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PROCESS SIMULATION AND DESIGN OF GREEN AMMONIA PRODUCTION PLANT FOR CARBON NEUTRALITY

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Abstract: This study investigated the viability of green hydrogen as an essential component in the global energy transition. Despite intensified efforts prompted by the ongoing global energy crisis, impediments have arisen, notably in the area of green hydrogen storage techniques. The inherently hazardous nature of hydrogen gas, resembling an explosion when stored conventionally, presents a significant challenge. In response, this study proposed an environmentally friendly, carbon-neutral, and secure storage technique. The focus is on utilizing green hydrogen in the production of ammonia, serving as both a hydrogen carrier and energy storage medium on an industrial scale. The versatile application of green ammonia extended beyond storage, encompassing fertilizer production, refrigeration, and chemical manufacturing, all aligned with principles of sustainable development, green energy transition, and achieving net-zero carbon emissions. The comprehensive study involved the plant design, process flow diagrams, Aspen HYSYS simulation, plant layout, HAZOP study, and an in-depth economic analysis to evaluate feasibility and profitability. The Haber-Bosch simulated process encompassed the entire production line, starting from sustainably sourced hydrogen to the separation unit ensuring a green nitrogen source. Further optimization was achieved through a heat exchanger network utilizing Aspen Energy Analyzer. The study yielded a substantial ammonia production rate of 7058 kg/hr with an impressive conversion rate of nearly 85%, minimizing waste through the recycling of excess hydrogen within the process. The resultant liquid form of stored ammonia in the refrigeration loop facilitates convenient and safe storage of hydrogen.

Keywords: Green Hydrogen; Process Design; Green Ammonia; Energy Transition; CO2 Reduction

1 INTRODUCTION

For the purpose of limiting climate change and its detrimental consequences, greenhouse gas (GHG) emissions and global warming must be reduced [1-4]. Several tactics and steps can be taken to accomplish this objective [5-7]. Reducing GHG emissions can be accomplished by switching from fossil fuels to

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renewable energy sources including solar, wind, and hydropower [8-10]. Infrastructure for renewable energy should be funded by governments, companies, and individuals, who should also encourage its use [11,12]. In addition to increasing energy efficiency in industrial operations, transportation, and buildings can lower energy use and related emissions [13-15]. Improved insulation, energy-saving appliances, and innovative manufacturing processes are some ways to be provided [16,17]. Encouraging environmentally friendly mobility through promoting the use of electric automobiles, bicycles, walking, and public transportation can lower emissions from the transportation sector [18,19]. The production of green hydrogen via electrolysis and renewable energy sources is crucial for combating the effects of climate change [20].

There are several main arguments in favor of the necessity of green hydrogen such as decarbonizing hard-to-electrify sectors. Green hydrogen can be crucial in decarbonizing industries including heavy industrial, shipping, aviation, and long-distance transportation that are difficult to directly electrify [16,17]. These fields can lessen their dependency on fossil fuels and cut their carbon emissions by using green hydrogen as a clean fuel or feedstock [18,19]. Green hydrogen can also be used for grid balancing and energy storage, assisting with the balancing of intermittent renewable energy sources like solar and wind. During times of high production, excess renewable energy can be electrolyzed to produce hydrogen [20,21].

While green hydrogen has a number of advantages, it also has some drawbacks, notably in terms of storage. The following are some of the major difficulties with hydrogen storage [22].

Low energy density as known hydrogen has a lower energy density than fossil fuels, which means that to store enough energy, a large volume or high-pressure storage is needed. Because handling and storing hydrogen under high pressure calls for specialized infrastructure and security measures, this presents logistical and safety issues.

Storage technologies for example, compressed gas, liquid hydrogen, and solid-state storage are a few of the ways hydrogen can be kept in storage. Each storing technique presents unique difficulties. High-pressure tanks, which can be big and expensive, are necessary for compressed hydrogen. Storage of liquid hydrogen needs cryogenic temperatures.

Leakage and permeation are common problems, hydrogen possesses small molecules that easily pass through materials, such as storage tanks and pipes, or leak or permeate through them. To stop hydrogen loss and keep safety, leaks must be controlled, and storage systems must be reliable.

Price represents a significant problem making hydrogen storage systems can be expensive, particularly when taking into account large-scale applications. The total economics of hydrogen storage and use can be affected by the price of high-pressure tanks, cryogenic equipment, or new materials for solid-state storage.

construction of infrastructure Investments in hydrogen storage facilities, pipelines, and transportation infrastructure are necessary to develop a dependable infrastructure for hydrogen storage. The establishment of such infrastructure is essential for enabling the widespread adoption of green hydrogen, but it can be challenging due to the costs involved and the need for cooperation from multiple stakeholders.

Market demand of ammonia is used in fuel cells, agriculture, and chemical production in addition to energy storage. This broad spectrum of market demand could promote economies of scale and reduce ammonia production and storage costs.

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It is crucial to keep in mind that the use of ammonia as a hydrogen transporter is still in its infancy and has its difficulties. The efficiency of ammonia cracking operations must be increased, costs must be cut, and ammonia production's impact on the environment must be addressed. In addition, nitrogen is produced as a byproduct of the conversion of ammonia back to hydrogen, which could have its own effects on the ecosystem if released in significant amounts into the atmosphere. Ammonia must be handled, stored, and used properly to guarantee safety and reduce environmental impact. Ammonia (NH₃) is a real possibility for the delivery and storage of hydrogen. It can assist in overcoming some of the difficulties related to hydrogen storage and has certain advantages over direct hydrogen storage [23].

