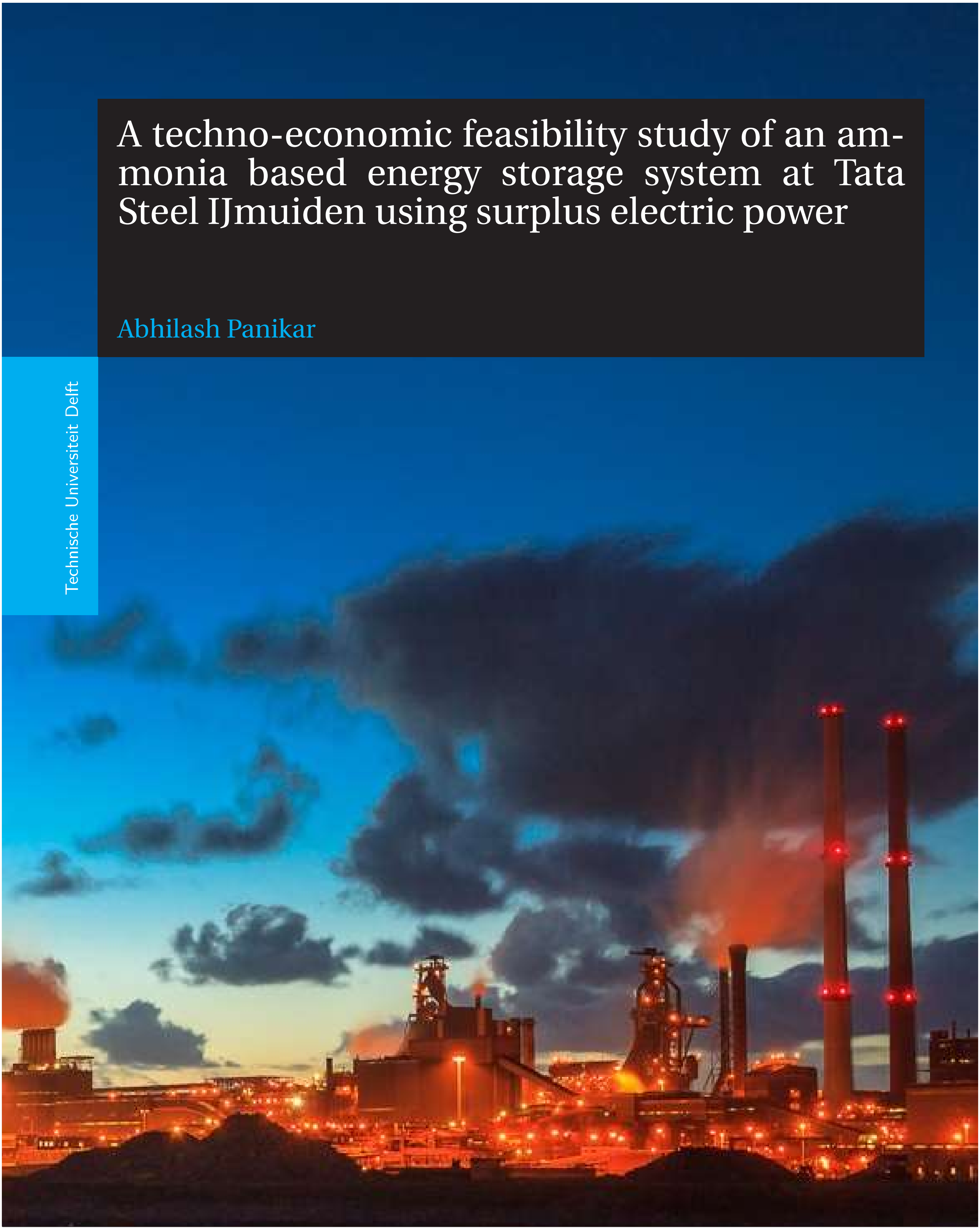
A techno-economic feasibility study of an ammonia based energy storage system at Tata Steel IJmuiden using surplus electric power

Abhilash Panikar

Technische Universiteit Delft



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A TECHNO-ECONOMIC FEASIBILITY STUDY OF AN AMMONIA BASED ENERGY STORAGE SYSTEM AT TATA STEEL IJMUIDEN USING SURPLUS ELECTRIC POWER

by

Abhilash Panikar
Student number: 4466063

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Supervisor:	Prof. Dr. ir. W. de Jong	TU Delft
Supervisor:	Dr. ir. G. van Zee	Proton Ventures BV
Supervisor:	ing. T. van der Velde	Tata Steel, IJmuiden
Thesis committee:	Prof. dr. ir. C.A. (Andrea) Ramirez Ramirez,	TU Delft
	Dr. ir. C.A (Carlos) Infante Ferreira	TU Delft

This thesis is confidential and cannot be made public until October 30, 2019.

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Ever since I was a child, mountain tops have fascinated me. There is something about enduring the pain and pushing yourself beyond your breaking point that brings out a special appreciation of the view once you reach there.

I received support from a lot of people during the course of this project and I take this opportunity to acknowledge them. I would like to thank Wiebren, my supervisor at TU Delft and Tom from Tata Steel for their continual support and guidance throughout the project. I wish to thank Jeanne from Tata Steel and Hans from Proton Ventures without whom this project would not have been possible. Each and every member at Proton Ventures BV made me feel welcome and helped to maintain a stress free environment to work in and I appreciate that. I am grateful to the Proton Ventures team to include me in the first European ammonia conference in Rotterdam. It was a very enriching experience. I would specially like to thank Kevin, Yasmina, George, Stefano and Vincent for answering my queries and providing all necessary data promptly. Gerard has played a huge role in constantly pushing me to question and improve myself at every step. I could not have asked for a better mentor.

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Life at Delft has definitely changed me in a positive way. As I write the last lines of this report I feel like I've reached a mountain top and the view is splendid!

Abhilash Panikar
Delft, October 2017

ABSTRACT

Renewable energy is continuously increasing its penetration in the energy supply network around the world. Due to the intermittent nature of renewable energy sources like solar and wind, storage of excess energy during its availability is vital. Energy storage, especially on the large scale, has recently received a lot of attention from the scientific world and ammonia has been identified as a promising energy storage medium suitable for this application. Factors like high energy density, potential to have minimal carbon footprint and ready existence of suitable infrastructure for handling and transport especially make it an attractive choice. Moreover, ammonia is a bulk feedstock in the chemical and fertiliser industry making it a valuable commodity.

A generic model has been developed in MATLAB® to assess the economic feasibility of producing ammonia from varying availability of electric power. The model estimates the optimum plant capacity at which levelised production cost is minimum thereby resulting in minimum energy storage cost. Steel industries like Tata Steel produce electric power to satisfy the plant's operational demand using by-product gases (termed as work arising gases) evolved during the steel making process. An intermittent availability of surplus electric power has been reported at Tata Steel, IJmuiden. The economic feasibility of utilising ammonia to store the surplus available electric power using the developed MATLAB® model has been assessed in this study. It has been found that the variable cost due to electric power consumption, the fixed cost of the system and capital cost of the electrolyser significantly influence the production cost of ammonia. The minimum levelised production cost estimated in this study is €997/ton which is almost three times the current market price of ammonia. The system shows potential to produce ammonia at a competitive price when sufficient electric power is continuously available at an electricity price of €10/MWh or lower. Utilising part of the hydrogen produced from the work arising gases in the ammonia production process helps to lower the levelised production cost to around €913/ton. Availability of sufficient hydrogen simplifies the system and it may be possible to produce ammonia at a competitive price when hydrogen price is lower than €1.26/kg.

The power to ammonia process shows an efficiency of around 50%. Using gas turbines to produce electricity from ammonia are expected to result in roundtrip efficiencies of around 15%-25%. Research and pilot plants have shown good potential of using ammonia as a fuel in combustion engines and commercial applications are expected to be realised in the near future.

