you know. You made this whole thing way less intimidating.

And to my friends, thanks for keeping me sane.

Boudjemline seyf el islam

Dédicace

To my family, for their unwavering support and love.

To my friends, for their constant encouragement and companionship.

And to everyone who supported me through the years.

Thank you for your kindness and belief in me.

Bebboukha Safouane

Remerciements

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We would like to thank all those who have contributed directly or indirectly to the accomplishment of this work.

Abstract:

This study addresses the conceptual design of a sustainable green ammonia production system, focusing on hydrogen generation via water electrolysis using renewable energy, with the goal of achieving carbon-neutral manufacturing. Using advanced simulations in Aspen Plus V12.1, the integration of air separation, electrolysis, and the Haber-Bosch cycle was analyzed. The results showed a hydrogen flow rate of 2529.91 kmol/h and a production of 1032.21 kmol/h of high-purity ammonia with zero carbon dioxide emissions.

Keywords:Haber-Bosch process, Hydrogen production, Electrolysis, Green ammonia.

ملخص :

تتناول هذه الدراسة التصميم المفاهيمي لنظام إنتاج الأمونيا الخضراء المستدامة، مع التركيز على توليد الهيدروجين عن طريق التحليل الكهربائي للماء باستخدام الطاقة المتجددة، بهدف تحقيق تصنيع محايد للكربون. باستخدام عمليات المحاكاة المتقدمة في Aspen Plus V12.1، تم تحليل تكامل فصل الهواء والتحليل الكهربائي ودورة هابر-بوش. أظهرت النتائج معدل تدفق هيدروجين يبلغ 2529.91 كيلومول/ساعة وإنتاج 1032.21 كيلومول/ساعة من الأمونيا عالية النقاء مع انبعاثات ثاني أكسيد الكربون الصفرية.

كلمات مفتاحية: عملية هابر-بوش، إنتاج الهيدروجين، تحليل الكهربائي للماء، أمونيا

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Nomenclature

Symbol	Definition	Unit
H_2	Hydrogen used or recycled	kg/h – kmol/h
N_2	Nitrogen supplied from the Air Separation Unit (ASU)	kg/h – kmol/h
NH_3	Ammonia produced by synthesis	kg/h – kmol/h
ASU	Air Separation Unit	
PEM	Proton Exchange Membrane electrolyzer	/
AEL	Alkaline Electrolyzer using KOH solution	/
KOH	Potassium hydroxide used as electrolyte	/
T	Process temperature	°C
P	Process pressure	bar
$\dot{m}$	Mass flow rate	kg/h
$\dot{n}$	Molar flow rate	kmol/h
H	Specific enthalpy	kJ/kg
s	Specific entropy	kJ/kg·K
ρ	Fluid or mixture density	kg/m^3
η	Conversion or efficiency	%
Q	Heat exchanged in the process	kW
Elec	Electrical energy consumed	kWh
EP	Photovoltaic energy supply	kWh/year
EH_2	Energy contained in the produced hydrogen	MJ

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General introduction

General introduction

Ammonia is used extensively in industry, particularly in the production of fertilizers, and it is also being discussed as a renewable energy source these days. The issue is that the conventional method of producing ammonia—the Haber-Bosch process—requires natural gas and emits a lot of CO_2, which somewhat negates the goal of green energy. Therefore, the goal is to build a facility that produces hydrogen and ammonia in an environmentally friendly manner by splitting water using renewable energy rather than fossil fuels. Just ammonia doing its thing without destroying the planet—no carbon, no guilt.

This is significant since the manufacture of ammonia was responsible for roughly 1.3% of the total CO_2 emissions from the worldwide energy system, or about 450 million tons of CO_2, and nearly 2% of the entire final energy consumption, or 8.6 exajoules. This highlights the substantial environmental impact of conventional ammonia production. [1] In essence, we're investigating if producing ammonia in a more environmentally friendly manner can truly be more effective than the conventional method, both in terms of efficiency and environmental friendliness. We're using a tool called Aspen Plus to combine computer simulations and some plain old-fashioned theory in order to determine this.We're focusing on the crucial details, such as how we separate air, split water to produce hydrogen, and really combine ammonia. The main goal is to determine whether this cleaner method can survive in the actual world.

Chapter 1: covers the basics of ammonia, or NH_3. It walks through what ammonia actually is and how it behaves chemically. There's some talk about how we normally make ammonia and newer, cleaner ways to produce itespecially methods involving green hydrogen from splitting water and better ways to pull nitrogen from the air.

It also gets into alternatives to the old-school Haber-Bosch method, which has been the go-to for ages. Safety stuff comes up too, because ammonia can be tricky to handle, and there's a bit about storing large amounts of it without things going sideways and transportation methods.

Chapter 2: begin with literature review of many studies in the field of ammonia production using Aspen plus software, then its covers all the gear and programs we used for this project. It's mostly about how we planned out a system to make ammonia in an eco-friendly way. We explaining how we used Aspen Plus software, version 12.1, to run simulations of the whole process. There's stuff about what numbers we plugged in for nitrogen and hydrogen, plus how we set up the simulation to mimic the actual production line from start to finish.

Chapter 3 : this chapter is dedicated to the comprehensive presentation and in-depth interpretation of the results obtained from the Aspen Plus simulations. It meticulously examines the operational performance of the integrated green ammonia production facility, providing a thorough analysis of its mass and energy balances. Furthermore, this chapter quantifies the significant reductions in CO_2 emissions achieved through the proposed green methodology and underscores the enhanced efficiency realized via optimized resource recovery and strategic process integration.

Finally, we will conclude this study with a general conclusion, present a summary ofthe work done and the main results obtained, and then give some perspectives for future workin this domain.

Chapter 1

Green Hydrogen and Ammonia

1. Introduction

Ammonia (NH_3) is a vital chemical used extensively in agriculture and industry. Traditionally, it is synthesized via the haber-bosch process, which reacts nitrogen with hydrogen under high temperature and pressure. While efficient, this process is energy-intensive and generates significant co_2 emissions. Recently, more sustainable approaches, such as green ammonia production using renewable hydrogen and nitrogen extracted from air, have emerged to foster a greener ammonia industry. Ammonia can also be stored and transported as a liquid under pressure or at low temperatures i.

In this chapter introduces ammonia, highlighting its properties, conventional production methods, and their environmental impact. It emphasizes the transition from fossil-based to green ammonia production using renewable energy and electrolysis. Emerging technologies like electrochemical synthesis and photocatalysis are briefly presented. The chapter also outlines ammonia's transport, storage, and safety considerations, reinforcing its role in a low-carbon future.

2. Ammonia production

2.1. General characteristics

- Chemical formula: NH_3
- Chemical name: ammonia, anhydrous ammonia
- Molecular weight: 17.03
- At ambient temperature and atmospheric pressure, ammonia is an alkaline, colourless gas with a pungent and suffocating odour. Ammonia gas is very soluble in water.
- The gas is strongly irritant/corrosive to the skin, eyes and respiratory tract and has
- Toxic properties. Ammonia gas condenses into a colourless liquid when cooled and
- Compressed. The liquid can cause severe cold burns on contact with the skin [2]

2.1.1 Physical properties of ammonia

table 1.1: physical data[2]

property	**liquid**	**Gas**
colour	colourless	Colourless
smell	pungent	Pungent
density (0°c, 101.3 kpa)	638.6 kg/m3	0.7714 kg/m3
density (-33.43°c, 101.3 kpa)	682 kg/m3	0.888 kg/m3
boiling point (101.3 kpa) -	-33.43°c	

melting point	-77.71°c	
critical temperature	132.4°c	
critical pressure	11.28mpa.	

2.1.2. Chemical properties of ammonia

- ammonia is an alkaline gas. the ph of a 1% aqueous solution is approximately 11.7.
- ammonia in contact with certain other chemicals including mercury, chlorine, iodine,
- bromine, calcium, silver oxide or hypochlorites can form explosive compounds.
- gaseous ammonia can react violently with nitrogen oxides and strong acids.
- ammonia is very corrosive to copper and copper containing alloys and therefore,
- equipment in contact with ammonia must be free of them**.** [2]

3. Conventional ammonia production

3.1. Methane-based haber-bosch.

ammonia is generally produced in high-capacity plants (1,000 to 1,500 t/d) utilizing the haber-bosch process. over 90%of ammonia produced worldwide comes from fossil fuels approximately 96% of the hydrogen (H_2) needed for themanufacturing of ammonia through the haber-bosch process comes from fossil fuels, while the remaining 4% isproduced by electrolysis. a typical steam methane reforming (smr) process produces nearly 9–10 tons of carbondioxide (CO_2) comparable to each ton of hydrogen produced. worldwide, 72% of the hydrogen generated for ammoniaproduction is through the smr process. this process is complex to decarbonize due to the direct release of CO_2 as ansmr side reaction. [3]

3.2. Definition and classifications (green, blue, gray)

the ammonia industry has informally adopted a color scheme to describe the carbon intensity of different production methods (figure 1.1). brown and gray ammonia refers to ammonia produced from fossil fuel feedstocks (from coal and natural gas, respectively) which involves high levels of co_2 emissions. blue ammonia also refers to ammonia produced from fossil fuel feedstocks but associated with carbon capture and storage (CCS) technology to capture the generated CO_2 instead of releasing it to the atmosphere. blue ammonia production is just ~1mt/year based on existing CCS projects (located in us, canada, and china), which can be increased to 4mt/year by 2030 based on the announced projects. green ammonia is produced using electrolysis powered by renewable electricity to produce H_2 instead of using hydrocarbon feedstocks, resulting in no CO_2 emissions. current and announced electrolysis projects could bring the green ammonia production to more than 3mt/year by 2030. [1]

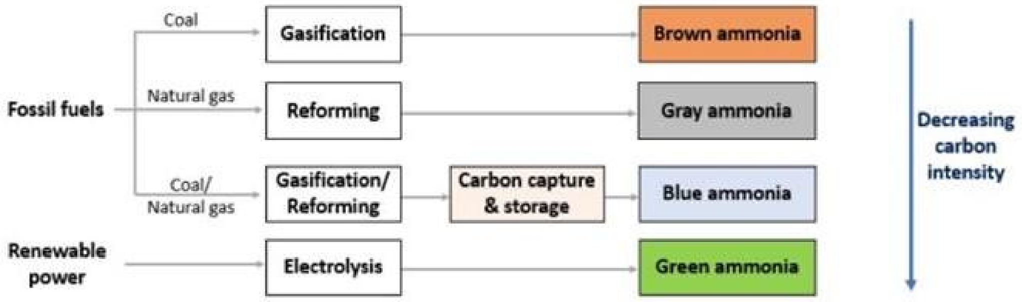


figure 1.1 categorizing ammonia production pathways based on the carbon intensity[1]

3.3. Environmental drawbacks of fossil-based ammonia

Ammonia, produced via the haber-bosch process, is the most energy-intensive commodity chemical, responsible for 1%–2% of global energy consumption and 1.44% of co_2 emissions.[5]

More than 96 % of the ammonia produced nowadays with this process uses fossil fuels asfeedstocks. Of this 96 %, a 50 % is produced from natural gas, a 31 % from oil and a 19 %from coal.

This causesthe process to be responsible for 1,2 % of the global anthropogenic emissions.[6]

It belched up to about 451 million t of CO_2 in 2010, according to the institute for industrial productivity. That total accounts for roughly 1% of global annual CO_2 emissions, more than any other industrial chemical-making reaction.[7]

4. Sustainable ammonia synthesis technologies

To produce green ammonia, the main steps remains but instead of using methane as a fuelandfeedstock, the process is powered by electricity from renewable source and smr isreplaced by electrolysis. Both the source of energy and theelectrolyser must be selected wisely. Furthermore,hydrogen exiting the electrolyser is purebut nitrogen must also be purified before entering the hb reactor, through a cryogenic.[8]

4.1 Green hydrogen

The current total market of hydrogen consumption is about us$115 billion, mainlydriven by the demand for petroleum refining and ammonia and methanol production.

There are three main pathways to produce hydrogen: steam methane reforming, coalgasification, and water electrolysis.

The first two methods dominate the global hydrogen production, but they use a lot of fossil fuels and emit CO_2 as a by-product.

Thistype of hydrogen is known as “gray hydrogen”. The CO_2 emissions can be reducedby capturing and storing the carbon (ccs or ccus), but this also increases the production cost andrequires strict control of methane emissions. This type of hydrogenis known as “blue hydrogen”. Thecleanest way to produce hydrogen is to split waterusing renewable energy sources, such as wind, solar, hydro, geothermal, or nuclearpower. This type of hydrogen is known as “green hydrogen” and does not emit anyCO_2 [9,10].