Ammonia has a higher energy density than hydrogen gas, allowing for the storage of more energy in a given volume. This improves its suitability for long-term storage and shipping. Alongside its extensive use in the fertilizer business, ammonia has a global infrastructure for production, storage, and delivery. This infrastructure's acceptance as a hydrogen transporter might be sped up by repurposing it for ammonia-based energy systems. Ammonia is easier to handle and store than hydrogen gas since it is a liquid at standard ambient temperature and atmospheric pressure. It can be transported using already-built infrastructure, including pipelines and tankers, and conventional tanks for storage. As for extracting back green hydrogen back ammonia, A procedure known as ammonia cracking or decomposition can quickly convert ammonia back to hydrogen. Ammonia may be split up into hydrogen and nitrogen using a catalyst, enabling the creation of hydrogen whenever it is required. As for safety concerns, ammonia has its own safety concerns, although compared to pure hydrogen, it is less likely to leak and permeate. Ammonia has a distinctive smell and may be detected at low amounts, making it possible to find leaks and take action to stop them. On the market level, ammonia has other uses besides energy storage, including fuel cells, agriculture, and chemical manufacturing. This wide range of market demand may encourage economies of scale and lower production and storage costs for ammonia. It is crucial to keep in mind that the use of ammonia as a hydrogen transporter is still in its infancy and has its difficulties. The efficiency of ammonia cracking operations must be increased, costs must be cut, and ammonia production's impact on the environment must be addressed. In addition, nitrogen is produced as a byproduct of the conversion of ammonia back to hydrogen, which could have its own effects on the ecosystem if released in significant amounts into the atmosphere. Ammonia must be handled, stored, and used properly to guarantee safety and minimize the environmental impact [24].

In this paper, the production of green ammonia will be discussed as a means of storage for green hydrogen, where green ammonia can be considered a power-to-x technology. The project consists of a full-on plant design study, where a preliminary design is made using process simulation and diagram sketching, which is then converted into a detailed plant design to assess the selected design's feasibility and profitability, while considering other plant design steps such as plant layout and equipment spacing.

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2 METHODOLOGY

After assessing the importance of green ammonia in its role towards the green energy transition and applications, a methodological plan is made for designing the most optimum, feasible and recent method to produce green ammonia. Several software programs were used as means of providing figures and data, including Aspen HYSYS V10, Aspen Energy Analyzer, Capcost and Microsoft Visio 2013. *Table 1* lists the tools used and their main purposes.

Table 1 Software Programs Used

Program	Purpose							
Aspen HYSYS V10	Process simulation							
Aspen Energy Analyzer	Process optimization (heat exchanger network)							
Microsoft Visio 2013	Block flow diagrams (BFD) and process flow diagrams (PFD) sketching							
Capcost (Microsoft Excel macro-enabled file)	Equipment cost analysis.							

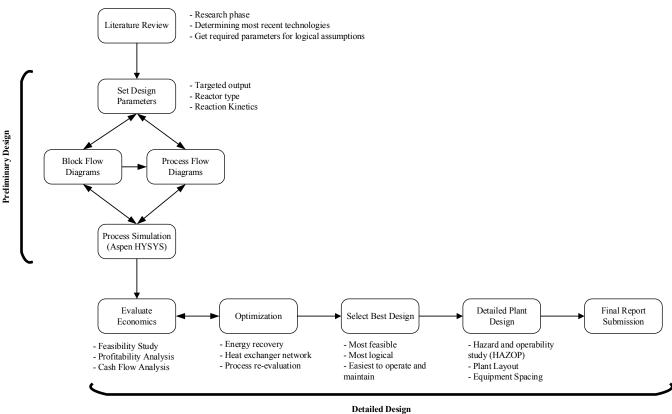


Figure 1 Design steps flowchart.

A series of steps were taken for the construction of a detailed plant design, as seen in **figure 1.** The plant design methodology is divided into two main design sections: preliminary and detailed design. The preliminary design stage is the first section of the plant design study, it first starts with collecting required data and assumption through research and literature review, which is then used to set the design

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parameters, as in the inputs, outputs, flowrates, reaction kinetics, suggested BFD's and PFD's and the sorts. The parameters are then used to construct a simulation model of the entire process on Aspen HYSYS V10, the process is then economically evaluated as well as optimized using Aspen Energy Analyzer, which aided in the development of a heat exchanger network whose main function is perform energy recovery and heat integration between heat exchanger systems. The design is then chosen at its most optimum and feasible form to assess its profitability, and create a plant layout for the process lines, and modify in the process according to the hazard

and operability (HAZOP) study. Egypt has been chosen as the region to perform the plant design study. **Figure 1** is sketched based on the Coulson's general steps of plant design [25].

I. Process Overview

The process of green ammonia is revolved 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 [26].

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

II. Nitrogen Source

As previously mentioned, ammonia is produced by a Haber-Bosch process where the two main reactants are hydrogen and nitrogen [26]. Obtaining nitrogen can be via several ways. Nitrogen is a very readily available source in air making up 79% of it; therefore, air as a source nitrogen is the most viable option. The main issue is the withdrawal of nitrogen from the air; there are several ways to extract nitrogen from air other than the use of Air Separation Unit (ASU), like the use of a combustion reaction to get rid of the oxygen in air leaving the unreacted nitrogen behind [27]. Although it is considered economically feasible option compared to installing an air separation unit, the downside of such process is the formation of Carbon monoxide as a byproduct and additionally the energy needed to burn the hydrocarbon source is also taken in consideration when calculating the capital cost needed. Nitrogen Purification technologies can be divided into three main methods [28].

- 1- Air separation unit (ASU), Cryogenic distillation.
- 2- Pressure swing adsorption (PSA).
- **3-** Membrane permeation.