Keywords: ammonia, large scale energy storage, steel industry, techno-economic assessment model, power to ammonia, alkaline electrolyser, ammonia market, applications of ammonia, energy storage cost, ammonia fired gas turbines, levelised cost of ammonia, small scale ammonia production

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NOMENCLATURE

ABBREVIATIONS

ASU	Air Separation Unit
BFG	Blast Furnace Gas
BLEVE	Boiling Liquid Expanding Vapour Explosion
BOFG	Basic Oxygen steel making Furnace Gas
C&F	Cost and Freight
COG	Coke Oven Gas
CNG	Compressed Natural Gas
GT	Gas Turbine
HHV	Higher Heating Value
ICE	Internal Combustion Engine
LFL	Lower Flammability Limit
LHV	Lower Heating Value
RF	Risk Factor
SOEC	Solid Oxide Electrolyser
SOFC	Solid Oxide Fuel Cell
TPD	Tonnes Per Day
UFL	Upper Flammability Limit
WAG	Work Arising Gas(es)

LIST OF SYMBOLS

γ_x	Isentropic exponent for gas x, -
ΔT_{cw}	Temperature rise of cooling water, °C
η_f	Faradaic efficiency, -
η_{isen}	Isentropic efficiency, -
η_{gen}	Generator efficiency, -
η_{gt}	Gas turbine cycle efficiency, -
η_{p2a}	Efficiency of power to ammonia process, -
η_{rt}	Round trip efficiency, -
μ	Mean of a distribution, -
ρ_x	Density of x , $\mathrm{kg/m^3}$

σ	Standard deviation of a distribution, -
b	Loan interest rate, %
C_T	Total capital cost of the system, €
$Cp_{H_2 mol}$	Specific heat capacity of hydrogen, kJ/mol K
Cp_x	Specific heat capacity of x, kJ/kgK
Cap_{act}	Actual capacity of equipment, -
F	Faraday's constant, 96485 C/mol
FC_{act}	Actual fixed cost of equipment, €
HHV_{H_2}	Higher heating value of hydrogen, 3.54 kWh/Nm^3 H$_2$
i	Inflation rate, %
Inv_{act}	Investment of equipment corresponding to actual capacity, €
$I_{el}(t)$	Current passing through the electrolyser at instant t, kA
$m_{cwx}(t)$	Cooling water requirement for x at instant t, kg/s
$m_{T_{NH3}}$	Total ammonia produced in plant lifetime, tonnes
$\dot{m}_x(t)$	Mass flow of gas x at instant t, kg/s
MW_x	Molecular weight of x, kg/mol
N_c	Number of electrolyser cells, -
n_{life}	Plant life, years
n_{loan}	Loan life, years
n_{stages}	Number of compression stages, -
$n_x(t)$	Number of moles of x at instant t, moles
OC_T	Total operating cost of the system, €/year
P_a	Annual payment, €
P_d	Downpayment on the system, €
$P^{ELY}(t)$	Operating capacity of the electrolyser at instant t, kW
P^{ELY}_{ins}	Installed capacity of the electrolyser, kW
P_{final}	Outlet pressure of compression unit, bar
P_{h_c}	Heat generated by a cell of electrolyser, kW
$P_h(t)$	Heat generated by the electrolyser at instant t, kW
P_{in}	Inlet pressure to compression unit, bar
$P_{stage}(t)$	Power requirement for compression unit, kW
PC_{H_2}	Production cost of hydrogen, €/ton
$Q_x(t)$	Heat duty of compressor unit x at instant t, kW
$\dot{Q}_x(t)$	Volumetric production of x at instant t, Nm^3
r	Discount rate, %

r_p	Pressure ratio of compression unit, -
$r_{p_{stage}}$	Pressure ratio of a compression stage, -
R_x	Gas constant for x, kJ/kg K
T_{in}	Inlet temperature to a compression stage, °C
T_{out}	Outlet temperature of a compression stage, °C
$U_c(t)$	Actual cell potential at instant t, V
U_{tn}	Thermoneutral cell potential, 1.48 V
$W_{stage}(t)$	Compression work for a single stage at instant t, kW
X_{design}^{ELY}	Electric power consumption by electrolyser at installed capacity, kWh/Nm^3 H$_2$
$X_{sp}^{ELY}(t)$	Specific electric power consumption by the electrolyser at instant t, kWh/Nm^3 H$_2$
z	Number of electrons transferred per molecule of hydrogen, -

SUBSCRIPTS

air	Air
asu_{comp}	Air separation unit compressor
cw	Cooling water
dw	Demineralised water
$elec$	Electrolyser
$elec_{comp}$	Hydrogen compressor

1

INTRODUCTION

The world energy demand has shown a steady increase from the year 1990 to 2015. Figure 1.1 shows the rising trend of electricity generation in Europe to cope with the rising demand.

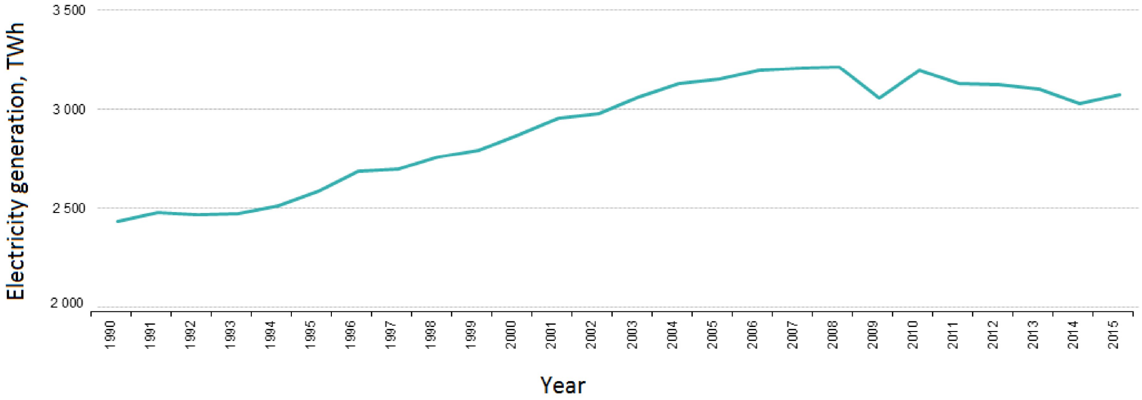

Figure 1.1: Net electricity generation in Europe

Source: Electricity production, consumption and market overview[17]

During the period 1990-2010 the electricity generation methods have a seen a gradual change. Figure 1.2 shows the change in electricity generation methods in Europe during this period. The contribution of electricity generation via oil and coal have shown a decreasing trend especially from 2005 and a rise in contribution by renewable energy sources is observed. This is attributed to the Kyoto Protocol which entered into force from 2005.