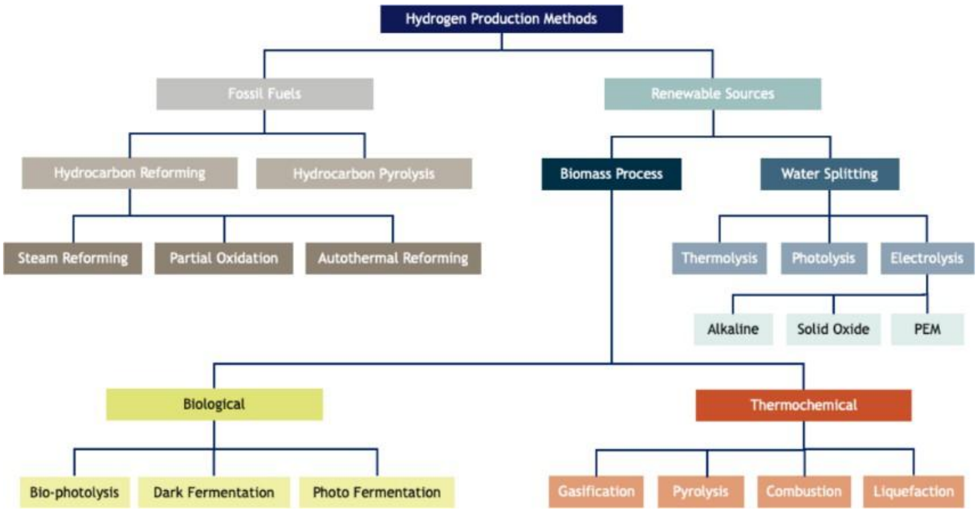


Figure 1.2 overview of various hydrogen production approaches. **[10]**

4.1.1 Electrolysis water electrolysis

Is an electrochemical process based on the use of direct electric current for splitting water into hydrogen and oxygen. An electrolyzer is composed of: two electrodes (anode and cathode, positive and negative respectively) and a conductive liquid designed as the electrolyte, in which the electrodes are immersed. Typically, potassium hydroxide (koh) is added to increase the conductivity of water. The process is based on the passing of an electric current between anode and cathode through the electrolyte. In this way, the water will split in hydrogen, released from the cathode, and oxygen from the anode. The general chemical equation for the electrolysis reaction is:

$$2h_2o \rightarrow 2\ h_2\ + o2$$

Two electrodes (anode and cathode, positive and negative respectively) and a conductive liquid designed as the electrolyte, in which the electrodes are immersed. Typically, potassium hydroxide (koh) is added to increase the conductivity of water.

The three most common and commercially available electrolysers are listed below:

A. Alkaline electrolysers

B. Proton exchange membrane (pem) electrolysers

C. Anion exchange membrane (aem) electrolysers. [11]

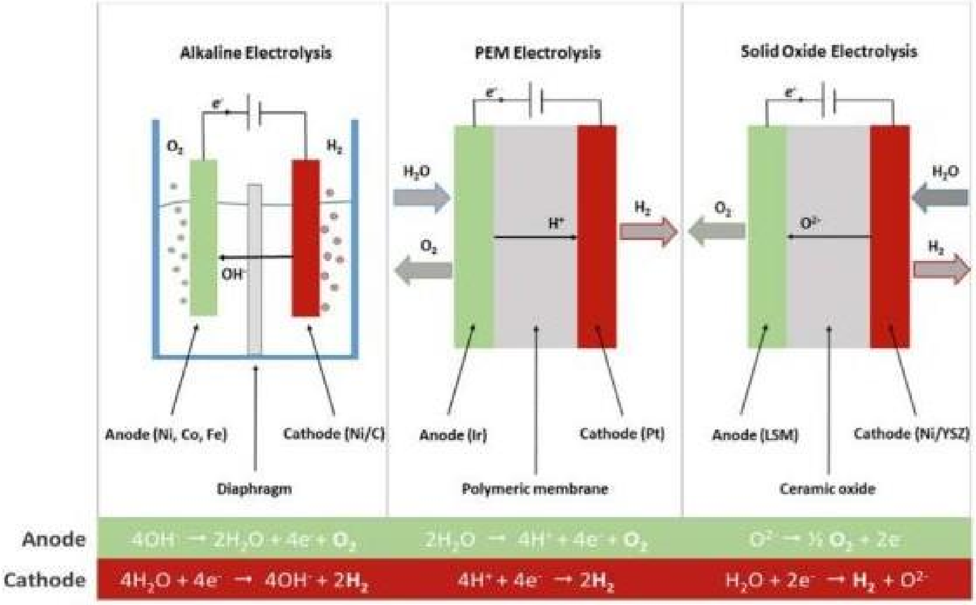


Figure 1.3 operating principles of three types of electrolysis technologies source: electrocatalysts for the generation of hydrogen, oxygen and synthesis gas[12]

4.2. Air production routes

Whenever one of the components of air is required, air separation units (asu) are built toprovide the plant the species of interest. Different techniques can be used to obtain the desiredresult and those are: membranes, pressure swing adsorption and cryogenic distillation of air.[13]

42.1. Air separator unit (asu)

Today, the only large-scale commercially available technology for use in air separator devicesis the cryogenic distillation. Although it possesses remarkablethermodynamic properties, its complicated architecture makes it challenging to operatair is gathered from the atmosphere, which mainly contains nitrogen (N_2), oxygen (O_2)and argon (ar)11(ucar, n.d.). Then the air is compressed (which generates heat)before it is cooled using a heat exchanger in the following step.

The air continues to the first condenser, a high-pressure condenser, which performs thefirst separation. In this condenser, only a portion of the air's nitrogen is filtered out.therefore, the remaining air passes through the low-pressure condenser to extract moreof the nitrogen from the air.

In this condenser, the majority of nitrogen is filtered out,and the final product is >99 percent clean nitrogen. Additionally,filtered oxygen and argon are available for use in other applications if needed. After thelast filtering process, the gases stays cooled and depending on the application, reheatingmight be appropriate for further use. [14]

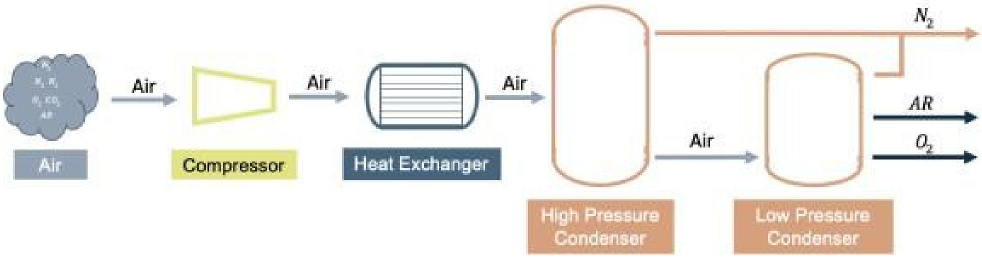


Figure 1.4 asu flowchart[10]

4.3. Electrolysis-driven haberbosch (green ammonia)

Green ammonia can be manufactured from renewable energy. Carbon-free hydrogen is produced using renewableelectricity by water electrolysis, so-called power-to-hydrogen (pth) as shown in figure1.5 .therefore, the coupling of pthand the haber-bosch process avoids the use of fossil fuels [16].

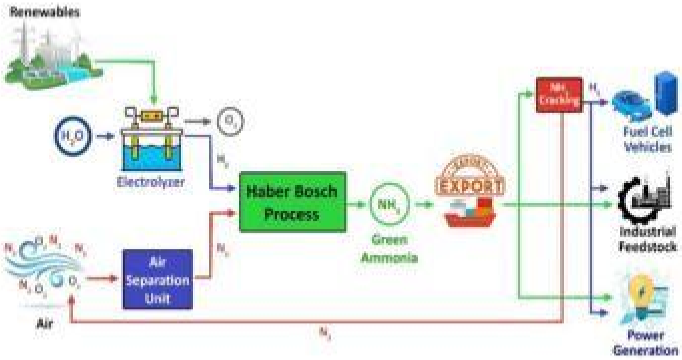


Figure 1.5 illustrates the power of the hydrogen process for ammonia production.[17].

Table 1.2 pros and cons of electrolysis-drivenammoniasynthesismethod and the common haber-bosch method [18,19,20].

Processname	**Advantages**	**Disadvantages**
Methanebasedhaber- Bosch	1.2. It is the most efficient way. 3.4. It has a high overallyield, 5. makingit a commercially viable method for large-scaleammonia production. The methodis scalable. It iswell-established. It isrecommended for continuousammonia production.	1. 2. Its high-energyconsumption. 3. There wereenvironmentalproblemsrelated to the process, especially due to the large quantities of greenhousegasesemissionsafetyconcernswhile operating in high pressure and high-temperatureenvironments.

Electrolysisdrivenh aberbosch (green Ammonia)	1.2. No direct 3. carbondioxideemissions. 4. Use of green ammonia in 5. agriculture as a 6. fertilizerprovides a sustainable alternative, contributing to improvedsoilhealth. It offersflexibility in scale, allowing for both large-scalecentralized and smaller-scaledecentralizedfacilities. Reduction of fossil fuel consumption and greenhousegasemissions, It can beused as a vector to transport hydrogen. It has betterenergydensity	1.2. Stillunderdevelopment. 3. There were challenges in terms of efficiency, cost-effectiveness, and scalabilitythat must bedealtwith. It ispriceycompared to traditionalprocessesbecause of the presentexpensesrelated to Renewableenergy technologies

5. New ammonia generation routes

5.1. Nonthermal plasma process

The proposed novel non-thermal plasma (ntp) gas-liquid nitrogen fixation process that generated plasma in situ within the liquid body using concentrated high-intensity electric field (chief) aims to increase ammonia production, partially replacing the energy intensive harbor-bosch process [21].

A synthesis has emerged as a promising strategyfor green NH_3 production because of its ability to operate under ambient conditions,efficiently activate inert molecules, respond rapidly to system variations, and integrate wellwith renewable energy sources [22].

Ntps are characterized by high-energy electrons (104-105 k) that cancause non-thermal activation of molecules, while the gas temperatureremains between 300 k and 1000 k. As a result, reactions cantake place at lower pressures and temperatures compared to thermalcatalysis.

Yet, combining ntps with catalysts can lead to a synergistic effect with the efficiency of the combined system surpassing that of the individual parts. Further, ntps allow for quick on/off operation making the technology compatible with thefluctuating renewable energy sources such as wind energy and solar power, enabling a novel green way to synthesize NH_3 [23].

5.2. Electrochemical ammonia synthesis

Electrochemical synthesis

Electrochemical ammonia synthesis is a process inspired in the enzyme nitrogenase, that fixes nitrogen by proton-coupled electron transfer under mild conditions. The method isemerging as a future compelling alternative to the haber-bosch process due to its mild operating conditions. It can also bepowered by renewable energies [24] and enables the delivery of modular production solutions on small and medium scales [25]. Additionally, it is considered that its simple configuration can reduce system configuration and control complexity, as the hydrogen production from water and the nitrogen fixation are integrated in a single unit [26]

The reactions involved are as follows:

$$\text{Anode: } 3h_2 \leftrightarrow 6h^+ + 6e^-$$

$$\text{Cathode: } N_2 + 6h^+ + 6e^-$$

$$\leftrightarrow 2$$

This technology also allows to eliminate the hydrogen production stage by using water oxidation directly as a counter reaction in an electrochemical cell [27], in this case the reactionat the anode is as follows:

$$3h_2o \leftrightarrow 6h^+ + 6e^- + {}_3/_2\ O_2 ++$$

The electrochemical process utilises pure hydrogen and nitrogen produced externally through hydrogen production and nitrogen separation. These diatomic synthesis molecules12 are then transported to the electrochemical ammonia synthesis. Hydrogen is led to the anode section of the unit, with nitrogen led to the cathode side when electricity is introduced, the reaction starts. Electrons e travels from the anode side over to the cathode side of the synthesis through the power unit, while the h+ travels through the separator to the cathode side .

at this stage, h+ and n2 react and form NH_3 at the cathode. After the reaction at the cathode, all substances are led out of the unit and into the NH_3 separator, which separates the NH_3 from the unreacted nitrogen N_2 and hydrogen H_2 [28].

A lot of complex strategies are required for electrochemical ammonia synthesis to become feasible for practical application, which is an interesting scientific challenge. [29]. For now, electrochemical ammonia synthesis should not be considered as a potential replacement of the haberebosch process for large-scale ammonia production, but rather as a technology for small-scale, intermittent ammonia production. When aqueous electrolytes are used, this would allow for localized, on-demand ammonia production for fertilizer application[33].