All three technologies have a very seminal purity, but they differ in the operating temperature as well as the energy consumption of each. So, choosing Cryogenic air distillation was based on a selection criterion, having the lowest energy consumption and the lowest investment cost on the long term. One might argue that it has the highest operating temperature but this can be easily fixed with a heat exchanger network discussed on later sections [29].

Cryogenic distillation works on the basis of separating the elements in air after extreme cooling in a refrigerating system and high compression. The main application

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of this separation technique is oxygen separation so usually the nitrogen is a byproduct in such application but a main one in ammonia production [30].

III. Green hydrogen Input

Scientists and researchers are working to advance the proton exchange membrane water electrolyzing (PEMWE) technology, which is now only accessible in a few developed nations, to manufacture green hydrogen from clean and renewable sources. The biggest problem with this technology is that it requires pricy metal catalysts and proton exchange membranes made of perfluorocarbons (PFC), which increase the expense of production. Because of this, a research team in South Korea has created a new technique for advanced generation electrolyzes that increases lifespans and performance while reducing the price. Additionally, the researchers were able to create an anion exchange membrane fuel cell (AEMFC)-equipped electrolyze, which is expected to take the place of the currently pricey PEMWE. AEMWE's technique does not require pricey platinum-group metal (PGM)-free catalysts because it uses iron instead of titanium for the separation plate of the electrolytic cell [31]. Therefore, the manufacturing cost is decreased by roughly 3000 times compared to the manufacturing cost of PEMWE technology when comparing the price of the catalyst and the separator material in the electro catalyst. However, because of the poor performance compared to PEMWE technology and the problem with the catalyst durability and lifetime of fewer than 100 years of continuous operating hour, this technology has not been used commercially. Additionally, the research team was successful in creating anion exchange materials based on (polyfluorenyl aryl piperidinium) (PFAP) (electrolyte membrane and electrode bonding), a membrane with high conductivity and durability. The material they created has excellent durability over 1,000 runs and a new record cell performance of 7.68 A/cm2. This created material performs roughly 1.2 times better than the PEMWE technology, which has a performance of 6 A/cm2, and about six times better than the performance of the existing anion exchange materials. Due to its great efficiency and low cost, AEMWE technology overcomes the limitations of the most recent electrolyze technology for hydrogen generation. Therefore, it is predicted that this technology will pave the way for the launch of next-generation electrolyze technology in a short amount of time and make it a strong competitor commercially [32]. Figure 2 demonstrates a PFD for production of green hydrogen. PFD is sketched based on the most common method used for green hydrogen synthesis, which is water electrolysis [33].

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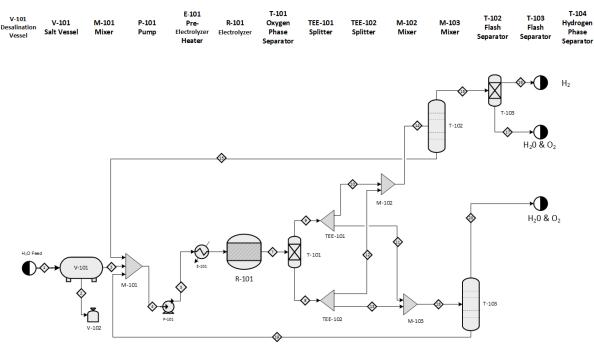


Figure 2 Green hydrogen from water electrolysis PFD.

IV. Green Ammonia Production

In figure 3, green ammonia production requires two inputs, similar to the conventional ammonia pathway. It requires a hydrogen stream and a nitrogen stream. The nitrogen stream can be obtained from cryogenic distillation (ASU), while the hydrogen can be obtained through the process of electrolysis of water which divides the water molecules into hydrogen and oxygen. This is the main reason that this synthesis method is called green; it is because the ammonia produced is via green hydrogen. Collectively, there are three main units. The hydrogen production unit, the nitrogen extraction unit, and the ammonia synthesis unit. The nitrogen extraction unit will remain the same while the hydrogen production unit will be assumed in the form of single hydrogen stream with authentic composition [34-36]. This is due to the absence of the required electrolyzer in Aspen HYSYS10. The ammonia synthesis process will consist of mixers, compressors, and heat exchangers in order to reach a mixture of nitrogen and hydrogen at certain pressure and temperature so that it can activate the reaction kinetics. The output stream is separated to obtain a stream with as much product ammonia as possible to be used at room temperature and atmospheric pressure.

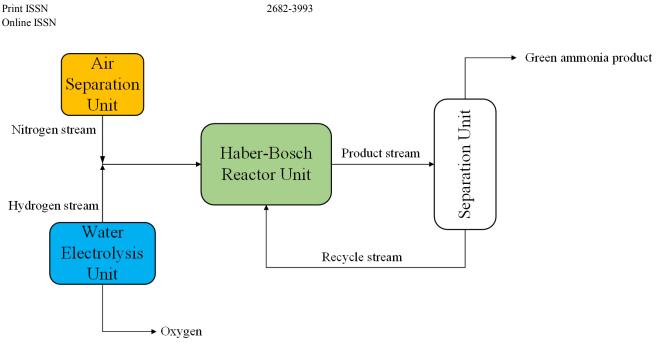


Figure 3 Green ammonia synthesis BFD.

3 SIMULATION RESULTS

The process flowcharts generated and the results discussed as a PFD (Figure 4) extracted from HYSYS V10 (Figure 5), a datasheet regarding the stream properties, the conversion rate, the purity of the product and an energy savings report before and after optimization and/or heat integration with an economic evaluation of the equipment purchasing costs. Aspen Energy Analyzer has been used to suggest possible heat integration between the heat exchangers to reduce amount of heat input and utilize on the internal heat energy of the streams.