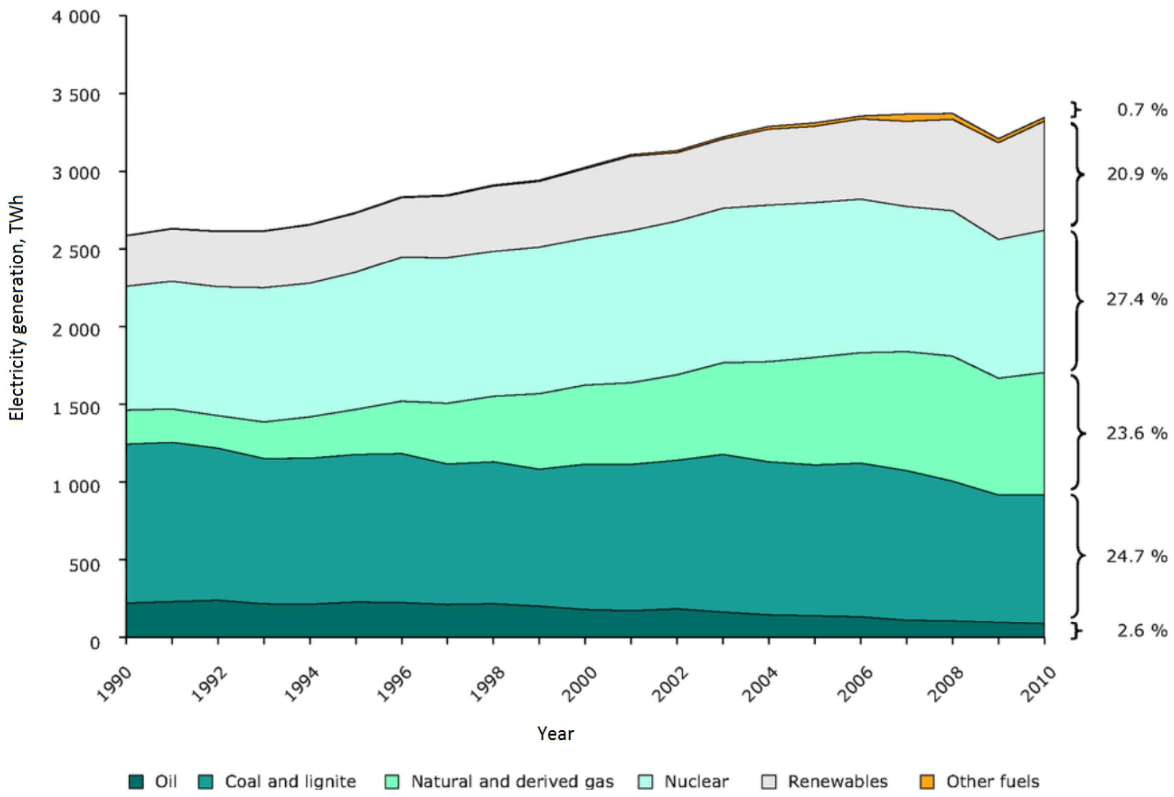

Figure 1.2: Electricity generation methods in Europe

Source: European Environment Agency [16]

The steel industry is a very energy intensive sector and responsible for significant carbon dioxide emissions as well. Tata Steel Europe has two main operating centres in the UK and the Netherlands. The main steel making plant in the Netherlands is located in IJmuiden and is responsible for emitting nearly 12 million tonnes of carbon dioxide per year. This plant, in collaboration with Nuon, produces nearly 3500 GWh of electricity annually using by-product gases termed as work arising gases(WAG) evolved during the steel making process. WAG are energy rich gas streams with an energy content close to 3000 GJ/hr mainly accounted by hydrogen and methane in them. The energy is utilised for the plant's operation in the form of electricity and heat. The power production by the plant is not synchronised with the demand resulting in over and under production of electricity. Energy storage is one of the solutions to create a balance and reduce dependency on the electricity grid.

Proton Ventures BV is an engineering company based in Schiedam, The Netherlands. They have been offering their expert services to the ammonia industry since 2001. Producing ammonia via electrolysis is a technologically proven process, however, it was never economically competitive enough compared to conventional production process using natural gas. As a result, this technology received little attention in the past. However, the Paris climate agreement(COP21) has changed this. Higher penetration of renewable energy and stricter carbon emission taxes have caused a surge in research and development focusing on carbon-free routes for ammonia production. Ammonia has also been identified as a potential large scale energy storage medium. Apart from conventional ammonia plants, Proton Ventures BV is now also focusing on small scale power to ammonia plants with capacities as low as 1000 tonnes per year. The aim of this study is to assess the feasibility of a power to ammonia plant.

Availability of surplus electric power and hydrogen rich gas streams make Tata Steel IJmuiden an interesting case study for this research. Moreover, availability of carbon dioxide creates the possibility of producing chemicals like urea via a carbon free path. The ammonia industry and the steel industry have a synergistic relationship. This study assesses the feasibility of using ammonia as an energy storage medium for the available surplus electric power. This builds a bridge between the steel-making and the ammonia industry which was never considered hitherto making this study unique.

The study has been structured in the form of 9 chapters including this one. Chapter 2 gives a background on the technology of power to ammonia and discusses market potential of ammonia and its role as an energy carrier. Chapter 3 describes the energy network at Tata Steel IJmuiden. The problem statement and research objectives are defined in this chapter. Chapter 4 statistically analyses the nature of the available surplus electric power. Chapter 5 and chapter 6 describe in detail the approach taken to complete the techno-economic assessment. Chapter 7 describes and interprets the results from the study. Chapter 8 describes the prospects of using ammonia as a fuel in gas turbines. Chapter 9 concludes the study by reflecting on the key findings and by proposing directions for future studies.

2

BACKGROUND

Section 2.1 highlights the importance of energy storage and compares different energy storage technologies available. Section 2.2 gives an insight into the market of ammonia and section 2.3 describes ammonia's role as an energy carrier. Section 2.4 reviews the technology to produce ammonia from electric power and describes the important components in the power to ammonia system.

2.1. CONCEPT OF ENERGY STORAGE

Renewable energy sources are playing a very important role in today's energy supply network and their contribution is expected to grow in the future. Intermittency is a key characteristic of renewable energy sources like solar and wind in particular. This limitation is overcome by storing energy during its abundance and recovering it during its deficit. This specially makes energy storage a very interesting topic in the current world. However, this does not imply that energy storage is exclusive to renewable energy. This technology finds application where energy availability is characterised by intermittency.

Figure 2.1 shows the best applicability range of some energy storage technologies based on capacity and storage time capacity. Typically, energy storage technologies greater than 1 MWh are best suited for grid scale energy storage and termed as large scale energy storage. Capacitors, super-capacitors, superconducting magnetic energy storage and flywheels are usually employed for small scale energy storage solutions. Advanced battery systems make it now possible to use them for large scale energy storage applications. For example Tesla Inc. is on its way to build the world's largest lithium ion battery for grid scale application in South Australia. It is estimated to have a storage capacity of about 130 MWh[52].

Pumped hydro is the most prevalent method to store energy at grid scale[5]. It utilises potential energy of water created by a height differential between reservoirs. However applicability of this technology is greatly dependant on the geographical location. The Netherlands, due to its low lying topography, is not well suited for this technology.

Thermal heat storage extracts heat from a process stream and stores it in a medium which can be recovered to drive a turbine-generator system using steam. They are classified further depending on the temperature of operation and characteristics of the storage media.

Compressed air energy storage utilises surplus electric power to operate a compressor. Air is compressed and stored in underground caverns. The compressed air is later heated up to recover electric power using an expansion or gas turbine. A detailed classification of energy storage technologies has been included in Appendix H