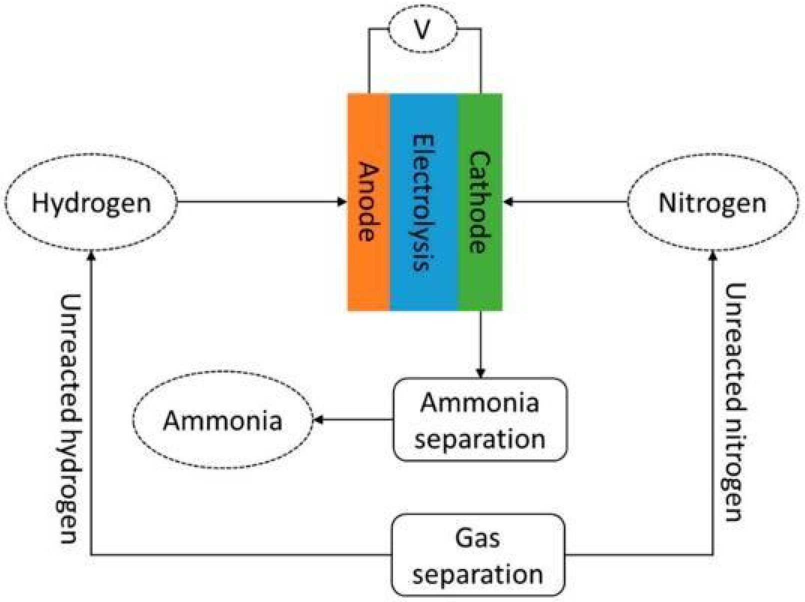


Figure 1.6 electrochemical ammonasyntesis process flow [30].

5.3. Photocatalysis synthesis

Photocatalysis offers a promising method for converting molecular nitrogen into ammonia, gaining significant interest in recent years. Like electrochemical ammonia synthesis, its primary benefit is the potential to use water as a reducing agent for nitrogen fixation under ambient conditions. Instead of an electrocatalyst, a semiconductor is employed. The photochemical reaction involves three key steps. Initially, a semiconductor absorbs light, generating charge carriers. For this to happen, the energy of the absorbed photons must be equal to or greater than the semiconductor's bandgap. Next, electrons are excited from the valence band to the conduction band, creating photo-generated electrons and holes in the valence band. Finally, these electrons and holes migrate to the semiconductor's surface, where redox reactions occur. Water can be oxidized to O_2 and h^+ by surface holes if the valence band potential is more positive than 1.23 v relative to the normal hydrogen electrode safety during transport of ammonia

6. safety during transport of ammonia

6.1 sea transport

Sea transport deserves a high degree of attention and careful management as relativelylarge quantities of materials, long distances of travel and often international shipmentsare involved. For safe transportation a number of requirements have been specifiedfor classified materials in regulations, e.g.

Restrictions concerning stowage of other goods must be adhered to as specified in thesea transport regulations.

The holds of ships should be checked to ensure:

- Cleanliness (including on top of the beams)
- No moisture
- No impurities
- All hatches can be tightly closed prior to loading and are so closed after loading.

Hatches should be designed, constructed and maintained so as to prevent the ingressof water. They should be fully closed once loaded to keep the cargo dry.

The design of electrical installations and fittings in holds should be such as to minimize the risk of mechanical or chemical damage[31].

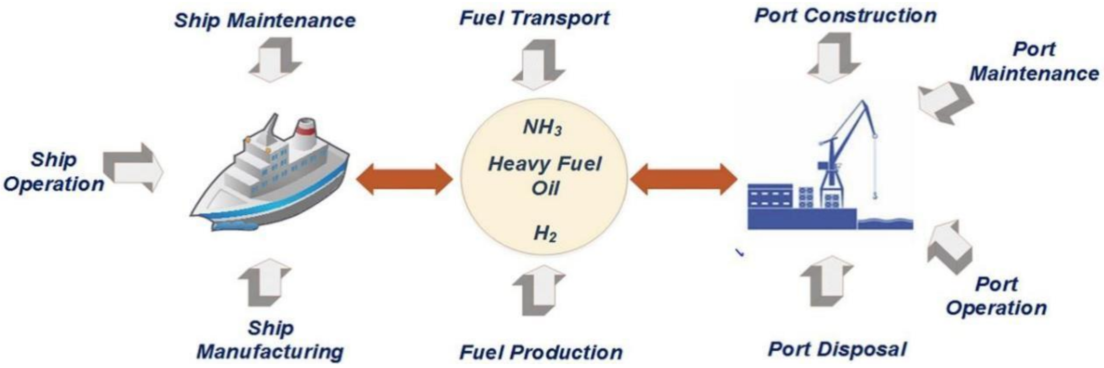


Figure 1.7 life cycle marine fuel use n sea transport [32].

6.2 pipeline transportation

Transporting large quantities of ammonia by pipeline over longdistances is more economical than transport by barge or rail, butthe use of pipeline routes is limited to certain locations.

There are several important aspects to consider in this transportalternative, mainly related to the integrity of the pipelines.

Ammonia transportation by pipelines requires the ammonia tobe heated to at least 2 °c to avoid brittle fracture in the pipeline,which in most cases means that it must be warmed at the supply Terminal and cooled again to -33 °c at the receiver terminal.

Ammonia shall also be transported at a minimum pressureof 20 bar to prevent gas formation this is because thevaporisation of some of the ammonia could reduce the transport capacity, make flow measurement and controldifficult, and cause cavitation damage to the inner wall of the Pipelines

Regarding materials, steels are used in ammonia transfer lines.stainless steel in particular is highly resistant to corrosion, buthas the disadvantage of being very expensive. Materials such as copper, zinc, and aluminum are not used as they are easilycorroded by ammonia [33].

7. ammonia storage

Ammonia can be stored as a liquid at atmospheric pressure if a fluid temperature of -33°c is maintained. A two-stage refrigeration system, which uses the stored ammonia directly as the refrigerant in the refrigeration cycle, is used to keep the ammonia at the low temperature and to cool it upon entry to the storage facility the energy density of the cooled ammonia is 15.37 mj/l, which is slightly denser than ammonia contained in pressurized storage at 13.77 mj/l. Ammonia storage vessels are constructed in a range of sizes from 4,500 t to 45,000 t, although typical facilities store between 15,000 t and 60,000 t the low temperature system can store 41- 45 t of ammonia per tonne of steel, which is nearly 15 times more efficient in than pressure storage this lower steel usage compared to pressurized storage, and the resulting lower capital cost, is one of the main factors why low-temperature storage is widely in use for large-scale ammonia storage[34].

7.1. Ammonia storage facilities

Liquid ammonia is stored either at ambient temperature under high pressure or at -33°c under atmospheric pressure. (the description liquefied is also sometimes used for liquid, see glossary for explanation). In some cases, it is also stored at intermediate temperatures and pressures (semi-refrigerated). For pressure vessels, the inspection requirements in most countries are governed by the respective pressure vessel codes and regulations. The recommendations provided in this guidance are, therefore, limited to atmospheric pressure storage tanks, which operate at -33°c. 3.2[34].

7.2. Types of ammonia storage

The main types of atmospheric tanks operating at -33°c are:

- Steel tank with full height concrete bund wall close to it with capacity to contain the full contents of the tank and the space between the tank and the bund having an impervious floor and roof covering.
- Steel tank housed within another steel tank to contain the full contents of the tank, with a single roof (cup in tank) or independent roofs steel tank with a partial height concrete bund wall with impervious floor within the contained area and no roof over the space.

- Steel tank with an embankment of earth to contain the full contents of the tank and no roof over the space between the tank and the embankment • single steel wall tank with no secondary containment [35].

8. Utilization of green ammonia

Green ammonia is utilized across several key sectors, with the most prominent being fertilizer production, accounting for over 80% of global ammonia use. It also serves as an efficient hydrogen carrier, enabling effective hydrogen storage and transport. Moreover, green ammonia is used as an alternative fuel in gas turbines, engines, and furnaces, and it can generate electricity via direct combustion or fuel cells. In the maritime sector, it is increasingly considered a clean fuel for ships. Additionally, it plays a role in renewable energy systems by storing excess power in the form of chemical energy. Green ammonia is also employed for industrial and residential heating, and it significantly supports the transition toward a low-carbon global economy.[36].

9. safety and environmental considerations of hydrogen and ammonia

Ammonia is corrosive and toxic, and risks are elevated by high vapour pressure under standard conditions. However, ammonia is readily detectable by smell at concentrations well below those that cause lasting health consequences6 while both hydrogen and ammonia have been safely used across several industries for decades, new applications will need to be tested afresh. From an environmental perspective, new ammonia applications will need to be assessed as ammonia-based fertilisers contribute to ghg emissions via nitrous oxide, to biodiversity decline via excess nitrogen, and to air pollution by reacting with other pollutants to form particulates. Research into hydrogen suggests it has only very small effects on the climate or ozone layer12. In both cases there will be challenges of public acceptability, even if some perceptions do not reflect the real risk. .[37].

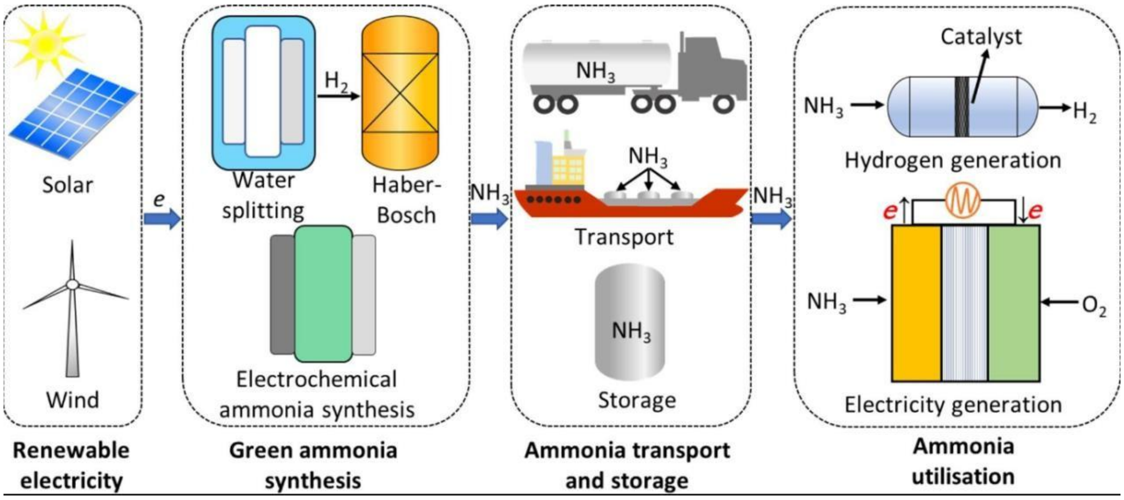


Figure 1.8 green hydrogen and ammonia energy cycle[38].

10. Conclusion

The reviewed study concludes that green ammonia production demonstrates significant technical, economic, and environmental viability as an energy vector. Technically, it is feasible by replacing conventional steam methane reforming (smr) with electrolysis powered by renewable energy. Environmentally, it offers substantial benefits, reducing carbon emissions by approximately 78% compared to traditional methods. Economically, although electricity remains the dominant cost, decreasing renewable energy prices and stable natural gas prices improve investment attractiveness. Accordingly, green ammonia emerges as a promising energy solution—particularly for energy-intensive sectors such as maritime transportation and heavy industry **[39].**

Chapter2

Equipment & Software

1. Introduction:

Addressing climate change requires reducing greenhouse gas emissions by shifting to renewable energy sources and improving energy efficiency across various sectors. Green hydrogen, produced via electrolysis powered by renewable energy, is a key solution for decarbonizing hard-to-electrify sectors like heavy industry and aviation but faces significant storage challenges due to low energy density and high costs [40–41]. In this context, green ammonia emerges as a promising hydrogen carrier with higher energy density, compatibility with existing infrastructure, and the ability to be converted back into hydrogen when needed. Despite technical challenges such as cracking efficiency and nitrogen emissions, ammonia's widespread use in agriculture and industry supports its economic and environmental viability. This project focuses on the preliminary design of a green ammonia production plant using simulation tools, along with equipment layout and site planning, within the framework of "Energy to X" technologies.

2. Literature review of green ammonia production with aspen plus:

Aspen Plus is a key tool in green ammonia production research, enabling simulations of process optimization, CO_2 capture cycles, advanced reactor designs, and renewable hydrogen pathways.

Abdulla and Walke (2015) optimize pump operation in conventional ammonia synthesis to lower production costs and environmental hazards. Concentrate on optimizing specific components like pumps within the ammonia synthesis process, demonstrating the potential for incremental improvements in existing technologies [42].

Byun et al. (2021) integrate the Haber–Bosch process with a supercritical CO_2 Allam power cycle, achieving CO_2 reductions of 68–96% at scales of 2–30 ton/hr. Alsoropose integrating the Haber-Bosch process with a supercritical CO_2 Allam power cycle, achieving significant CO_2 emissions reduction (68-96%). This approach addresses the carbon intensity of traditional ammonia production while potentially improving overall process efficiency [43].