I. Process Flow Diagrams

After looking into each process line, the whole production flow can be assembled into the following process flow diagrams (PFD's).

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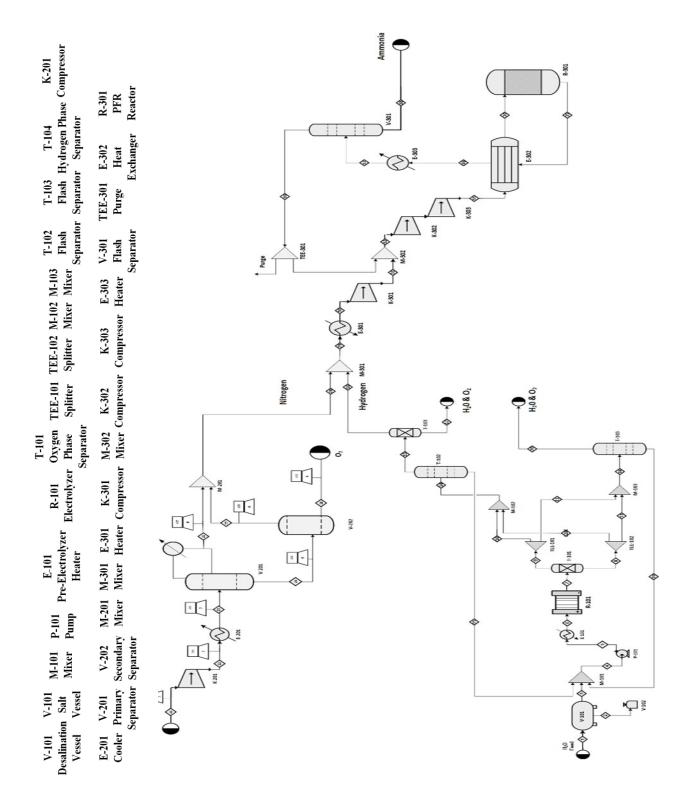


Figure 4 Green ammonia PFD. Landscape

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II. Aspen HYSYS Simulation

This process flowchart illustrates green ammonia synthesis using aspen HYSY v10 by Haber-Bosch reaction. First, nitrogen and hydrogen are mixed at 25c and 101.3 kPa, then pass through a certain number of heat exchangers and compressors for heating up the mixture temperature and pressure until it reaches 438 °C and 2.533e+004kpa which assists Haber-Bosch reaction to start in plug flow reactor as shown in figure 6. Before ammonia could be stored in a tank, the temperature and pressure should be dramatically decreased to around -35.52 °C and 101.3kpa respectively.

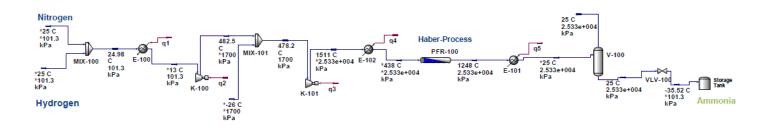


Figure 5 Process flowchart of green ammonia synthesis on Aspen HYSYS V10.

Table 2 shows the values of hydrogen and nitrogen as an input and the final product (ammonia) as an output regarding their vapor fraction, temperature, pressure, and mass flow rate. The temperature of inputs is almost the same at 25 °C while the ammonia was kept in at extremely low temperature of -35.52 to stay in liquid form in the refrigeration loop.

Table 2 Datasheet for input and output streams.

Name	Vapour Fraction	Temperature [C]	Pressure [kPa]	Molar Flow [kgmole/h]	Mass Flow [kg/h]	Liquid Volume Flow [m3/h]	Heat Flow [kJ/h]
Nitrogen	1.0000	25.00	101.3	249.2	7000	8.632	-1944
Hydrogen	1.0000	25.00	101.3	646.1	1400	18.62	-4.138e+005

Table 3 shows the detailed and total purchasing equipment cost for utilities needed. Total purchased equipment cost is 22,556,800 Dollar, bare module cost is 61,487,600 Dollar, base equipment cost is 10,598,280 Dollar and base bare module cost is 29,079,800 Dollar. Materials of construction and cost are listed in table 4.

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Table 3 Purchasing equipment cost of utilities.

ser Added	Equipment									
ompressor s	Compressor Type	Power (kilowatts)	# Spares	мос		Purchased Eq Cost	uipment	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
C-101	Centrifugal	3440	1	Stainless Steel		£ 7,*	190,000	£ 19,700,000	£ 3,420,000	£ 9,380,00
C-102	Centrifugal	8410	1	Stainless Steel		£ 15,0	000,000	£ 41,100,000	£ 7,150,000	£ 19,600,00
xchangers	Exchanger Type	Shell Pressure (barg)	Tube Pressure (barg)	e MOC	Area (square meters)	Purchased Eq Cost	uipment	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
E-101	Double Pipe		20.7	Stainless Steel / Stainless Steel	4	£	17,600	£ 38,600	£ 6,460	£ 21,20
E-102	Double Pipe		260	Stainless Steel / Stainless Steel	4	£	54,100	£ 95,000	£ 6,460	£ 21,20
E-103	Double Pipe		260	Stainless Steel / Stainless Steel	4	£	54,100	£ 95,000	£ 6,460	£ 21,20
Mixers	Туре	Power (kilowatts)	# Spares			Purchased Eq Cost	uipment	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
M-101	Impeller	100	1							
M-102	Impeller	100	1							
Reactors	Туре	Volume (cubic meters)				Purchased Eq Cost	uipment	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
R-101	Mixer/Settler	6								
Channel		Volume				D 1 1 F				
Storage Tanks	Tank Type	(cubic meters)				Purchased Eq Cost	uipment	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
Tk-101	Fixed Roof	90								
Vessels	Orientation	Length/Height	Diameter	MOC Demister MOC	Pressure (barg)		uipment	Bare Module	Base Equipment	Base Bare Module
V-101	Vertical	(meters) 4.19	(meters) 0.762	Carbon Steel	345	£ Cost	241,000	Cost £ 459,000	Cost £ 8,900	£ 36,20
V-101	venucar	4.13	0.702	Carbon Steel	340	~ 4	-+1,000	~ 409,000	r 9,900	~ 30,20
					Totals	\$ 22.5	56 000	\$ 61,487,600	\$ 10,598,280	¢ 20.070.90
					Iotais	ə 22,	008,000	\$ 01,487,600	a 10,598,280	\$ 29,079,80