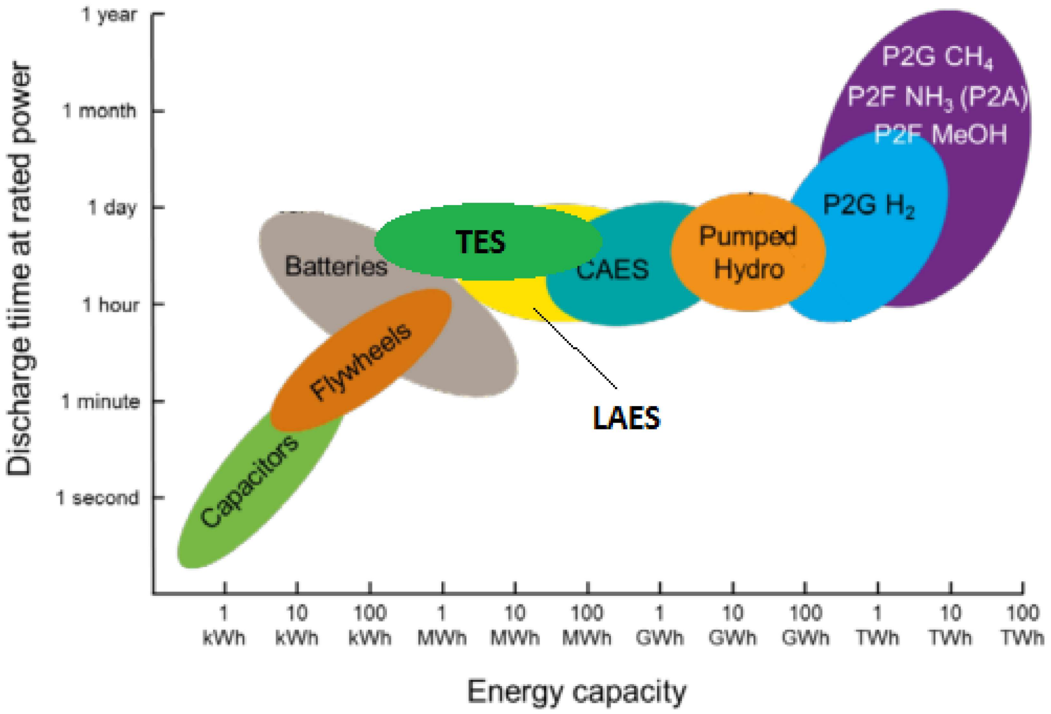

Figure 2.1: Comparison of energy storage technologies [1]

Source: Adapted from ISPT (2017)[27]

1

The different energy storage technologies are compared and the main parameters are summarised in table 2.1.

SMES and flywheels show excellent round trip efficiency but are very expensive and applicable for low capacity storage. Power to chemical technology is particularly attractive for large scale energy storage and has a lower environmental impact compared to pumped hydro or CAES. It is the only large scale energy storage solution offering convenient transportation of energy. Utilising an existing carbon stream makes this technology carbon neutral[2]. There are some power to chemical demonstration plants in Europe, especially in Germany, and focus on hydrogen and methane production[23]. Appendix C gives a list of some of these plants.

This study focuses on power to ammonia (chemical) and hence other technologies will not be discussed further.

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[1] TES: Thermal Energy Storage; LAES:Liquid Air Energy Storage; CAES: Compressed Air Energy Storage; P2G: Power to Gas; P2F: Power to Fuel

[2] System is totally carbon neutral only if power requirement for the entire conversion process is met by renewable sources

Table 2.1: Comparison of energy storage technologies

Source: Evans et al. (2012)[18], Banares Alcantara et al. (2014)[3], Lehner et al.[29], Bennani et al.(2016)[7]

Technology	Round trip efficiency (%)	Capacity rating (MW)	Energy density (Wh/kg)	Capital USD/kWh[1]	Storage time	Self discharge (% per day)	Environmental impacts
CAES	70-89	5-400	30-60	50	Hours-months	Low	High
Pumped hydro	75-85	100-5000	0.5-1.5	100	Hours-months	Very low	High
Flywheels	93-95	0.25	10-30	5000	Seconds-minutes	100	Very low
Capacitor	60-65	0.05	0.05-5	1000	Seconds-minutes	40	Low
Supercapacitor	90-95	0.3	2.5-15	2000	Seconds-minutes	20-40	Low
SMES[2]	95-98	0.1-10	0.5-5	10000	Minutes to hours	10-15	Moderate
CES[2]	40-50	0.1-300	150-250	30	Hours-months	0.5-1	Very low
HT-TES	30-60	0-60	80-200	60	Hours-months	0.05-1	Low
Pb-acid battery	70-90	0-40	30-50	400	Minutes-days	0.1-0.3	Moderate
Li-ion battery	85-90	0.1	75-200	2500	Minutes-days	0.1-0.3	Moderate
Power to chemicals	30-75	0.01-1000	4318-39000	6-725	Minutes-months	Very low	Low

---

[1] Operating cost, maintenance and other ownership costs have been neglected

[2] SMES: Superconducting Magnet Energy Storage; CES: Cryogenic Energy Storage

Power to chemicals: The fundamental building block for power to chemicals is hydrogen. Electric power is utilised to generate hydrogen by electrolysis of water. Hydrogen itself can be used as the end product or combined with other gases to produce different products. Figure 2.2 gives an overview of routes for power to chemicals.

Main advantages:

- High energy density
- High storage capacity
- Long storage duration
- Multiple applications including fuel for mobility, electricity production, chemical feedstock and heat generation

Main disadvantages:

- Low round trip efficiency
- Needs existing infrastructure for product utilisation (eg. a natural gas grid for methane)

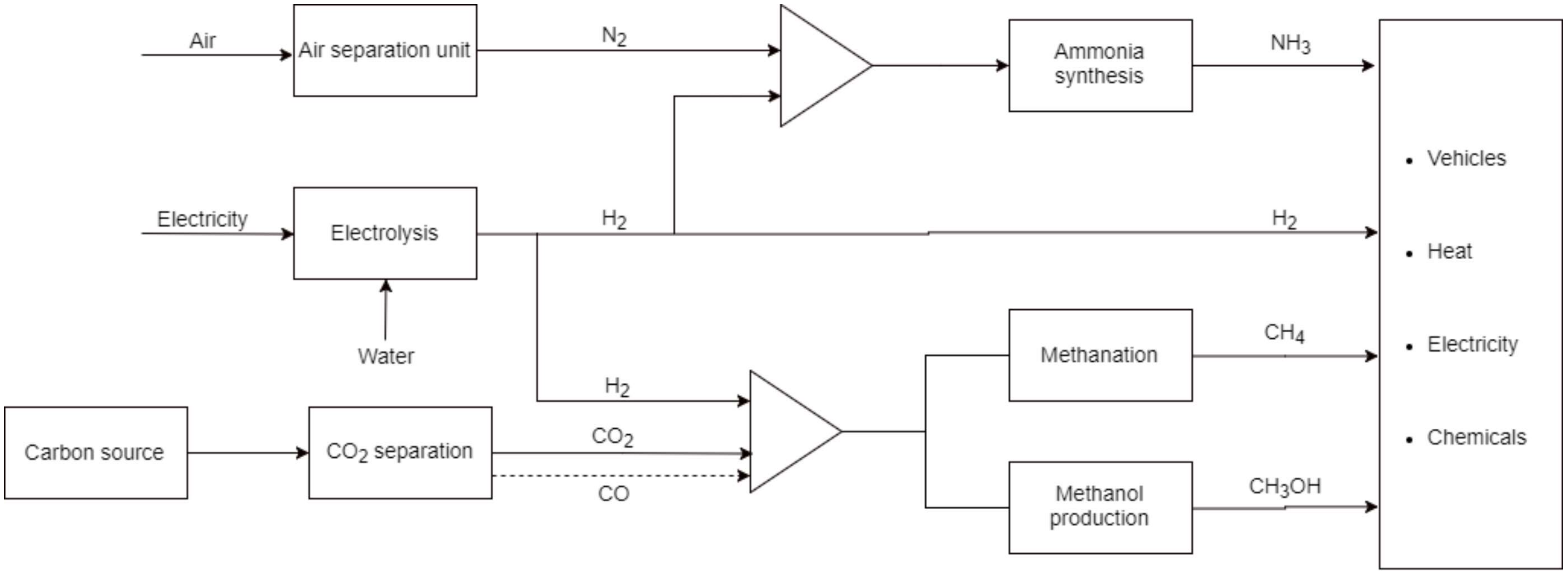

Figure 2.2: Routes for power to chemicals [1]

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[1] An example of carbon source is flue gas from industries like steel, cement, aluminium etc.

2.2. AMMONIA MARKET AND DERIVED PRODUCTS

Ammonia is a gas at ambient conditions having a pungent odour and colourless appearance. It is a rich source of nitrogen, highly soluble in water and is an important compound in the chemical industry.[57].