Kappagantula et al. (2024) introduce a Three Reactor Chemical Looping technology that reaches 67.5% conversion efficiency with an energy consumption of 21.5 GJ per ton NH_3. The study explores the use of Three Reactor Chemical Looping (TRCL) technology, which involves the continuous circulation of a solid Oxygen Carrier between three reactors. This innovative approach aims to lower energy consumption and improve environmental performance compared to conventional processes [44].

Two studies report green ammonia production via hydrogen from electrolysis: Shaker et al. (2024) attain a production rate of 7058 kg/hr with 85% conversion efficiency using cryogenic air separation in conjunction with the Haber–Bosch reaction [45]. While de la Hera et al. (2024) design a flexible, small-scale process (5.60–56.7 kmol/h for 1–10 MW capacities) that couples alkaline electrolysis with membrane air separation. De la Hera et al. (2024) investigate flexible small-scale ammonia production with capacities ranging from 5.60 to 56.7 kmol/h for 1-10 MW electrolyzer capacities. This approach aims to enable distributed, on-site production of ammonia, potentially reducing transportation costs and improving overall efficiency [46].

Shaker et al. (2024) and de la Hera et al. (2024) focus on using electrolysis for hydrogen production, coupled with air separation techniques for nitrogen supply. This approach aligns with the goal of reducing the carbon footprint of ammonia production by utilizing renewable energy sources.

Table 2.1: summarize of green ammonia production with aspen plus literature

Study	Software	Production scale	Process type	Energy consumption	CO_2 reduction	Conversion efficiency	Ref
Abdulla and Walke, 2015	Aspen plus	No mention found	Conventional ammonia synthesis with focus on pump optimization	No mention found	No mention found	No mention found	[41]
Byun et al., 2021	Aspen plus	2-30 ton/hr	Haber-Bosch process integrated with supercritical carbon dioxide (CO_2) Allam power cycle	No mention found	68-96%	No mention found	[42]
Kappagantula et al., 2024	Aspen plus	No mention found	Three Reactor Chemical Looping (TRCL) technology	21.5 GJ/t NH_3 at 67.5% conversion	No mention found	67.5% (Steam Reactor)	[43]
Shaker et al., 2024	Aspen HYSYS	7058 kg/hr	Green ammonia production using	Not explicitly detailed	No mention found	85%	[44]

			electrolysis and cryogenic air separation				
de la Hera et al., 2024	Aspen plus	Small-scale: 5.60-56.7 kmol/h for 1-10 MW capacities	Flexible small-scale green ammonia production using alkaline electrolysis	214-217 kWh/kmol NH_3	No mention found	Not explicitly detailed	[45]

3. ProcessOverview:

The process of green ammonia revolves around one main reaction, which is the Haber-Bosch reaction. The Haber process as shown (equation 1), consists of one mole of nitrogen gas and 3 moles of hydrogen gas react in a dynamic equilibrium to produce ammonia gas; due to exothermic nature of the reaction (Illustrated by the negative value ΔH) is favored under relatively low temperature conditions. Furthermore, high pressure is also favored since there are fewer ammonia molecules on the right-hand side [47]

$$N_2 + 3H_{2(g)} \rightleftharpoons 2NH_{3(g)} \quad \Delta H^\circ = -92\ kJ.mol^{-1} \quad ...(1)$$

4. Aspen plus:

Aspen Plus is a robust process simulation tool extensively utilized for modeling and optimizing chemical processes, such as green ammonia production. It allows engineers to create comprehensive process flow diagrams, specify feed streams (e.g., nitrogen from air separation and hydrogen from water electrolysis), and simulate unit operations like compressors, heaters, reactors, coolers, and separators. The software facilitates precise mass and energy balances, incorporates reaction kinetics, and handles recycle loops to effectively represent the Haber-Bosch process under defined conditions (e.g., elevated temperature and pressure).

4.1. Definitionofequipmentanditsfunctionsinammoniaproductionprocessflowchart:

4.1.1. B1. B3–Mixer:

Themixerisresponsibleforcombiningnitrogenandhydrogengasesinuniformproportionstoensurea well-distributed and optimal mixture for the reaction in the reactor.

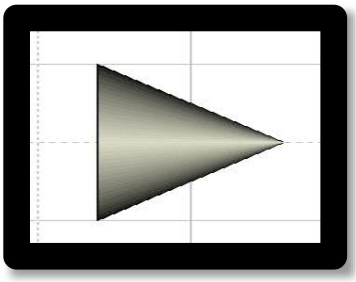


Figure2.1ofMixer

4.1.2. Compressor:

The compressor increases the pressure of the nitrogen and hydrogen gas mixture to the required levels beforeenteringthenextunit.Thishighpressureisessentialtopromotethechemicalreactioninsidethe reactor and improve production efficiency.

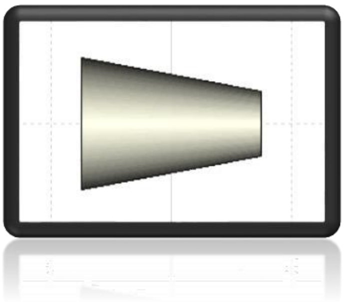


Figure 2.2 Compressor

4.1.3. Cooler/Heat Exchanger:

Afterleavingthereactor,thegasiscooledtoreduceitstemperature,whichhelpscondensethe produced ammonia, facilitating its separation from the unreacted gases.

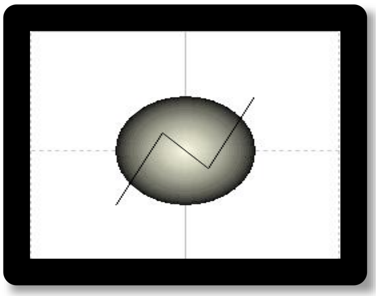


Figure 2.3 Cooler

4.1.4. B5–Reactor(AmmoniaSynthesisReactor):

Inthisreactor,nitrogenreactswithhydrogenunderhightemperatureandpressureinthepresenceofa catalyst to produce ammonia. It is considered the core unit of the production process

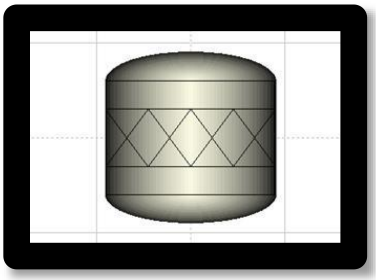


Figure 2.4 Reactor

4.1.5. B7– Separator:

Thisseparatorisresponsibleforseparatingunreactedgasesthatdidnotundergoreactioninthereactor. These gases are then recompressed and returned to the reaction cycle to enhance material utilization.

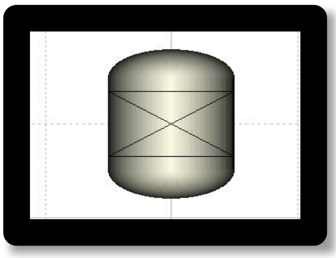
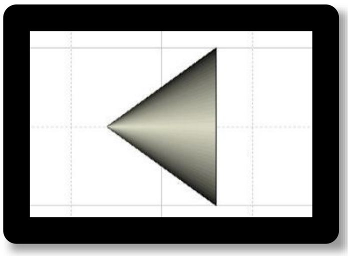


Figure 2.5Separator

4.1.6. B8–Purge Splitter:

Thisdeviceremovesaportionoftheunreactedgasesfromthesystemtopreventtheaccumulationof impurities and undesired gases, ensuring stable operational conditions.

Figure2.6Splitter



5.Methodotology:

Afterassessingtheimportanceof green ammonia and itsroleinthetransitiontogreenenergyand its applications, a systematic plan was developed to design the optimal, most feasible, and most modern method for producing green ammonia. Aspen Plus V12.1 software was used to provide figures and data.

6. GreenAmmonia Production:

In Figure II.10, green ammonia production requires two inputs, similar to the conventional ammoniaprocess.Itrequiresahydrogenstreamandanitrogenstream.Thenitrogenstreamcanbe obtainedfromcryogenicsubsurfacedistillation(ASU),whilethehydrogencanbeobtainedthrough water electrolysis, which splits water molecules into hydrogen and oxygen. This is the primary reason this method is called green, as the ammonia produced is produced via green hydrogen.

Thismethodconsistsofthreemainunits:ahydrogenproductionunit,anitrogenrecoveryunit,and an ammonia synthesis unit. The nitrogen recovery unit will remain the same, while the hydrogen productionunitwillassumeasinglehydrogenstreamwiththeoriginalcomposition.Thisisdueto theabsenceoftherequiredelectrolyzerintheAspenPLUSV12.1.Theammoniasynthesisprocess consists of mixers, compressors, and heat exchangers to achieve a mixture of nitrogen and hydrogen at a specific pressure and temperature, which activates the reaction kinetics. The outlet stream is separated to obtain a stream containing the maximum possible amount of ammonia produced, for use at room temperature and atmospheric pressure

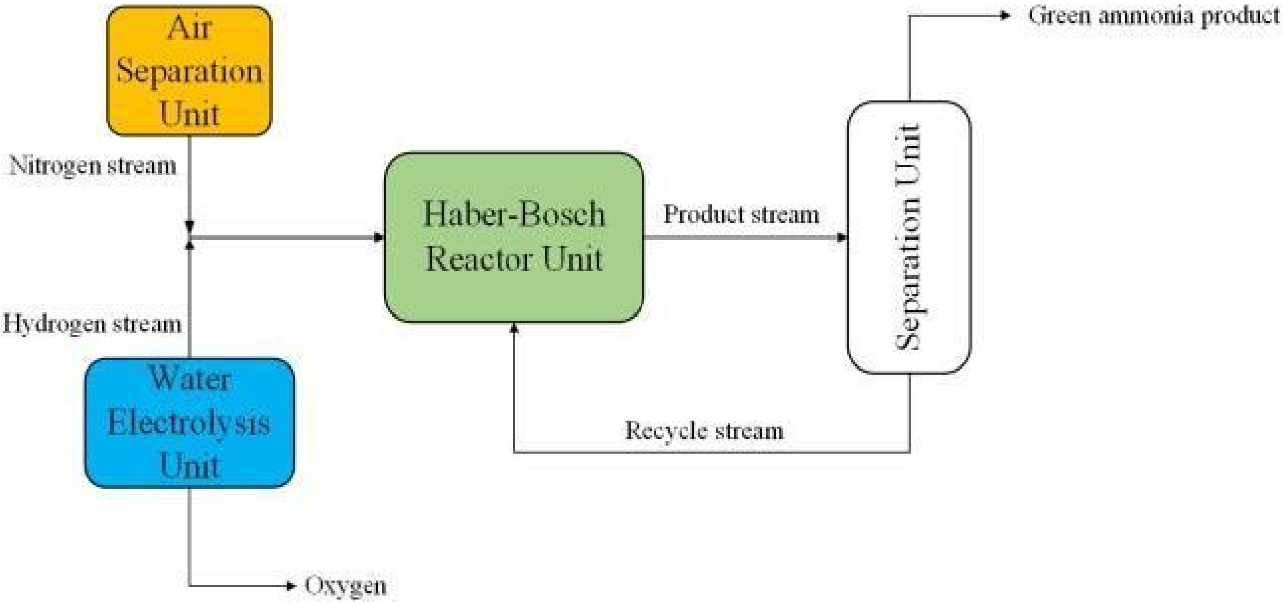


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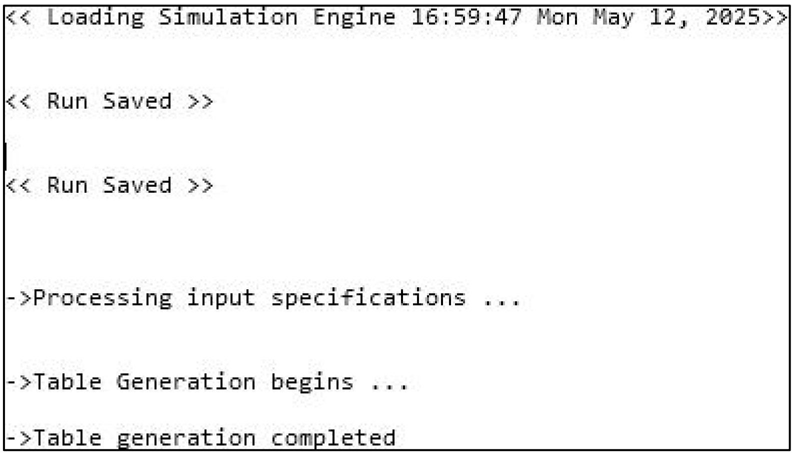
Figure2.7GreenammoniasynthesisBFD

7.NitrogenSource:

The Haber-Bosch process relies heavily on high-purity nitrogen extracted from atmospheric air, which contains about 79% nitrogen. Among the main nitrogen purification technologies—cryogenic air separation units (ASUs), pressure swing adsorption (PSA), and membrane permeation—cryogenic distillation stands out as the most cost-effective and energy-efficient solution for large-scale ammonia production. This process separates nitrogen at extremely low temperatures (-196 °C) and high pressures, delivering ultra-pure nitrogen (≥99.999%) essential for efficient ammonia synthesis. Recent advances in flexible cryogenic unit designs enable seamless integration with variable renewable energy sources through innovative thermal management and load tracking, enhancing both economic feasibility and sustainability. Consequently, cryogenic separation technology is positioned as the ideal method to supply high-purity nitrogen for green ammonia projects within a low-carbon economy framework.. [52]



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->Table generation completed
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7.1. AspenPlusSimulation:

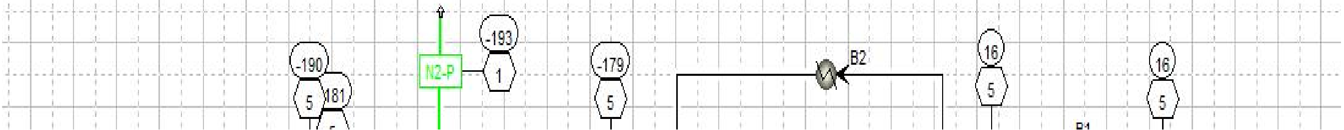


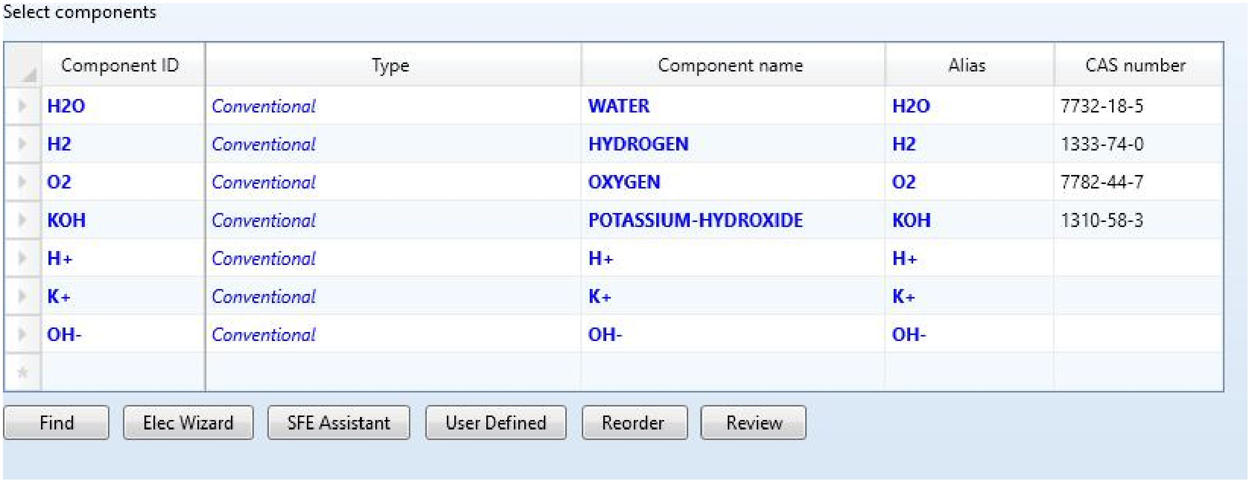
Figure2.8Nitrogenproductionprocesssimulationbyaspenplus

8.GreenHydrogenInput:

In this project, green hydrogen is produced through alkaline water electrolysis, utilizing a potassium hydroxide (KOH) solution as the electrolyte. This process is known for its robustness, lowcapitalcost,andsuitabilityforlarge-scalehydrogengeneration.Theelectrolyzeunitoperates by passing an electric current through a mixture of water and KOH, which facilitates the dissociation of water molecules into hydrogen and oxygen.

IntheAspenPlussimulation,theelectrolyteinputstream(S1)consistsof102833kg/hofahighly concentratedKOH-H_2 Osolutionat25°Cand1bar.Anadditionalstreamofdeionizedwater(S2), at a flow rate of93376.1 kg/h, is introduced to maintain proper hydration and electrolytebalance.

The electrolyze operates at an elevated temperature of 93°C and a pressure of 29 bar, which enhancesionicconductivityandgasseparationefficiency.Theresultinghydrogenstream(S12)is separated and conditioned for further use in the ammonia synthesis process.



Select components

Component ID	Type	Component name	Alias	CAS number
H2O	Conventional	WATER	H2O	7732-18-5
H2	Conventional	HYDROGEN	H2	1333-74-0
O2	Conventional	OXYGEN	O2	7782-44-7
KOH	Conventional	POTASSIUM-HYDROXIDE	KOH	1310-58-3
H+	Conventional	H+	H+	
K+	Conventional	K+	K+	
OH-	Conventional	OH-	OH-	

Figure2.9 INPUTFORGREENHYDROGEN

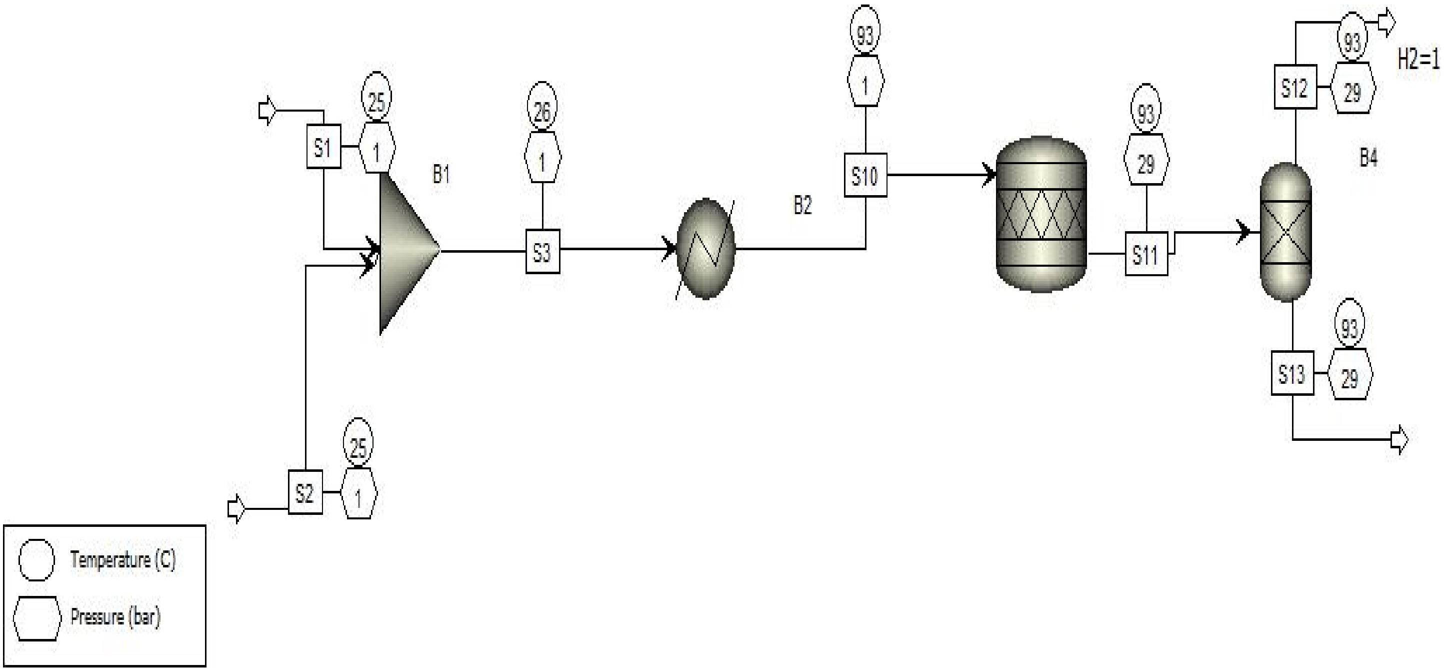


Figure2.10SIMULATIONOFGREENHYDROGENPRODUCTIONBYWATERELOCTROLYSIS(KOH)

Afterlookingintoeachprocessline,thewholeproductionflowcanbeassembledinto the following process flow diagrams (PFD)

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- ->Processinginputspecifications...

➢ **Information**

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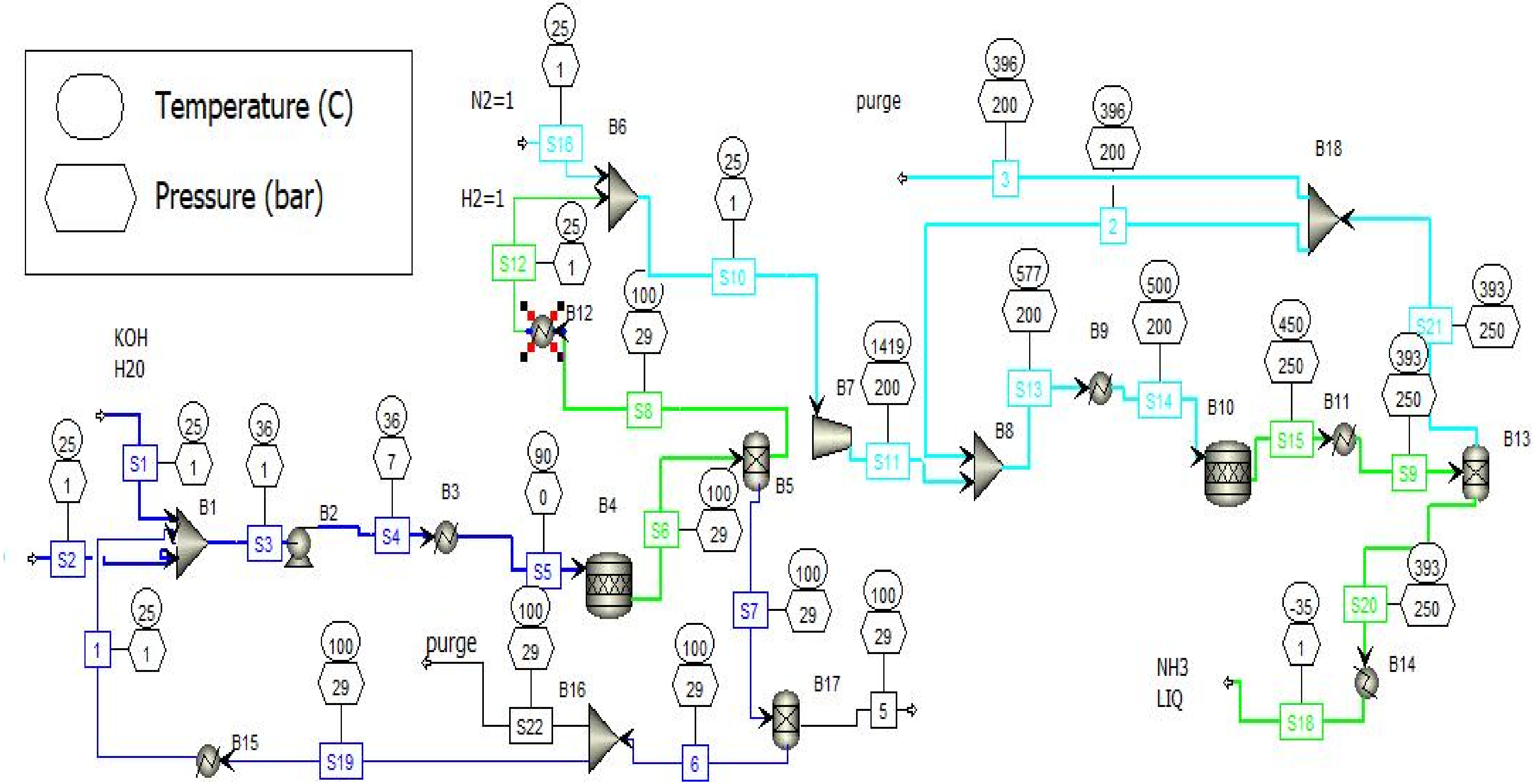

Figure2.11GreenammoniaPFD.Landscape

9. AspenPlusSimulation:

Thisprocessflowchartillustratesgreenammoniasynthesisusingaspenplusv12.1byHaberBoschreaction. First, nitrogen and hydrogen are mixed at 25c and 1Par, then pass through a certain number of heat exchangers and compressors for heating up the mixturetemperature and pressure until it reaches 500°C and 200par which assists HaberBosch reaction to start in plug flow reactor as shown in figure 5 . Before ammonia could be stored in a tank, the temperature and pressure should be dramatically decreased to around -36 °C and 1par respectively