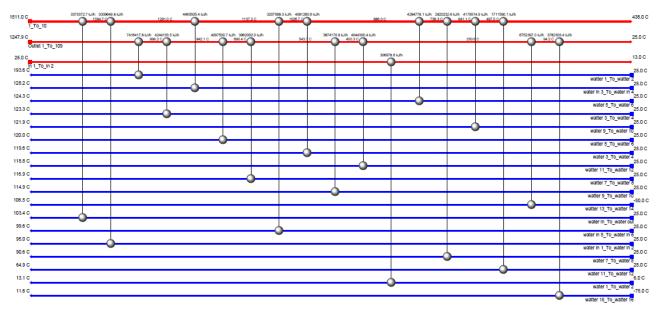


Figure 6 Heat exchanger network of green ammonia synthesis.

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Power (kilowatts)	# Spares	MOC			Purchased uipment Cost	Ba	are Module Cost	Bas	e Equipment Cost	Bas	
(kilowatts) 3440	1	Stainless Steel		£	uipment Cost 7,190,000	£	19,700,000	6	3,420,000	6	Cost 9,380,00
8410	1	Stainless Steel		£		£	41.100.000	£	7,150,000		19,600,00
				-	10,000,000	-	10,000,000	-	1,100,000	-	,0,000,00
Shell Pressure	lube Pressure	MOC	Area (square meters)		Purchased uipment Cost	Ba	are Module Cost	Bas	e Equipment Cost	Bas	e Bare Modul Cost
	2.01	Stainless Steel / Stainless	4	£	17,600	£	38,600	£	6,460	£	21,20
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200	£	6,460	£	21,20
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200	£	6,460	£	21,20
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200	£	6,460	£	21,20
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200	£	6,460	£	21,20
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200	£	6,460	£	21,20
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200	£	6,460	£	21,20
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200	£	6,460	£	21,20
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200	£	6,460	£	21,20
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200	£	6,460	£	21,20
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200	£	6,460	£	21,20
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200	£	6,460	£	21,20
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200	£	6,460	£	21,2
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200	£	6,460	£	21,2
	254	Stainless Steel / Stainless	4	£	51,600	£	91,200 31,200	£	6,460	£	21,20
	254	Stainless Steel / Stainless	4	£	51,600	t t		۲ £	6,460	t £	2%2% 21,20
	254	Stainless Steel / Stainless	4	£	51.600		91,200		6,460		21,20
	254	Stainless Steel / Stainless	4	£	51,600		91,200		6,460		21,20
Volume (cubic					Purchased uipment Cost	Ba	are Module Cost	Bas	e Equipment Cost	Bas	e Bare Modu Cost
6											
Volume					Purchased	Ba	are Module	Bas	e Equipment	Bas	e Bare Modu
(cubic				Eq	uipment Cost		Cost		Cost		Cost
90											
.ength/Heigh t (meters)	Diameter (meters)	MOC Demister MOC	Pressure (barg)		Purchased uipment Cost	Ba	are Module Cost	Bas	e Equipment Cost	Bas	e Bare Modu Cost
4.19	0.762	Carbon Steel	345	£	241,000	£	459,000	£	8,900	£	36,2
			Totals	\$	23,738,600	4		\$	10,746,860	\$	29,588,60

Table 4 Materials of construction and cost

4 PIPING AND INSTRUMENTATION DIAGRAM

One must note that the P&ID has been single-handedly made on the refrigeration loop which can be found in both production lines. A P&ID (Piping and Instrumentation Diagram) is a graphical representation of a process system that shows the interconnection of process equipment, piping, and instrumentation, along with their associated control and monitoring devices. P&IDs are important tools for engineers, operators, and maintenance personnel to understand the configuration and operation of a process system. They are used for various purposes, including design, construction, operation, maintenance, troubleshooting, and safety analysis as shown in figure 7.

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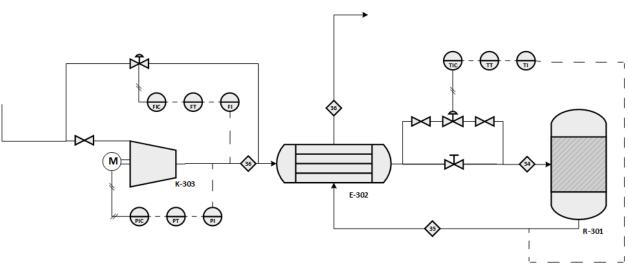


Figure 7 P&ID for ammonia refrigeration loop.

5 HAZARD AND OPERABILITY STUDY

The importance of conducting a Hazard and Operability (HAZOP) study cannot be overstated. This systematic process safety management tool serves as a cornerstone for risk assessment and mitigation in industries prone to hazardous operations. Through a HAZOP study, potential hazards and deviations from normal operation are meticulously unearthed, enabling organizations to take initiative-taking measures to minimize or eliminate these risks. Such preventive actions not only safeguard against accidents and injuries but also prevent environmental harm and property damage. Furthermore, HAZOP studies are often a legal requirement, ensuring compliance with regulatory standards and reducing the likelihood of legal repercussions. Beyond compliance, these studies offer the opportunity for process optimization, enhancing operational efficiency and cost-effectiveness.