2.2.1. APPLICATIONS OF AMMONIA

Nitrogen based fertilisers are the most popular fertilisers in the world. Ammonia is the building block of the world nitrogen industry[31] and is used as a feedstock for production of a variety of fertilisers like urea, di-ammonium phosphate, mono-ammonium phosphate, ammonium nitrate etc. Anhydrous ammonia is also used directly as a fertiliser especially in the USA, but is not very common elsewhere[43]. The various applications of ammonia are represented in figure 2.3. Ammonia is used as a refrigerant especially in large scale industrial processes and food preservation. It shows enhanced thermodynamic properties compared to other refrigerants[1]. Ammonia is used to reduce nitrogen oxide emissions (NOx) using selective catalytic reduction[37]. Ammonia has the potential to be used as a fuel in ICE, GT and even SOFCs. In case of ICE, mixing ammonia with another fuel, like hydrogen or diesel is required for a stable performance[10]. Ammonia can be directly fed into SOFCs or used in the form of hydrazine[1]. Ammonia is the most popular stabilising agent used in rubber industries to prevent coagulation of latex[24]. Ammonia also finds application in water treatment plants to control pH levels and to produce potable water when used with chlorine. Dissociated ammonia is used for metal treating processes like nitriding, carbonitriding, bright annealing, sintering etc. Ammonia neutralises acid content in crude oil and helps protect equipments in the oil and gas industry against corrosion. Ammonia is used as a casein dispersant in coating of paper and as a curing agent in the leather industry[7][46].
Ammonia is used as a feedstock for important chemicals like urea formaldehyde, hydrogen cyanide, nylon, nitric acid etc. Some of the pathways are shown in figure 2.4.