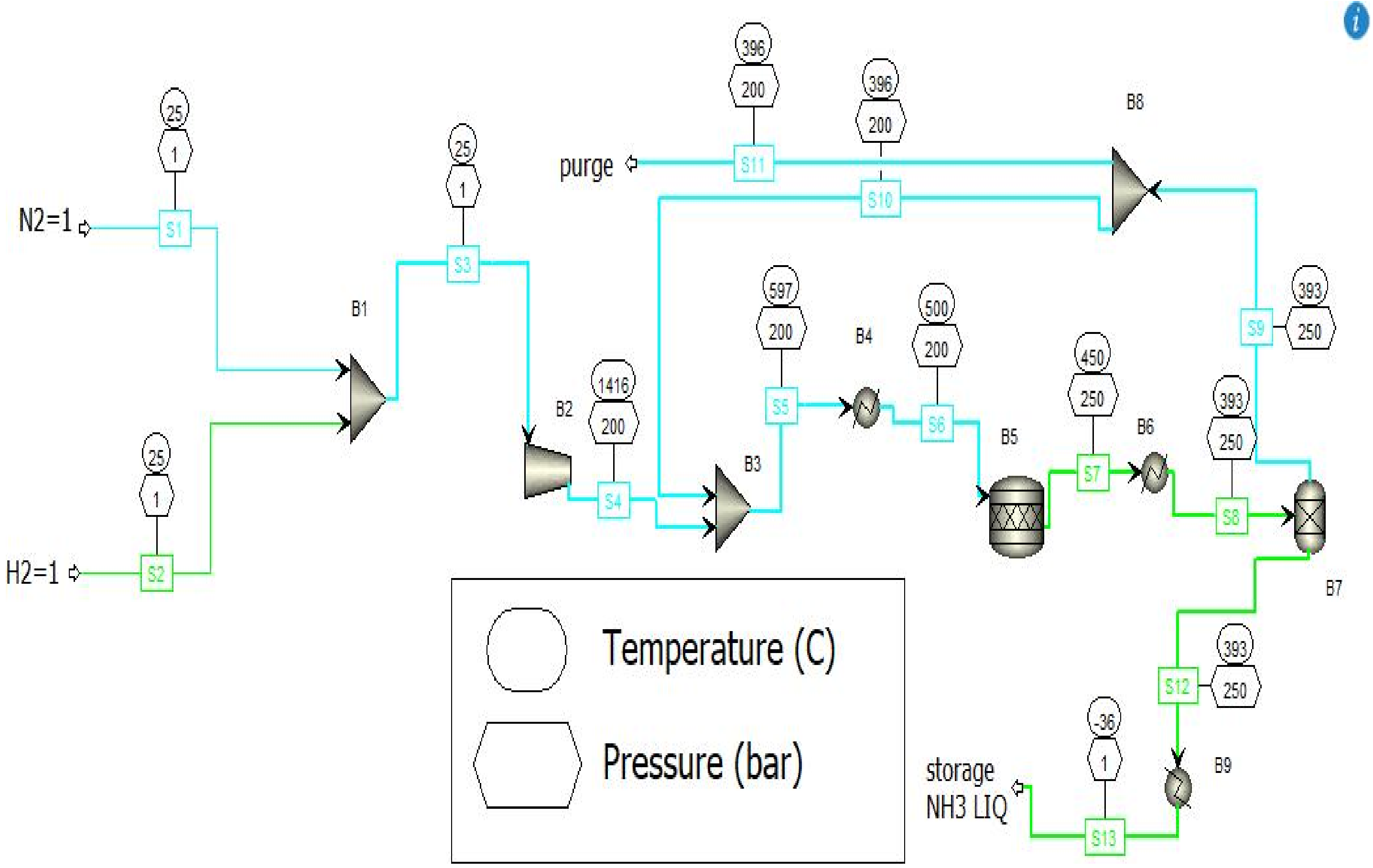

Figure2.12ProcessflowchartofgreenammoniasynthesisonAspenPLUSV12.1.

10. Conclusion:

The Aspen Plus simulation framework effectively models the green ammonia production process, enablingdetailedmassandenergybalance analysesessentialforprocessoptimization.Thisapproach providesarigorous basis for designing sustainable, low-carbonammoniasynthesispathways,thereby advancing the development of environmentally benign chemical manufacturing.

Chapter3

Results and discussions

1. Introduction:

This new method relies on a combination of modern technologies that combine the production of clean electricity, converting it into green hydrogen, and then converting that hydrogen into sustainable ammonia. The whole idea is to move away from the old fossil fuel-based methods, while reducing emissions and increasing energy efficiency.In this installment, we'll go over some of the numbers and findings from our simulations, focusing on how the thermal systems involved in the production of hydrogen and ammonia work. We'll take a look at the flow of materials, how basic units such as electrolysis cells and reactors perform, not forgetting the positive environmental impact of this shift towards a zero-emissions model.Everything here feels like a step towards a cleaner future, but it's not just a dream, it's a reality proven by numbers and analysis.

2. Problematic:

Making ammonia the old-school way, using the Haber-Bosch process with hydrogen from natural gas, is a huge contributor to CO_2 emissions. It's not great for the planet and kinda goes against what we're trying to do with sustainability these days. That's where green ammonia comes in - it swaps out the fossil fuel hydrogen for clean hydrogen made by splitting water using renewable energy. In this chapter, we'll use Aspen Plus to model a green ammonia setup, checking how well it works energy-wise, figuring out how to make it more efficient, and seeing if we can actually pull off making pure ammonia without any carbon footprint.

3. Result of Simulator:

3.1 Nitrogen Input:

In this section, we present the thermodynamic properties of the nitrogen feed used in the green ammonia production process. The data was obtained through process simulation using Aspen Plus and serves as a basis for understanding energy balances and optimizing system performance.

Table 3.1 Thermodynamic Properties of Nitrogen Feed Stream

Settings	**Value**	**Unit value**
Temperature	25	C
Pressure	1	bar
Mass Enthalpy	-228.886	J/kg

Mass Entropy	3.2537	J/kg-k
Mass Density	1.1305	Kg/cum
Enthalpy Flow	-3433.29	KJ/hr
Average MW	28.0135	/
Mass Flows	15000	Kg/hr
Mass Vapor Fraction	1	/

Here's the nitrogen gas data we used for the green ammonia project. We ran the numbers through Aspen Plus to get these specs. The nitrogen comes in at room temperature, around 25°C, and normal pressure. It's got an enthalpy value sitting at -228.886 J/kg, and the entropy's at 3.2537 J/kg·K - basically tells you about its energy state and how chaotic the molecules are. The gas isn't very dense, just 1.1305 kg per cubic meter. Total energy flow works out to -3433.29 kJ every hour, which is what we're working with heat-wise. We're pushing through 15,000 kg of nitrogen every hour, and since it's all gas (vapor fraction shows 1), that molecular weight of 28.0135 stays consistent. These numbers really matter when we're figuring out how to make the whole process more efficient and

3.2 GRENN HYDROGN INPUT:

The following section outlines the key thermodynamic parameters of two distinct liquid input streams—S1 and S2—used in the green hydrogen production pathway. Stream S1, a potassium hydroxide solution, functions as an electrolyte, while S2 consists of demineralized water used in electrolysis. Understanding their thermal behavior and flow characteristics is essential for assessing system performance and ensuring process stability.

Table 3.2 Thermodynamic Data of Green Hydrogen Input Streams (S1 and S2)

Settings	**Value**		**Unit value**
	S1	S2	
Temperature	25	25	C
Pressure	1	1	bar
Mass Enthalpy	-9.81864e+06	-1.58757e+07	J/Kmol
Mass Entropy	-4325.04	-9056.91	J/Kg-k
Mass Density	1856.27	997.167	Kmol/cum

Enthalpy Flow	-1.00968e-09	-1.48241e-09	KJ/hr
Average MW	25.2402	18.0153	/
Mass Flows	102833	93376.1	Kg/hr
Mass Liquid Fraction	1	1	/

So, this table breaks down the properties of two liquid streams used in making green ammonia. The first one, S1, is mostly potassium hydroxide mixed with some water, while S2 is just plain water. Both come in at room temperature and normal pressure. That KOH solution in S1 helps conduct electricity in the electrolysis part of the process, and the water in S2 gets used directly in the reactions.

The numbers show they behave differently - S1's got way less enthalpy than S2, and both have negative entropy values, which might mean they were cooled down or pressurized before this step.

They're definitely liquids though, with those high-density numbers. The molecular weight's different too - S1's mix makes it lighter than pure water in S2. Kinda interesting how these simple ingredients play such specific roles in the whole ammonia-making process.

3.2.1 GREEN HAIDROGEN OUTPUT

This section provides the thermodynamic data of the green hydrogen stream at the outlet of the electrolysis unit, as obtained from process simulation.

Table 3.3 Thermodynamic Properties of Green Hydrogen Output

Settings	**Value**	**Unit value**
Temperature	25	C
Pressure	1	bar
Mass Enthalpy	496.068	J/Kg
Mass Entropy	53.4473	J/Kg-K
Mass Density	0.0812716	Kg/cum
Enthalpy Flow	2529.95	KJ/hr
Average MW	2.01588	/
Mass Flows	5100	Kg/hr
Massvapor Fraction	1	/

Here's what the data from Table 3 tells us about the green hydrogen coming out of the electrolysis setup. This hydrogen is the end product of splitting water, and it's also what gets fed into the ammonia reactor. It comes out at room temperature and normal pressure - nothing fancy there. The numbers show it's in a stable gas form, with low density and all the other signs pointing to it being fully gaseous. We're looking at about 5100 kg of hydrogen flowing every hour, which is a solid amount for making ammonia. The heat energy it carries isn't huge, but it's there. And the molecular weight checks out - it's just regular H_2 , exactly what we'd expect. The simulation results from Aspen Plus back all this up. These parameters ensure that the hydrogen stream is pure, gaseous, and energetically stable, making it ideal for efficient and sustainable green ammonia synthesis when combined with nitrogen in the reaction system. Furthermore, the system achieves a water recovery rate of 85% in (S19), significantly enhancing resource efficiency and reducing freshwater consumption in the process.

4. Ammonia Input:

This section outlines the operating conditions of the nitrogen and hydrogen input streams used in the ammonia synthesis stage, as defined in the simulation results.

Table 3.4 Datasheet for input streams

NAME	Vapour Fraction	Temperature(C)	Pressure(bar)	Mass Flow (Kg/hr)
Nitrogen	1	25	1	15000
Hydrogen	1	25	1	5100

This table shows a basic comparison between nitrogen and hydrogen as they go through the process. You can use the gas to finish the vapor, but you'll need to set the temperature and pressure to standard conditions—around -25°C and 1 bar. The difference in fuel oil amounts is pretty big—hydrogen comes out to over 15,000 kg per hour, while nitrogen is only about 5,100 kg per hour. The key takeaway here is that you don't really need to stress over the gas conditions themselves. What matters more is keeping the volume and system equipment the same, since that's what helps you actually understand how the process works.

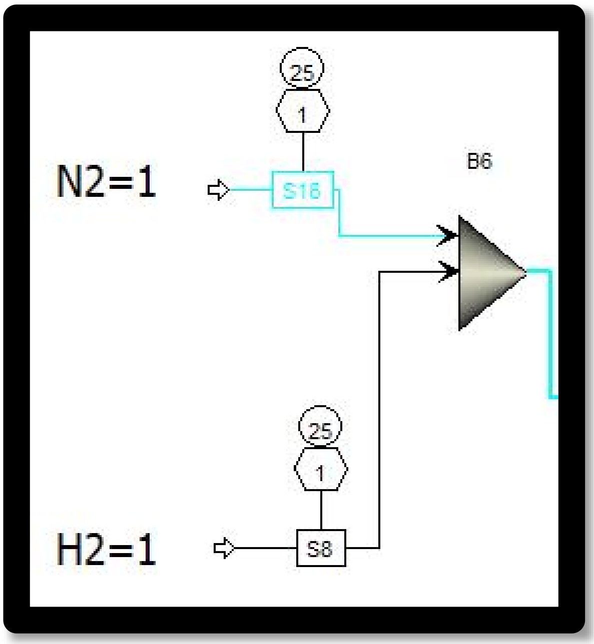

Figure 3.1 hydrogen and nitrogen input configuration

So, in this diagram, you have two main gas lines - one for nitrogen and one for hydrogen. Each one goes through its own controller (there's S16 for the nitrogen side and S8 for the hydrogen side) before they feed together into a centralized mixing unit called B6. That's where the two gases come together and mix together in one compact stream. It's pretty simple when you look at it this way.

5. Reactor Output:

So, the ammonia reactor spits out this super-hot, high-pressure vapor mix at around 450 degrees and 250 bars. That's just how the Haber-Bosch process rolls - it needs those crazy conditions to work. You'd think it'd be pure ammonia coming out, but nope. There's still a bunch of leftover hydrogen and nitrogen in there, plus the actual ammonia we want. The numbers show hydrogen's way more abundant than nitrogen at this stage, but the ammonia's holding its own too. Problem is, we can't just use this messy mix as-is. Gotta send it through another unit to separate the good stuff (ammonia) from the leftovers (hydrogen and nitrogen), which we'll just recycle back through the system. Makes the whole operation way more efficient that way.