I. HAZOP Study

The previously stated P&ID shows the refrigeration loop under normal operating conditions. However, it must be taken into consideration that there is a possibility of a cluster of hazards that may occur due to human and other interventions or deviations. Therefore, a hazard and operability study (HAZOP) has been made as database for as many hazards that may cause deviations and a precaution and monitoring solution to each hazard as listed in tables 5 & 6

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Guide word	Deviation	Cause	Consequences	Action	Recommendation
Reverse	Flow	High pressure level at reactor or heat exchanger or both	potential of pressure and temperature increase led to explosion hazard	Non return valve installation Pressure and temperature alarm or sensor	Non return valve. Temperature alarm. Pressure alarm Proper inspection and measuring on pressure and temperature level
No/none	Flow	Compressor failure – (small hole for example)	Possible hazardous NH ₃ concentration changes	Low concentration alarm	Low concentration alarm interlocked to shut-down NH ₃ flow
More	Flow	failure of compressor control	Temperature and pressure increasing High reaction rate	Temperature sensor Pressure Sensor	High Temperature sensor High Pressure Sensor Measure reaction rate by liquid level observation

Table 5 HAZOP study on compressor (k-303) Intention- increase pressure of hydrogen and nitrogen

Table 6 HAZOP study on reactor (R-303) Intention- increase temperature of hydrogen and nitrogen

Guide word	Deviation	Cause	Consequences	Action	Recommendation
Reverse	Reverse cooling flow	Loss of water control in the	Less cooling	Install check valve or non-	Install non return valve.
		opposite direction	Possible reaction	return valve.	Repeatedly measure on
			changing rate	~ ·	the reactor function
				Continuous	
N T				inspection	T . 11 1 * 1
No	No cooling	Cooling water	Temperature	Install high	Install high temperature
	effect	valve break down	increases in the	temperature	alarm.
			reactor above target.	alarm	
			Possibility of		Continuous inspection
Mana	Mana dhan	Less of controlin	explosion	Τ	I and tanks and tanks allowed
More	More than	Loss of control in	Temperature	Low	Low temperature alarm
	wanted cooling	cooling water	decreases	temperature	Install temperature check valve.
		valve	Reaction rate	alarm	
				Install	Repeatedly observation Install insulation for
			increases	temperature check valve	Install insulation for alternative heating
Less	Less cooling	Loss of control in	Temperature	High	high temperature alarm
2000	targeted	cooling water	decreases	temperature	Install high temperature
		valve		alarm	check valve.
			Reaction rate		Repeatedly temperature
			increases	Install High	measuring
				temperature	Install water jacket for
			Possibility of	check valve	alternative cooling
			explosion		

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As well	Unwanted	More pressure in	Contamination in the	Check	Install more control
as	product	reactor	product lead to	maintenance	valves.
	specifications		change in its	procedures and	Repeatedly observation
	_	Loss of pressure	specifications	schedules.	Instruct operators on
		control valve	Poisoning in the	Maintenance of	procedures.
			reaction	the control	
			Impurities	valves	
Other	Another material	Water source	May be cooling	If less cooling,	Temperature alarm high
than	besides water	contaminated.	ineffective and effect	TAH will	installation
			on the reaction.	detect. If	Water insulating system
				detected, isolate	
				water source.	

II. Modified P&ID

As a result of the previously constructed HAZOP study, a modification can be made on the P&ID in **figure 8**. This might be a safer alternative to the system which will result in fewer failure costs.

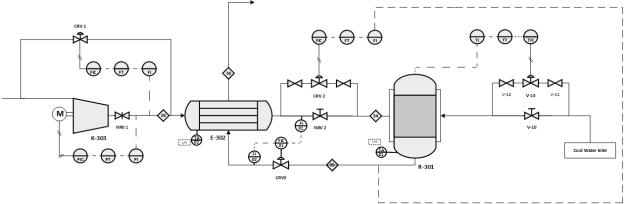


Figure 8 modified Refrigeration Loop P&ID.

6 GENERAL PLANT CONSIDERATIONS

Designing a plant involves a range of critical considerations to ensure its efficient and safe operation. First is the choice of site location, which should factor in geological stability, accessibility to transportation networks and resources, and environmental impact assessments to minimize harm to local ecosystems and communities. The plant layout is equally vital, encompassing equipment spacing to allow for maintenance access and potential expansions, as well as efficient material flow for optimized operations. Safety zones and areas for emergency response and fire protection must also be designated within the layout. Moreover, assessing wind direction and weather patterns is crucial when positioning equipment and emissions stacks to minimize pollutant dispersion and maximize safety, especially in regions prone to extreme weather conditions. Ensuring safety and security measures, including fire prevention and suppression systems and access control, is paramount for protecting critical infrastructure. Thinking ahead, plant designs should incorporate scalability and future expansion possibilities to accommodate growing energy demands or technological advancements. Aesthetic considerations should not be overlooked, as the visual impact on the local community can influence public perception. Finally, operational efficiency should be at the forefront of planning, with a focus on process integration and maintenance accessibility to optimize energy efficiency and reduce operational costs. By addressing these multifaceted considerations, plants can be designed to meet energy needs while minimizing environmental impacts and ensuring long-term sustainability.

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I. Equipment Spacing

Equipment spacing is necessary to ensure safe operations and minimize failures in case of accidents. Equipment Spacing has been made once for grey ammonia and green ammonia, however later the design is continued on the green ammonia since it is more environmentally friendly as shown in figure 9.