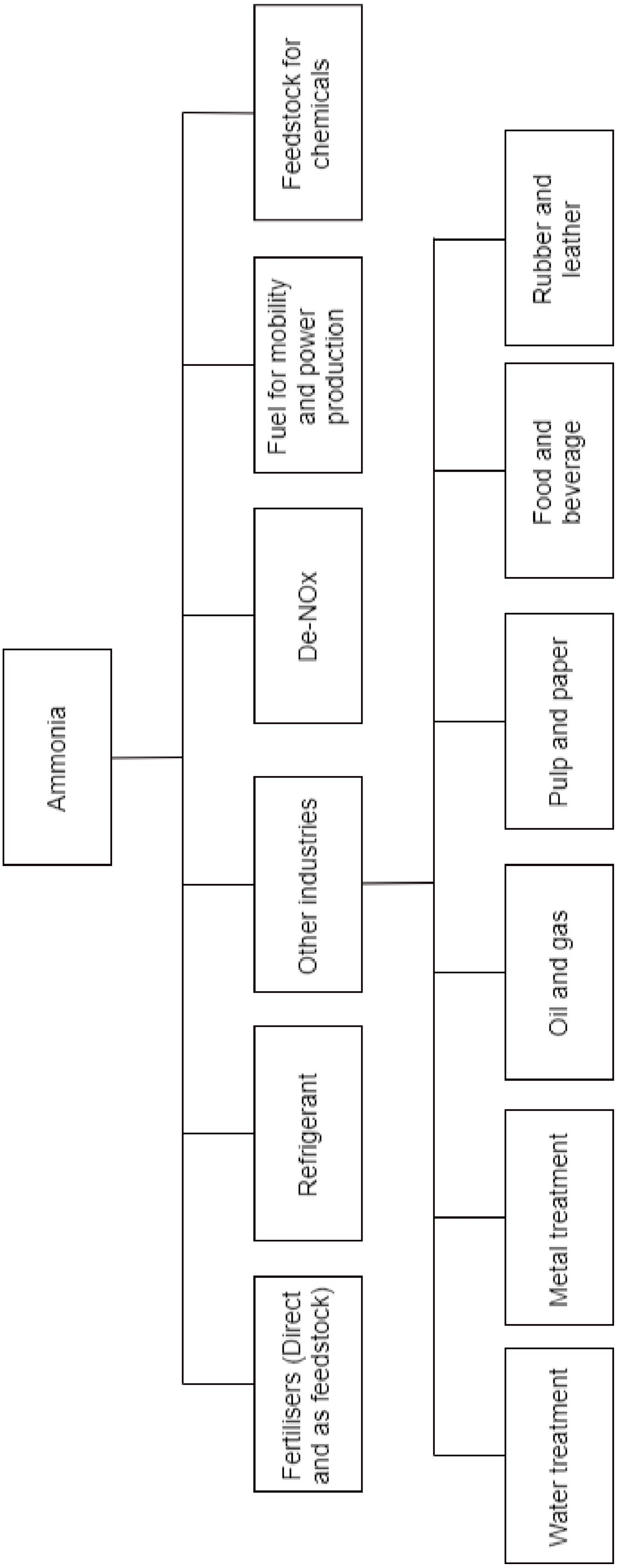

Figure 2.3: Applications of ammonia

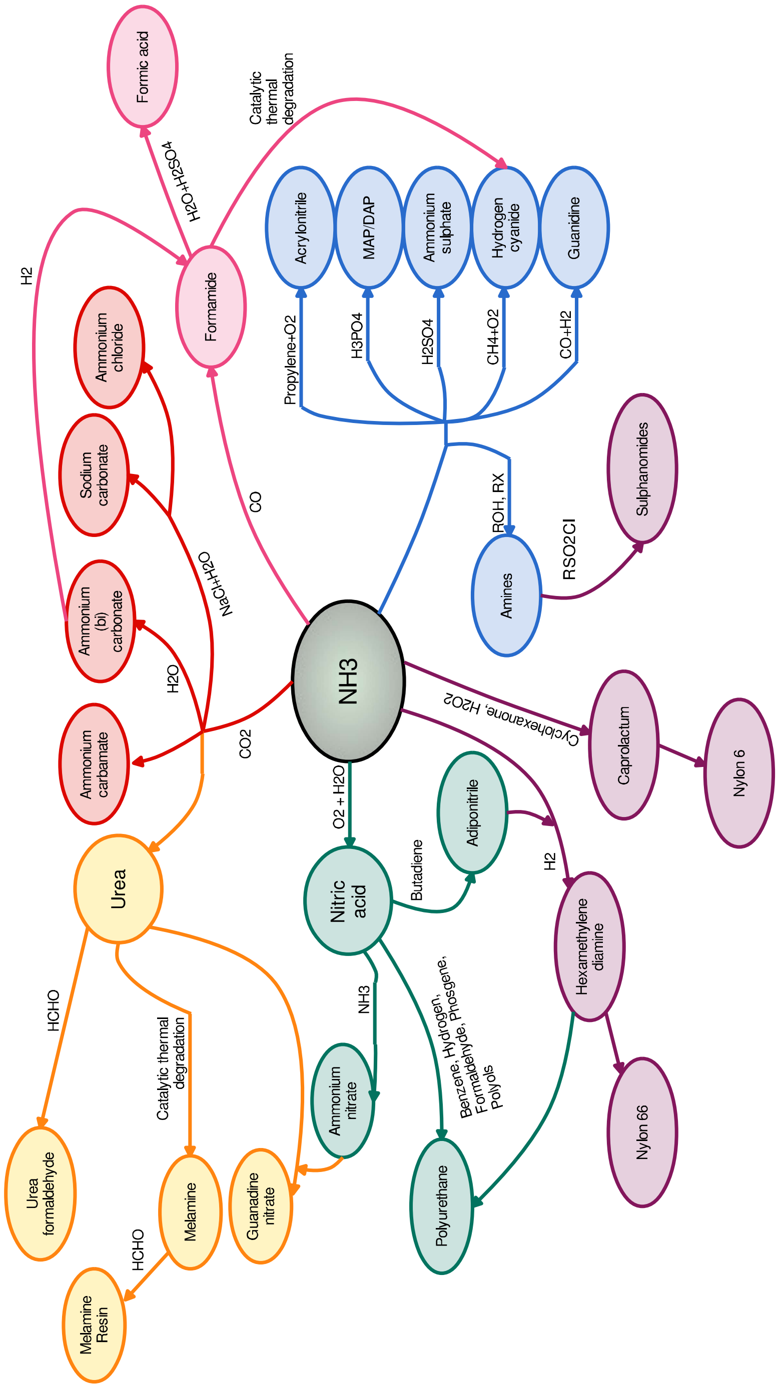

Figure 2.4: Pathway for chemical production from ammonia

2.2.2. GLOBAL AMMONIA MARKET OVERVIEW

AMMONIA PRODUCTION

The world production of ammonia in the year 2013 was close to 173 Million tonnes(approximately 3.2 Tera-Joule[1]). Compared to 2008, ammonia production showed an increase by 18%. It is expected that the world demand for ammonia will only keep increasing. A forecast of 14% increase has been made for the years 2013-2018.[31]. Haber Bosch is the most popular industrial process of producing ammonia and natural gas is the most common fuel used as a source of hydrogen in this process. An exception is China, which relies heavily on coal gasification for producing the necessary hydrogen[3]. Figure 2.5 shows the contribution of different regions around the world towards ammonia production. China leads the production with a share of almost 34%. Along with former USSR and Southwest Asia, these regions account for about 57% of global production.

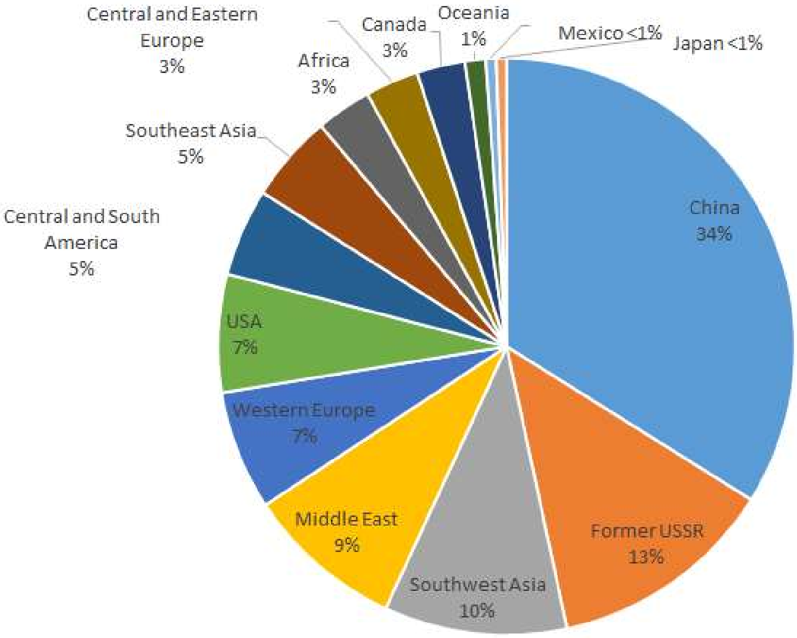

Figure 2.5: Global distribution of ammonia production in 2013

Source: Adapted from Malveda et al. (2014)[31]

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[1] Based on LHV of ammonia

APPLICATIONS OF AMMONIA

Figure 2.6 shows the global applications of ammonia. It is seen that the largest application of ammonia is used to produce urea, a popular fertiliser. Over 80% of all ammonia produced finds application within the fertiliser industry.

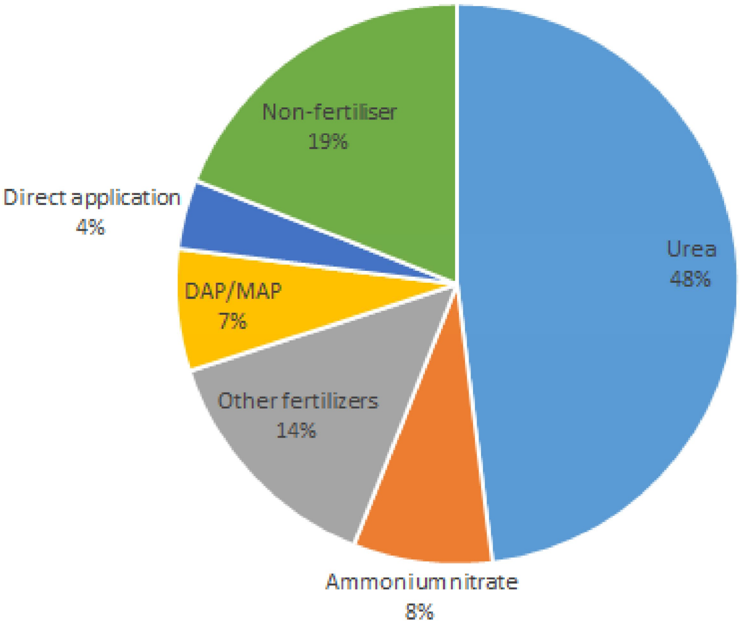

Figure 2.6: Global applications of ammonia during 2010-2013

Source: Potash Corp.(2008)[44]

2.2.3. WEST EUROPEAN AMMONIA MARKET OVERVIEW

TRADE CHARACTERISTICS

It is seen from figure 2.6 that western Europe accounts for 7% of the world ammonia production. However, compared to the year 1990, the share in the world production has decreased by almost 23% and is expected to fall further in the future[31]. This maybe attributed to high natural gas prices which is one of the most important cost drivers of ammonia[43]. The Netherlands and Germany are the main producers of ammonia in western Europe accounting for almost 54% of the production in this region. France, Belgium and the United Kingdom are other main producers of ammonia. In the year 2013, western Europe produced almost 12 million tonnes of ammonia and the Netherlands was responsible for almost 25% of this share. From a global perspective, the Netherlands contributes just over 1.5% of global ammonia production. Figure 2.7 puts production capacity of the Netherlands in perspective with production in western Europe and the world. Western Europe imports about 2 million tonnes of ammonia annually. This is equivalent to 17% of its production and almost 11% of the total world imports. Africa and USSR are the major import partners. Western Europe plays a very insignificant role as an exporter of ammonia and contributes to only 0.8% of global exports. Almost all the export is limited to be within western Europe.[31].
The trade trends suggest that western Europe is a significant consumer of ammonia and relies on import to meet its demand. Unfavourable natural gas price is one of the main reasons for such high imports.

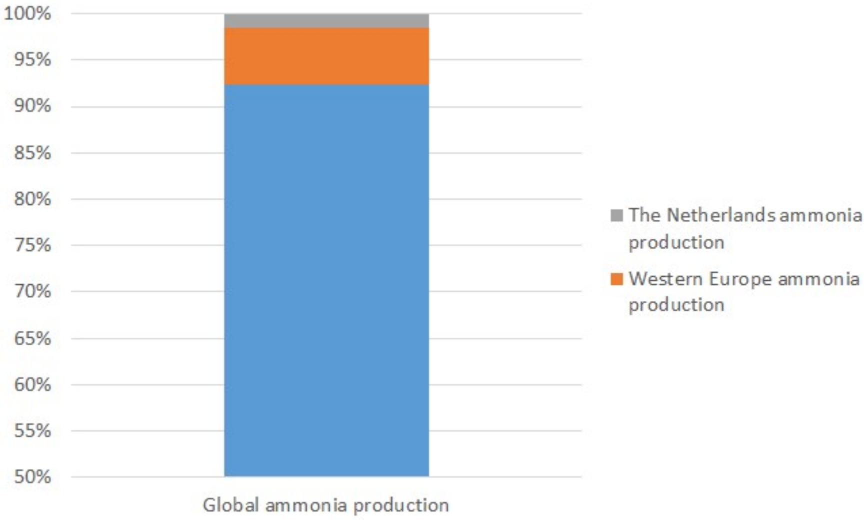

Figure 2.7: Ammonia production in western Europe and the Netherlands in year 2013

Source: Data from M.Malveda (2014)[31]

APPLICATIONS OF AMMONIA

In western Europe most of the ammonia produced is used in making ammonium nitrate followed by urea. Figure 2.8 represents the different application areas of ammonia in western Europe. The other applications constitute of chemicals like caprolactum, hydrogen cyanides, amines, other nitrogen fertilisers and also application in metallurgy, refrigeration, pollution control etc. Consumption of ammonia to make urea, nitric acid and ammonium nitrate is forecasted to increase from 2013 to 2018 with an annual growth of 0.8%, 0.9% and 0.9%, respectively. The other applications of ammonia have been forecasted to show an annual decrease of 14.2%[31]. Appendix E shows the evaluation of different products derived from ammonia with relevance to Tata Steel.