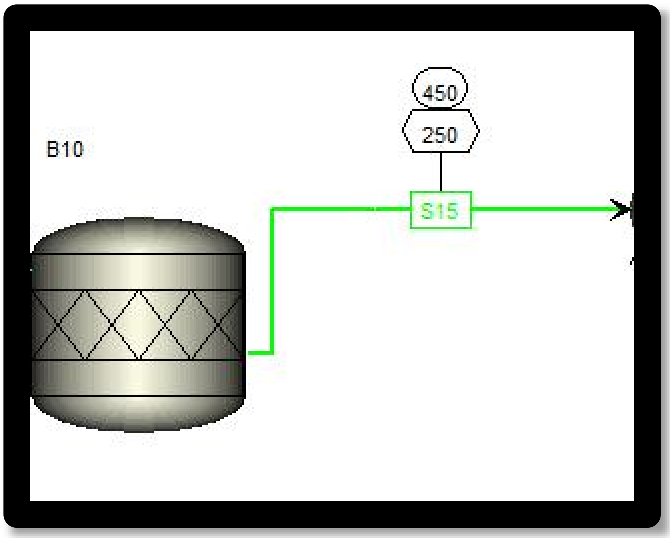

Figure 3.2 Output from reactor Unit

This drawing shows the main part of the process of making green ammonia. The main reactor (labeled B10) is where most of the work happens - it's essentially the heart of the entire sustainable ammonia production process. You can see the ammonia product flowing out as this green line. It passes through a monitoring or control unit of some sort (this is S15) where the numbers 450 and 250 appear - possibly temperature or pressure readings. After that, it goes to whatever comes next in the production line. It's not very technical, but it gets the idea across in a much clearer way while retaining all the important details.

Table 3.5 Reactor output properties.

Temperature	**450**	**C**
Pressure	250	Bar
Molar Vapor Fraction	1	/
Molar Enthalpy	1751.6	Cal/Mol
Mass Enthalpy	392.911	Cal/gm
Molar Enthalpy	-6.68	Cal/Mol*K
Mass Enthalpy	-1.49	Cal/gm*K
Molar Enthalpy	0.0039	Mol/cc
Mass Enthalpy	0.01747	Gm/cc
Enthalpy Flow	3.74 x 10^6	Cal/s
Average MW	4.49	Cal/gm

The tables show what you'd usually get from an ammonia reactor. It runs hot—around 450 °C—and under crazy high pressure, like 250 bar, which is pretty standard for the Haber-Bosch method. That keeps everything in gas form, no liquid hanging around. The low average molecular weight means there's still some leftover hydrogen and nitrogen in the mix, not just ammonia. But the big takeaway? The output is pumping out over 1000 kmol of ammonia every hour, and nothing else. That's a solid sign the reaction's working well, maybe even better than usual, since hitting full conversion in one go isn't something most industrial setups pull off.

Table3.6 Reactor output mole flows.

Mole Flows	**Total:7705.02**	**Unit value**
H_2	6543.79	Kmol/hr
N_2	129.026	Kmol/hr
NH_3	1032.21	Kmol/hr

So, looking at table six, we've got the molar fluxes coming out of the reactor, totaling about 7,705 kmol per hour. Hydrogen gas makes up most of that—around 6,543 kmol/hr—which makes sense since it's a key player in the reaction. Ammonia comes in second at roughly 1,032 kmol/hr, and nitrogen trails way behind at just 129 kmol/hr. The numbers tell us the reactor's doing its job pretty well. The fact that there's so much ammonia means the conditions inside are working like they should, and the tiny amount of leftover nitrogen suggests most of it got used up in the reaction. That's a good sign for conversion rates. Overall, this data helps us see how well the reactor's performing and whether it's hitting the targets we set for the industrial process.

Table 3.7 Reactor output mole fractions.

Mole Fractions	value
H_2	0.8492
H_2	0.016745
NH_3	0.1333

Here's what the numbers in **table 3.7** show about what's coming out of the reactor. Hydrogen makes up most of it at around 85%, which makes sense since we're using way more of it than we need for the reaction. Ammonia comes in second at about 13% - that's the good stuff we're actually trying to make. There's just a tiny bit of nitrogen left, less than 2%, which tells us most of it got used up like it should. Looking at these percentages gives us a pretty clear picture of how the reaction's going. When we see this much hydrogen hanging around, it means we've got plenty to work with. The ammonia amount shows the reaction's doing its job, and that barely-there nitrogen tells us we're not wasting much. It's all useful info for figuring out if the reactor's running right and how we might tweak things to get even better results.

6. Separator Output:

The mole flow data presented here reflects the composition of the stream exiting the separation unit, providing insight into the distribution of hydrogen and residual nitrogen following the separation stage.

Component	Mole Flow (kmol/hr)
H_2	6543.79
N_2	129.026
NH_3	0

Table 3.8 Separator Output Mole Flows (S21).

So, table 8 shows what's coming out of the separator, mostly hydrogen with a flow rate around 6544 kmol per hour. There's also a bit of nitrogen in there, about 129 kmol per hour. Altogether, it adds up to roughly 6673 kmol per hour. Basically, the separator does a pretty good job pulling out most of the hydrogen, with just a little nitrogen left over. This kind of info helps figure out how well the process is working and where we might tweak things down the line.

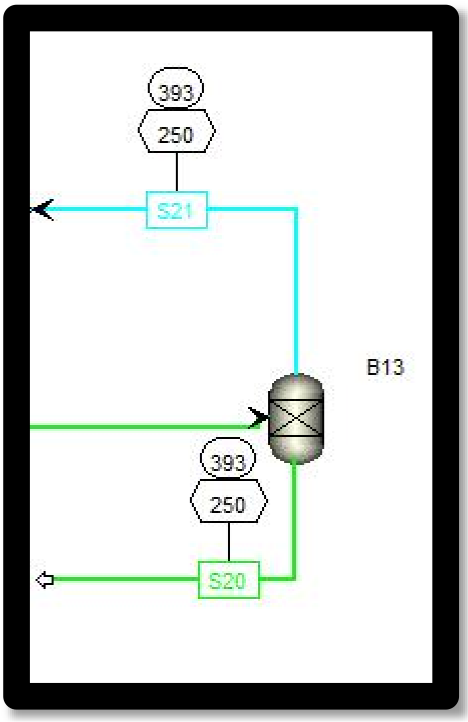

Figure 3.3 Output from Separation Unit

This diagram shows the separator unit, labeled B13, which is a key step in making green ammonia. It takes in two different flows - one with leftover gases through S21 and another with pure ammonia through S20. Both streams go through checkpoints 393 and 250 where they're monitored. Inside B13, the gases get split up so some can be reused, while the clean green ammonia moves on to the next part of the process. It's pretty neat how this setup helps keep everything running smoothly while making sure the ammonia stays pure.

7.Splitter Output:

Detailed below are the output characteristics of the splitter and subsequent separator stages, focusing on the recovered and purified product streams as defined in the simulation data.

Table 3.9 Fplit Output Mole Flow.

Component	**Mole Flow (kmol/hr)**
H_2	5562.19
N_2	109.672
Total	5671.86

The numbers in table show what comes out of the splitter, which is set up to grab back about 85% of the unused gases. Hydrogen is the big player here, flowing at over 5500 kmol per hour, while nitrogen trails way behind at just under 110. Altogether, you're looking at around 5670 kmol per hour coming out. The fact that nothing else shows up in the mix tells you this thing is pretty good at its job—just pulling out the hydrogen and nitrogen so they can be reused. That kind of efficiency is key for keeping costs down and making the whole process a little greener.

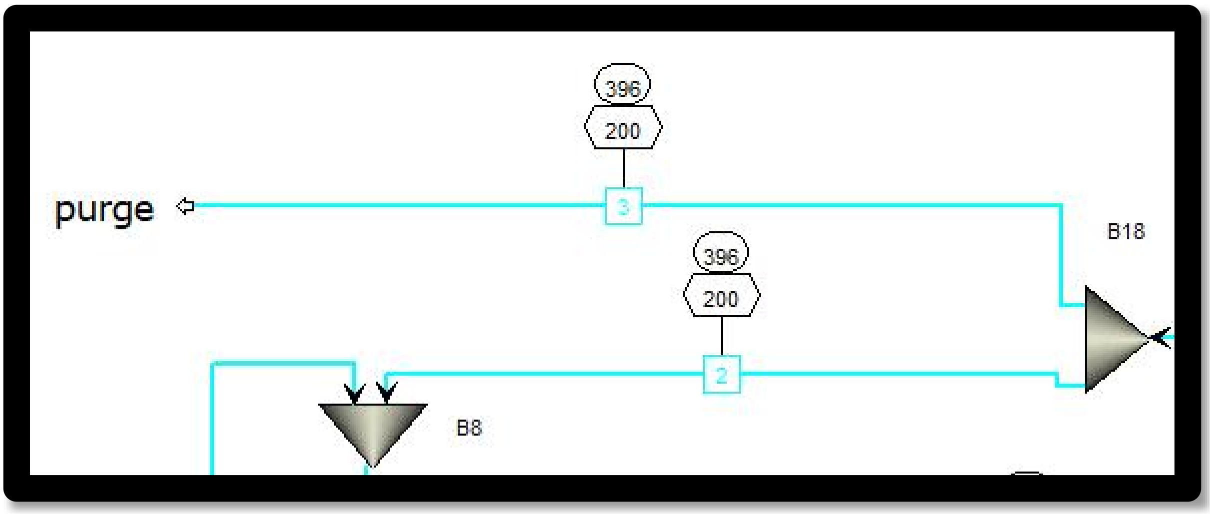

Figure 3.4 Output fromSplitter Unit

This diagram in **figure 3.2**shows how a gas recovery system works in some high-tech industrial setup. There's this unit labeled B18 that basically sorts out the gases that didn't react. Those gases get pushed back into the system under crazy high pressure and heat - we're talking 200 bar and nearly 400°C hot. To keep things running smooth and avoid gunk building up, they split the recovered gas. Most of it (like 85%) gets mixed back in with other gas streams in unit B8. The rest (that 15% bit) gets kicked out as waste gas. That purge step is super important because it stops impurities from messing with the whole system. It's all about keeping the process clean while making sure nothing useful gets wasted. Pretty clever how they balance it all out.

Table 3.10 Separator output properties.

Parameter	S18	Units

Temperature	-35.3	C
Pressure	1	Bar
Molar Vapor Fraction	1	/
Molar Enthalpy	-17022.1	Cal/mol
Mass Enthalpy	-999.504	Cal/gm
Molar Entropy	-48.9186	Cal/mol*K
Mass Entropy	-2.8724	Cal/gm*K
Molar Density	0.040285	Mol/cc
Mass Density	0.686075	Gm/cc
Enthalpy Flow	4800000	Cal/s
Average MW	17.0306	/

The data for stream S18 shows how the ammonia gets separated after the reactor stage. It's kept super cold at around -35 degrees and at a low pressure of 1 bar, which is perfect for turning the ammonia into liquid while the leftover hydrogen and nitrogen stay as gas. The numbers show it's all liquid at this point, which makes sense since that's what we want with ammonia. The molecular weight checks out too—it's exactly what you'd expect for pure ammonia. And those big negative enthalpy values? That just tells you how much cooling it took to get the ammonia to condense like that. It's all pretty straightforward when you look at the numbers.

Table 3.11 Separator output mole flows.

Mole Flows	**Total:1032.21**	/
H_2	0	Kmol/hr
N_2	0	Kmol/hr
NH_3	1032.21	Kmol/hr

Table 3.12 Separator output mole fractions.

Mole Fractions	**Quantity**
H_2	0
N_2	0
NH_3	1

Looking at the numbers in Table 11 and Table 12, it's pretty clear the separator is doing its job really well. The whole output stream, all 1032.21 kmol/h of it, is just pure ammonia - no leftover hydrogen or nitrogen hanging around. That tells us the separation process is working exactly like it should, pulling out the good stuff and leaving nothing behind. What's cool is how clean the ammonia comes out, which matters big time for both quality and keeping costs down. Any unreacted gases get sent back to try again, so nothing goes to waste. It's one of those things that makes the whole ammonia production process way more efficient and sustainable in the long run. The numbers don't lie - this setup is nailing it.

8. CO_2 emission:

This part focuses on the assessment of carbon dioxide emissions associated with various feed streams used in the green ammonia process. The evaluation is based on simulation outputs and serves to verify the carbon-neutral performance of the system.

Feed Stream Name	**Flow(kg/hr)**	CO_2**(kg/hr)**
S16	15000	0
S8	5100	0
3	2520.97	0
S18	17579	0

Table 3.13 CO_2 emission data.