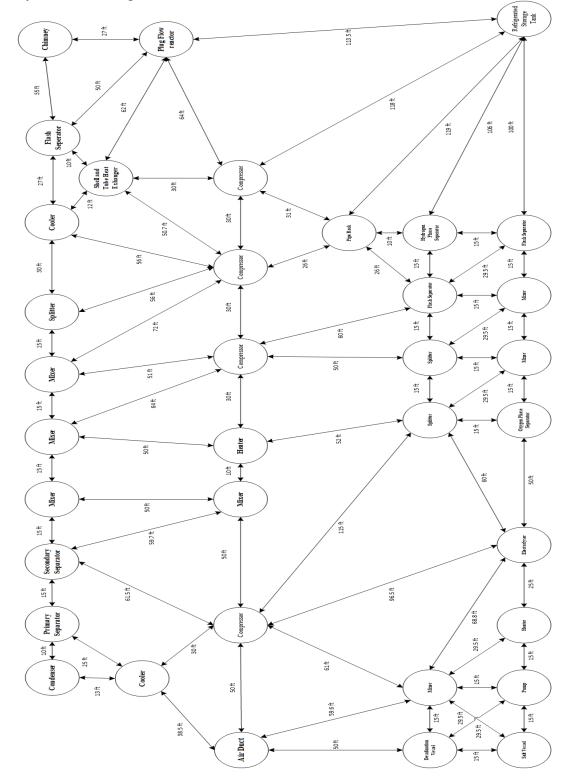


Figure 9 green ammonia equipment spacing

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II. Plant Layout

This section will discuss the overall plant layout with respect to equipment spacing and administrative area as well as potential areas for expansion. It is important to be aware of the wind direction and intensity to set up the orientation of the plant as shown in figure 10. Therefore, it would make sense to analyze the wind atlas or so-called wind rose of Al Ain Al

Sokhna. Although a Windrose for Ain Sokhna cannot be found, a wind rose of nearby gulf of Suez can be used to estimate the direction of wind in Ain Sokhna [37-40].

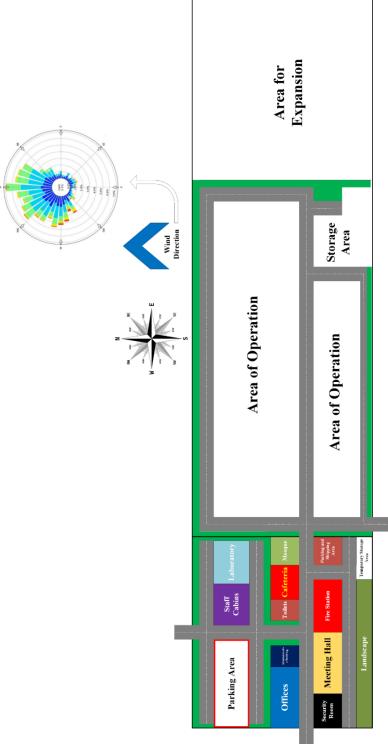


Figure 10 plant layout. 95

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III. Site Location

The following sites have been taken into consideration:

- October industrial zone
- 15 May industrial zone
- Abo Rawash industrial zone
- New Al Nubaria
- Tarboul
- Fayoum industrial zone
- Marsa Matrouh
- Al Shlallat Al Aulaqui Valley Industrial Zone Aswan
- Ras Ghareb, Red Sea Governate
- The following reasons have been used as a basis for choosing the best area:
 - Location, with respect to the marketing area.
 - Raw material supply.
 - Transport facilities.
 - Availability of labor.
 - Availability of utilities: water, fuel, power.
 - Availability of suitable land.
 - Environmental impact, and effluent disposal.
 - Local community considerations.
 - Climate.
 - Political and strategic considerations.

As result, one can assume that the Industrial Zone in Ain Sokna (SIDC Industrial Park) is the most optimum for green ammonia production plant while 6th October industrial zone is best for grey ammonia.

7 PROFITABILITY STUDY

Thorough examination of the various financial prospects is essential when conducting a profitability study to determine an estimate of how much profit the initial investment will generate. This study assessed the upfront capital costs associated with building and operating the plant, including the expenses related to green ammonia production technology and infrastructure as listed in table 6. It would also consider revenue generation potential, considering factors like electricity generation, potential government incentives for clean energy, and market demand for ammonia as a clean fuel or chemical feedstock. Additionally, the study would analyze ongoing operational expenses, maintenance costs, and environmental benefits such as reduced greenhouse gas emissions. Ultimately, this profitability study aims to determine if the long-term economic benefits, including potential profitability and positive environmental impact, justify the investment in a green ammonia plant.

PCE	\$ 761,145
PPC	\$ 259,427,437
Fixed Capital Cost	\$ 376,186,300
Total Investment	\$ 395,000,900

Table 6 Fixed and variable cost

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Variable Cost:

Raw Materials	\$ 5,495
Miscellaneous	\$ 1,976,590
Utilities	\$ 97,200
Shipping and Packaging	not applicable
Sub Section A	\$ 2,079,285

Fixed cost:

Maintenance	\$ 19,765,900	
Operating labor	\$646,200	
Supervision	\$ 129.240	
Plant Overhead	\$ 323,100	
Laboratory costs	\$ 1,421,640	
Capital charge	\$ 38,052,000	
Insurance	\$ 38,052,000	
Local taxes	\$ 752,584,000	
Royalties	not applicable	
Sub Section B	\$ 71,566,650	
Direct Costs (A +B)	\$ 73,645,935	