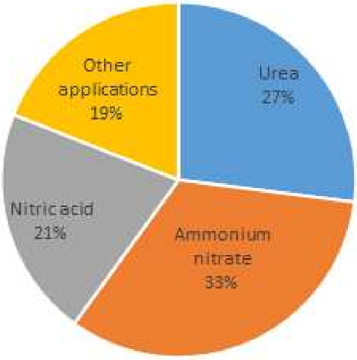

Figure 2.8: Application of ammonia in western Europe in 2013

Source: Data from M.Malveda (2014)[31]

PRICE OF AMMONIA

Ammonia market price is subject to variations and is highly influenced by the natural gas price. Figure 2.9 shows the trend of ammonia price (Western Europe C&F) for the period 2000 to 2013[31]. A wide range of price is observed from as low as \$130/ton to as high as \$780/ton. For this period the average price of ammonia is about \$344/ton.

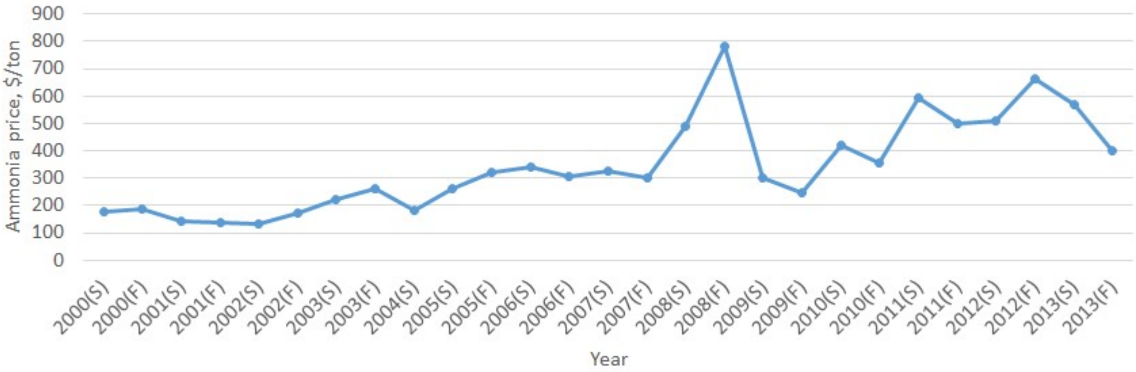

Figure 2.9: Price of ammonia in western Europe (C&F) for the period 2000-2013 [1]

Source: Data from M.Malveda (2014)[31]

AMMONIA IN THE NETHERLANDS

Yara, Sluiskil and OCI Nitrogen, Geleen are the two producers of ammonia in the Netherlands. About 10 users utilise the ammonia produced within the Netherlands and the remainder it exported[43].
Yara Sluiskil is one of the biggest ammonia producer in the world with a production capacity of 1.8 million tonnes annually. Yara is also a producer of nitric acid, urea and granulated nitrates. It consumes most of the produced ammonia for this purpose[43].
OCI Nitrogen in Geleen produces just over a million tonnes of ammonia annually. Like Yara, OCI Nitrogen also produces nitric acid, urea and some specialised fertilisers. OCI Nitrogen is also responsible for production of about 150,000 tonnes of melamine annually[43].
Some applications of ammonia within the Netherlands along with the concerned company is given in table 2.2.

Table 2.2: Applications of ammonia in the Netherlands

Source: Patil et al.(2016)[43]

Application	**Company**
De-Nox	AVR, EON
Refrigerant	Nijssen, Grenco
Formaldehyde, Resins	CALDIC, Chemcon Delfzijl
Nitrate, sulphate and phosphate fertilisers	Euro liquids, Van Iperen
Polyurethane	Huntsman Chemicals
Nitric acid solution for industrial cleaning	Freisland Campina

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[1] S:Spring; F: Fall

2.3. ROLE OF AMMONIA AS AN ENERGY CARRIER

Hydrogen has been recognised as a promising source of energy. As shown in figure 2.2, hydrogen is the building block for power to chemical technology. However, at present, a global hydrogen economy is not feasible due to the lack of a suitable storage medium[60]. A solution is to find a storage medium that is cheap, easy to handle and transport, and easy to retrieve the stored energy. Ammonia is a compound having 3 atoms of hydrogen for every atom of nitrogen which corresponds to 108 $kg_{eq,H_2}/m^3$ at 20°C. Comparing with metal hydrides for hydrogen storage, ammonia stores more than four times hydrogen by weight in the same volume[7]. Moreover, a well distribution network already exists for ammonia[60]. Table 2.3 compares the production, storage and transportation cost of ammonia and hydrogen[7]. The figures for ammonia are based on equivalent mass of hydrogen in order to make a direct comparison with hydrogen. Although ammonia production involves more steps and is more expensive than hydrogen, transportation costs are much lower and so is the storage cost. This shows that at present, long term storage of hydrogen is not economically attractive.

Table 2.3: Comparison of production, transportation and production cost of ammonia with hydrogen

Source: Bennani et al.(2016)[7]

	Hydrogen (€/kg H_2)	**Ammonia (€/kg H_2)**
Production[1]	2.7	3.4
Pipeline transport	1.69	0.17
Storage		
1 day	0.71	0.03
15 days	1.78	0.05
182 days	13.48	0.49

Hydrogen can be retrieved from ammonia using the following techniques[7]:

- Catalytic decomposition of ammonia: Ammonia decomposes into nitrogen and hydrogen under the influence of an iron based catalyst at a temperature of around 445°C. A conversion of over 98% is possible by this technique.
- Electro oxidation of ammonia: Ammonia decomposes into nitrogen and hydrogen under a thermodynamic potential of 0.77V in an alkaline medium.

Ammonia can also be used directly to recover energy using ICE, GT or SOFC. Table 2.4 compares the performance of ammonia as an energy carrier with some common fuels. Energy density of ammonia is comparable to methanol and CNG, but the specific energetic cost is lower by almost 75% and 50% respectively. Gasoline has the highest energy density, however it is expensive compared to ammonia. Moreover, combustion of gasoline and CNG results in emission of carbon oxides and sulphur oxides which are difficult to avoid. Combustion of ammonia may result in formation of nitrogen oxides like NO and NO_2, but they can be handled well using selective catalytic reduction. From a safety perspective, ammonia stored as metal amines are better than pressurised ammonia tanks when used for automotive purposes[60].
Ammonia shows bright potential to be a solution for energy storage. Research and development is being done all around the world to make ammonia a practical alternative fuel. Table 2.5 shows some of the institutes involved in this field.[51][38].