So, check out table 13 - it's got the CO_2 emission numbers for different feed streams. Kinda weird though, all the values are showing up as zero even though there's definitely stuff moving through the system. What this tells us is that these particular streams aren't adding to greenhouse gases at all. Maybe the materials just don't have any burnable carbon in them, or the process itself is super-efficient. Either way, it's good news for keeping things green and making the whole operation more sustainable.

9. Conclusion:

The results of this chapter demonstrate that the production of green ammonia using Aspen Plus is a feasible and efficient process, with zero CO_2 emissions. High conversion rates were achieved for both hydrogen and nitrogen, indicating an efficient reaction. Moreover, 85% of unreacted gases and water were recovered, enhancing process efficiency and minimizing waste.

These findings suggest that green ammonia could serve as a sustainable and environmentally friendly alternative to conventional ammonia production methods, which are associated with significant carbon emissions. This model supports the green hydrogen economy and contributes to achieving carbon neutrality goals.

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General conclusion

General conclusion

The need to replace high-emission industrial processes, especially the manufacture of ammonia from fossil-based hydrogen, has become more pressing due to growing environmental concerns and the worldwide push for carbon neutrality. This study investigated the intriguing idea of green ammonia, which uses hydrogen produced by electrolyzing water using renewable energy sources. The study was divided into three primary parts. The first part gave a theoretical review of ammonia production, identifying gray, blue, and green ammonia and stressing developments in hydrogen production and other synthesis methods.

Then, using Aspen Plus software, a conceptual design of a green ammonia plant was created, defining ideal operating conditions and describing key process units such air separation, alkaline electrolysis, gas mixing, compression, and the Haber-Bosch reactor. Lastly, the outcomes of the simulation were examined and compared to conventional procedures. The results indicated that the green ammonia system could generate 1032.21 kmol/h of high-purity ammonia with no direct CO_2 emissions, improve energy efficiency by integrating heat, and use resources sustainably by recovering water and recycling 85% of unreacted gases..

This study shows that it is possible to create green ammonia in a more sustainable manner, providing a workable way to decarbonize industries like power generation and future energy systems. The traditional Haber-Bosch method is still widely used because it is economical and technically advanced, but it has a high environmental cost and is no longer in line with international climate targets. Our study demonstrated that using renewable hydrogen instead of hydrogen derived from fossil fuels reduces carbon emissions without sacrificing production efficiency. However, a number of practical endure—exorbitant upfront expenses, the erratic nature of renewable energy, and the requirement for extensive new infrastructure. Investment and teamwork will be needed to overcome these obstacles. Priorities include developing a completely integrated supply chain, improving energy storage options, and reducing the price of electrolyzers and catalysts. Making the switch to green ammonia is a practical approach with revolutionary potential, not just an idealistic objective. A cleaner, more sustainable future may be mostly dependent on green ammonia if scientists, businesses, and legislators work together well. It is unquestionably a crucial component of the larger solution to global decarbonization, even though it is not a panacea. transformative potential. If scientists, industries, and policymakers collaborate effectively, green ammonia could play a pivotal role in creating a cleaner, more sustainable future. While it is not a silver bullet, it is undeniably a key part of the broader solution to global decarbonization**.**

Bibliographic references

Bibliographic references

[1] Banafsheh Jabarivelisdeh1 , Enze Jin1 , Phillip Christopher2 , Eric Masanet1,3 Ammonia Production Processes from Energy and Emissions Perspectives: A Technical Brief USA

[2] Product Stewardship GUIDANCE FOR TRANSPORTING AMMONIA BY RAIL 2007 Edition

[3] Maggie Nasry1, Noran Ashraf 1, Rawda Serag1, Shimaa Ahmed1, Omar Hatem1, Mai Abd Elbasset1,Fathy Shokry1, Amr Mansi1,2 , Mohamed Bassyouni 1,2 Application of water electrolysis for green ammonia production: a plant simulation study Egypt August 2024

[4] Vasileios Kyriakou,1,2,4, * Ioannis Garagounis,2,3 Anastasios Vourros,2,3 Eirini Vasileiou,2,3 and Michael Stoukides2,3 An Electrochemical Haber-Bosch Process
January 15, 2020 , Joule

[5] Joaquín Barrera Gajardo Technical-economic analysis of the electrosynthesis of ammonia POLITECNICO DI TORINO March 2021

[6] Leigh Krietsch Boerner, special to C&EN Industrial ammonia production emits more CO_2 than any other chemical-making reaction. Chemists want to change that June 15, 2019

[7] Palina Nicolas Technical, environmental and economic analysis of
green ammonia as an energy vector in Spain September 2022

[8] Xu, Q., et al., Anion exchange membrane water electrolyzer: Electrode design, lab-scaled testing system and performance evaluation. EnergyChem, 2022. 4(5): p. 100087

[9] Phillips, R. and Charles W. Dunnill, Zero gap alkaline electrolysis cell design for renewable energy storage as hydrogen gas. RSC Adv, 2016. 6(102): pp. 100643–100651

[10] Dr. Mridula Bharadwaj, Dan Millison A ROADMAP FOR DEVELOPING AND SCALING THE GREEN HYDROGEN ECOSYSTEM November 2023

[11] Tjahjono, B., Stevani, I., Siswanto, G. A., Adhitya, A., & Halim, I. (2023). Assessing the feasibility of gray, blue, and green ammonia productions in Indonesia: A techno-economic and environmental perspective. International Journal of Renewable Energy Development, 12(6), 1030–1040

[12] K. Kolmetz, J. Aprilia, Air Separation Units - Engineering Design Guidelines, 2013.www.klmtechgroup.com

Bibliographicreferences

[13] Palina Nicolas Technical, environmental and economic analysis ofgreen ammonia as an energy vector in Spain September 2022

[14] John Kristian Ellertsen & Sondre Gunnar Haugen Flexible Production of Green Ammonia Norwegian School of EconomicsBergen, Fall 2023

[15] G. Cheng et al., “Analysis and prediction of green hydrogen production potential by photovoltaic-powered waterelectrolysis using machine learning in China,” Energy, vol. 284, p. 129302, Dec. 2023, doi:10.1016/J.ENERGY.2023.129302.

[16] Maggie Nasry1 , Noran Ashraf 1 , Rawda Serag1 ,Shimaa Ahmed1 , Omar Hatem1 , Mai Abd Elbasset1 , Fathy Shokry1 , Amr Mansi1,2 , Mohamed BassyouniApplication of water electrolysis for green ammonia production: a plant simulation studyAugust 2024

[17] S. Ghavam, M. Vahdati, I. A. G. Wilson, and P. Styring, “Sustainable Ammonia Production Processes,” FrontEnergy Res, vol. 9, p. 580808, Mar. 2021, doi: 10.3389/FENRG.2021.580808/BIBTEX.

[18] H. Zhang, L. Wang, J. Van herle, F. Maréchal, and U. Desideri, “Techno-economic comparison of greenammonia production processes,” Appl Energy, vol. 259, p. 114135, Feb. 2020, doi: 10.1016/J.APENERGY.2019.114135

[19] S. Anwar, F. Khan, Y. Zhang, A. D.-I. J. of Hydrogen, and undefined 2021, “Recent development in

[20] Roger Ruan Sustainable Nonthermal Plasma Assisted Ammonia Production Environment and Natural Resources Trust Fund 2025 Request for Proposal

[21] . Xiaowang Yan 1 ,Dengyun Wang 1 , Lijian Wang 2,3, Dingkun Yuan 1 ,Zhongqian Ling 1 ,Xinlu Han 4 and Xianyang Zeng Research Progress of Nonthermal Plasma for Ammonia Synthesis Processes 2025, 13, 1354

[22] Callie Ndayirindea,* , Yury Gorbanev a , Radu-George Ciocarlan b , Robin De Meyer a,c,1 , Alessandro Smets a,b , Evgenii Vlasov c , Sara Bals c ,Pegie Cool b , Annemie Bogaerts a Plasma-catalytic ammonia synthesis: Packed catalysts act as plasma modifiers Catalysis Today 2023

[23] J. Deng, J. A. Iñiguez and C. Liu, “Electrocatalytic Nitrogen Reduction at Low Temperature,” Joule, vol. 2, p. 846-856, 2018.

[24] M. Aziz, A. TriWijayanta and A. B. D. Nandiyanto, “Ammonia as Effective Hydrogen Storage: A Review on Production, Storage and Utilization,” Energies , pp. 1-25, 2020

Bibliographicreferences

[25] S. Giddey, S. Badwal and A. Kulkarni, “Review of electrochemical ammonia production technologies and materials,” International journal o f hydrogen energy, vol. 38, pp. 14576-14594, 2013

[26] K. Rouwenhorst, P. Krzywda, N. Benes, G. Mul and L. Lefferts, “Ammonia production technologies,” in Techno-Economic Challenges of Green Ammonia as Energy Vector, Amsterdam, Elsevier, 2020, pp. 41-84

[27] John Kristian Ellertsen & Sondre Gunnar Haugen Flexible Production of Green Ammonia Norwegian School of Economics Bergen, Fall 2023

[28] John Kristian Ellertsen & Sondre Gunnar Haugen Flexible Production of Green Ammonia Norwegian School of Economics Bergen, Fall 2023

[29] Muhammad Aziz 1,* , Agung Tri Wijayanta 2 and Asep Bayu Dani Nandiyanto 3 Ammonia as Effective Hydrogen Storage: A Review on Production, Storage and Utilization 18 March 2020

[30] GUIDANCE FOR TRANSPORTING AMMONIA BY RAIL 2007 Edition Issue 2014

[31] Yusuf Bicer [a], Ibrahim Dincer [a b] Environmental impact categories of hydrogen and ammonia driven transoceanic maritime vehicles: A comparative evaluation March 2018

[32] Anny Santodomingo Rojas (Nitric Acid Climate Action Group (NACAG)) AMMONIA TRANSPORT & STORAGE Berlin, January 2024

[33] Hale CC. 1983 Survey of refrigerated ammonia storage in the United States and Canada. Plant Oper Progr July 1984;3(3):147e59

[34] Hale CC. 1983 Survey of refrigerated ammonia storage in the United States and Canada. Plant Oper Progr July 1984;3(3):147e59

[35] Haris Ishaq a b, Curran Crawford a Review of ammonia production and utilization: Enabling clean energy transition and net-zero climate targets Energy Conversion and ManagementVolume 300, 15 January 2024, 117869

[36] creativecommons.org/licenses/by/4.0 Ammonia: zero-carbon fertiliser, fuel and energy store POLICY BRIEFING : February 2020

[37] G. Cheng et al., “Analysis and prediction of green hydrogen production potential by photovoltaic-powered waterelectrolysis using machine learning in China,” Energy, vol. 284, p. 129302, Dec. 2023, doi:10.1016/J.ENERGY.2023.129302

Bibliographicreferences

[38] Palina Nicolas Escola Tècnica Superior d'EnginyeriaIndustrial de Barcelona September 2022

[39] Bassyouni, M., and Saud A. Gutub. "Materials selection strategy and surface treatment of polymercomposites for wind turbine blades fabrication." Polymers and Polymer Composites 21, no. 7 (2013)

[40] Elhenawy, Y., G. H. Moustafa, S. M. S. Abdel-Hamid, M.Bassyouni, and M. M. Elsakka."Experimental investigation of two novel arrangements of air gap membrane distillation module withheat recovery." Energy Reports 8 (2022)

[41] K. Abdulla, Dr. S. M. Walke (2015). Simulation of Pumps by Aspen Plus

[42] M. Byun, Dongjun Lim, Boreum Lee, A. Kim, I. Lee, and 2 more (2021). Economically feasible decarbonization of the Haber-Bosch process through supercritical CO_2 Allam cycle integration. Applied Energy

[43] Ratnakumar V. Kappagantula, Gordon D. Ingram, H. Vuthaluru (2024). Effectiveness of Three Reactor Chemical Looping for ammonia production using Aspen Plus simulation. International journal of hydrogen energy

[44] Islam Shaker, Moataz El-Bagoury, Salma Yaser, Habiba Emad, Omar Hamdy, and 3 more (2024). Process Simulation and Design of Green Ammonia Production Plant for Carbon Neutrality. International Journal of Industry and Sustainable Development

[45] Guillermo de la Hera, Gema Ruiz-Gutiérrez, J. Viguri, B. Galán (2024). Flexible Green Ammonia Production Plants: Small-Scale Simulations Based on Energy Aspects. Environments

[46] The Haber-Bosch Heritage: The Ammonia Production Technology," International Fertilizer Association, 2023

[47] Mao, C., Verma, P., Yang, Z., &Axelbaum, R. L.(2022). Dynamic Modeling and Control of a Rapidly-Ramping Cryogenic Air Separation Unit for Low-Carbon Fossil-Fuel Power Plants (Preprint). Department of Energy, Environmental and Chemical Engineering, Consortium for Clean Coal Utilization, Washington University in St. Louis.Electronic