Sub Section C

Sales expense	\$ 18,416,700
General overheads	not applicable
Research and Development	not applicable
Sub Section C	\$ 18,416,700

Profitability

Annual Production costs $(A + B + C)$	\$ 92,062,635 / year
Production Cost	\$ 3.62 / kg
Profit per kg	\$ 4.53 / kg
Total annual production	25,409,000 kg
Net Profit	\$ 23,122,190

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8. ENVIRONMENTAL IMPACT ASSESSMENT

Environmental Impact Assessment (EIA) is essential study that uses various data and prediction to insure sustainability in any project. Assessing the environmental impact especially in green projects is a necessary to build a common ground for competition with other alternatives in a growing sustainable green economy offering a plethora of alternatives and options. Due to ammonia being one of the most produced chemicals worldwide with already established facilities, [41-43] assessing the direct impacts like the resources consumption from water, energy and materials is already acknowledged. Although the process is green, analyzing the potential of any indirect pollutants and greenhouse gases (GHG) [44-46]. Some of the indirect emissions include the source of energy used in producing the hydrogen. Solar and wind power used can have unintended greenhouse gas emissions from the land use change that could have been utilized for other non-emitting practices [47-49]. Furthermore the emissions of maintenance and manufacturing of the systems including the end of life consideration and decommissioning of all the technology and the ammonia plant in general [50-52]. [3]. Hydrogen storage technologies is considered a gap hindering the progress of the green energy, the scaling up from pilot to industrial scale has a lot of factors to take in consideration; one of those is having a way to store the larger potential of hydrogen in an effective way as shown in figure 11.

Storing hydrogen using established methods like compressed gas or liquid hydrogen presents a number of limitations. Safety risks, high costs, and logistical hurdles associated with transportation can hamper their widespread adoption. However, emerging options like the liquid organic hydrogen carrier (LOHC) offer a glimmer of hope by addressing these critical concerns. Unlike conventional methods, LOHCs promise safe, cost-effective storage of large quantities of hydrogen for extended periods. This not only enhances safety but also simplifies long-distance transport, making LOHCs a potentially transformative solution for hydrogen utilization. It's important to note that LOHCs aren't the only contenders in the race for

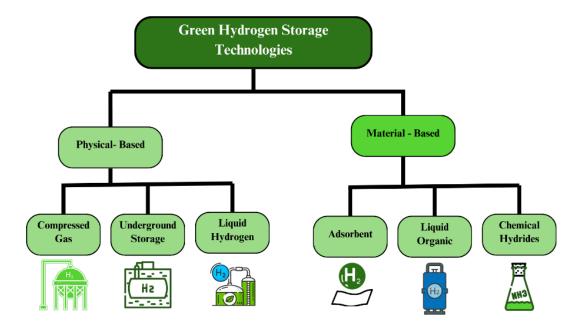


Figure 11 Classification of Hydrogen Storage Techniques

efficient hydrogen storage. Research explores various chemical hydrides like ammonia,

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methanol, and formic acid, each showcasing exciting potential. This diverse landscape of innovative approaches underscores the commitment to developing robust and practical solutions for harnessing the clean energy potential of hydrogen. So, while traditional methods face practical limitations, the emergence of LOHCs and other chemical hydrides paints a promising picture for the future of hydrogen storage and utilization. Technological advancements in this field hold significant promise for unlocking the true potential of hydrogen as a clean and sustainable energy carrier.

9. CONCLUSION

In summary, this research highlights the pivotal role of green hydrogen and green ammonia in advancing the global transition toward cleaner and more sustainable energy sources. By utilizing green ammonia as an efficient carrier for green hydrogen, coupled with meticulous process modeling and simulation, this study offers a promising pathway toward an environmentally friendly and energy-efficient future. As mentioned in the publication of The International Renewable Energy Agency (IRENA), one of the key points of the cost reduction strategy other than governmental support towards the renewable technology projects and finding cheaper alternatives materials used is increasing the size of the facility; the small scale facilities are considered a hindrance in relation to the amount of hydrogen produced. Taking a closer look in the overall process, ammonia synthesis compared to the hydrogen production itself is far less cheap regarding the capital needed for the process. As for global investments, an estimate of USD 2.8 trillion is invested in energy projects with USD 1.7 trillion of them is invested in clean energy projects of all sorts in the year 2023. It was recorded in 2022 according to the International Renewable Energy Agency (IRENA), hydrogen investments were tripled compared to 2021, with a very small portion going into energy storage technologies making the storage technologies economically challenging alongside the technical challenges of hydrogen storage methods. Therefore, storage must be commercialized, in order to achieve higher sustainability. Although the previous process flowcharts are a modified version from the literature, it can be assumed that there is always room for improvement. In addition, the use of fired heaters and high cooling systems instead of a series of heat exchangers could be more spacious but the purchasing cost difference between both options should be considered. The compressors used are prescribed with Aspen HYSYS default efficiency, one might consider finding ways to increase it. Another factor that must be considered is to recycle in order to avoid waste streams as much as possible and increase cost effectiveness. This was not possible to implement in the process simulation due to the program's maximum number of iterations. Some researches discussed the use of absorbing solvents for ammonia extraction. Moreover, to get a more accurate economic comparison, a cash flow analysis could be made to calculate the return on capital over time. In conclusion, green ammonia production has been discussed to convert it to store green hydrogen as well as reduce the carbon dioxide emissions, this is to contribute to the 2030 vision, especially goal 7 in providing clean and affordable fuel, while avoiding the distortion in the stability of the ammonia market and its applications on day-to-day basis. The goal can be achieved through the proposed project of green ammonia production for hydrogen storage, where the commercialization of the project on a larger scale can help in making the dream of clean fuel affordable to all a reality in the near future.

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