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[1] Production of ammonia is considered to be through electrolysis. Price of electricity has been neglected for both hydrogen and ammonia production

Table 2.4: Comparison of ammonia with some common fuels

Source: Zamfirescu et al.(2008)[60]

Fuel	**Storage**	**P(bar)**	**Density[1] (kg/m^3)**	**HHV (MJ/kg)**	**Energy density (GJ/m^3)**	**Specific volumetric cost (\$/m^3)**	**Specific energetic cost (\$/GJ)**
Gasoline	Liquid tank	1	736	46.7	34.4	1000	29.1
CNG	Integrated storage system	250	188	55.5	10.4	400	38.3
LPG	Pressurised tank	14	388	48.9	19	542	28.5
Methanol	Liquid tank	1	749	15.2[2]	11.4	693	60.9
Hydrogen	Metal hydrides	14	25	142	3.6	125	35.2
Ammonia	Pressurised tank	10	603	22.5	13.6	181	13.3
Ammonia	Metal amines	1	610	17.1	10.4	183	17.5

Table 2.5: Leading research institutes focusing on ammonia as a fuel

Source: Data from Soloveichik (2016)[51] and NH3 fuel association (2016) [38]

Institute/Company	**Location**	**Area of research**
Space propulsion group	California, USA	Gas turbine
Sturman Industries	Colorado, USA	ICE
Toyota	Japan	Car/SOFC
Korean Institute of Energy Research	South Korea	Car
HEC-TINA	Tennessee, USA	Generator set
AIST	Japan	Gas turbine (bifuel)
Kyoto university	Japan	SOFC

---

[1] Refers to the density of fuel under mentioned storage condition except for gasoline and methanol. The densities for these two fuels are in their liquid states

[2] It is assumed that methanol would be converted into hydrogen by reforming before using as a fuel in fuel cells. The HHV has been compensated to include energy requirement for the reforming process.

2.3.1. HEALTH AND SAFETY

Ammonia has been assigned the following hazard categories[50]:

- H221: Flammable gas
- H280: Contains gas under pressure; may explode if heated
- H314: Causes severe skin burns and eye damage
- H331: Toxic if inhaled
- H410: Very toxic to aquatic life with long lasting effects

To put the hazard level of ammonia in perspective, the hazard level of ammonia is compared with conventional fuels:

1. Fire/Explosion hazard: Ammonia has a lower heat of combustion and a narrower flammability limit compared to conventional fuels. This makes ammonia less of a hazard for explosion. RF[1] index is used to assess the explosion hazard and higher RF index implies higher hazard. Figure 2.10 compares hazard levels of different fuels with relevance to fire and explosion. It is observed that hydrogen is almost a 100 times more hazardous than ammonia in this respect.

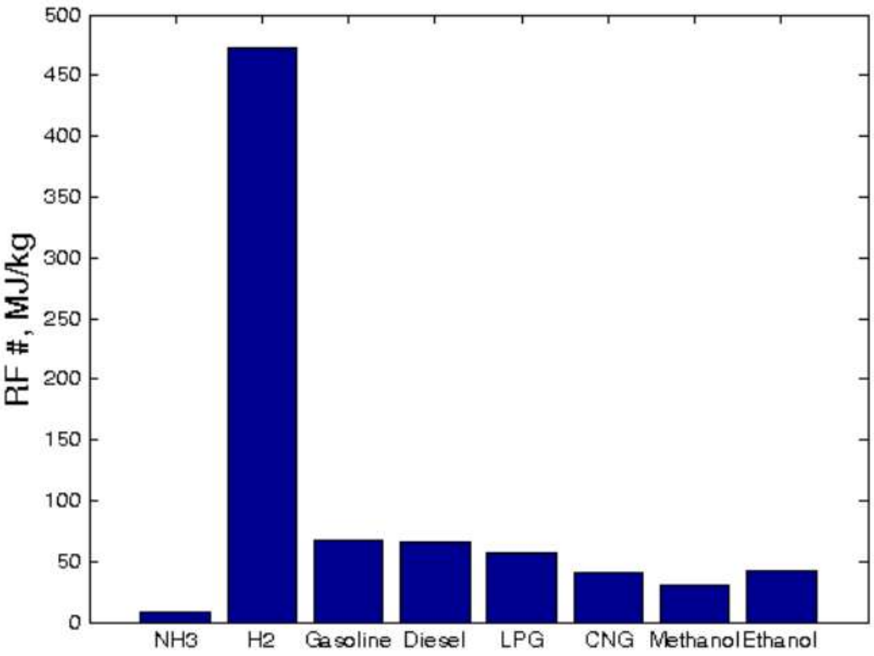

Figure 2.10: Explosion hazard level for different fuels

Source: Evans (2013)[19]

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[1] $RF=HHV\left(\frac{UFL}{LFL}-1\right)^{0.5}$

2. Toxicity hazard: Ammonia is a toxic chemical but not carcinogenic. Exposure to high levels of ammonia or low levels for a prolonged duration may be fatal. However, it should be noted ammonia is lighter than air. Unless in an enclosed space, ammonia gas will rise up and reduce human exposure. Ammonia has a strong odour and hence detectable even at safe concentrations without any detectors. Figure 2.11 shows chances of fatality as a function of concentration and exposure time.

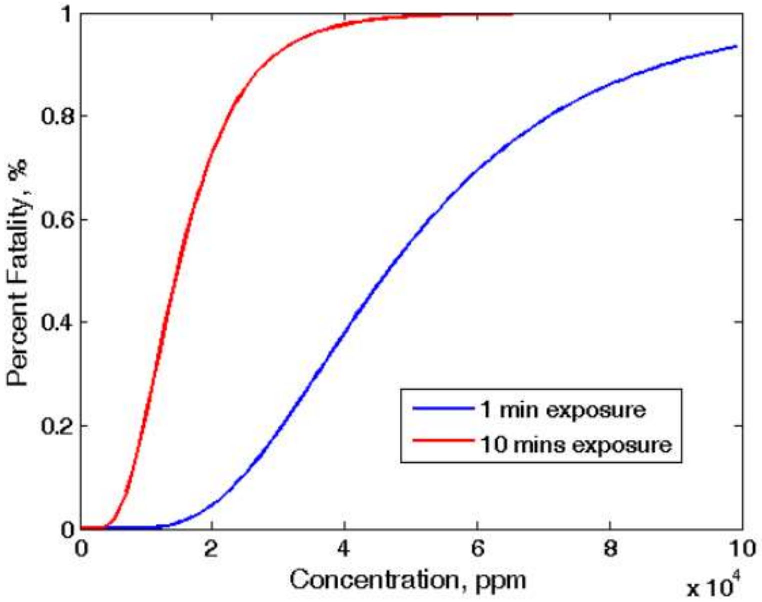

Figure 2.11: Influence of ammonia concentration and exposure time on fatality chance

Source: Evans (2013)[19]

3. Tank rupture hazard: Compared to hydrogen and CNG, ammonia is stored at relatively low pressure. Fatalities have been reported for ammonia subject to BLEVE incidents however, reported BLEVE have been limited to large industrial systems. BLEVE is unlikely in small tanks. Finally, blast wave and fragment hazard associated with BLEVE is insignificant for ammonia when compared to hydrogen or CNG[19].

Ammonia is a hazardous fuel, however, it can be concluded that compared to other fuels, it presents a much lower threat and is easier to handle.

2.4. TECHNOLOGY REVIEW: POWER TO AMMONIA

Ammonia production is dominated by natural gas as the feedstock. Although commercial applications of power to ammonia were started to be used since the 1980s, it did not expand as it could not compete economically with the traditional method using natural gas. Ammonia production using electrolysis represents only 0.5% of global production[3]. Currently, much research is focused on this route since this is a green way to produce ammonia and it fits well as a solution for energy storage. This is much more relevant because of the rise in energy production via renewables. Compared to the traditional ammonia production process, utilising electricity to produce ammonia via electrolysis has the potential to reduce carbon dioxide emissions by about 1.8 tonnes per ton of ammonia produced. However, this is applicable strictly to electricity production via renewables. If grey electricity[1] is used for ammonia production, CO_2 emissions are almost 3 times higher than the conventional process[27].

Figure 2.12 shows the block diagram for the power to ammonia process. It is followed by description of main components in the system.

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[1] Grey electricity is the term for electricity production using fossil fuels. Average CO_2 emission in the Netherlands is 0.54 ton/MWh_e and average power consumption for power to ammonia is 10MWh_e/ton of ammonia[27]

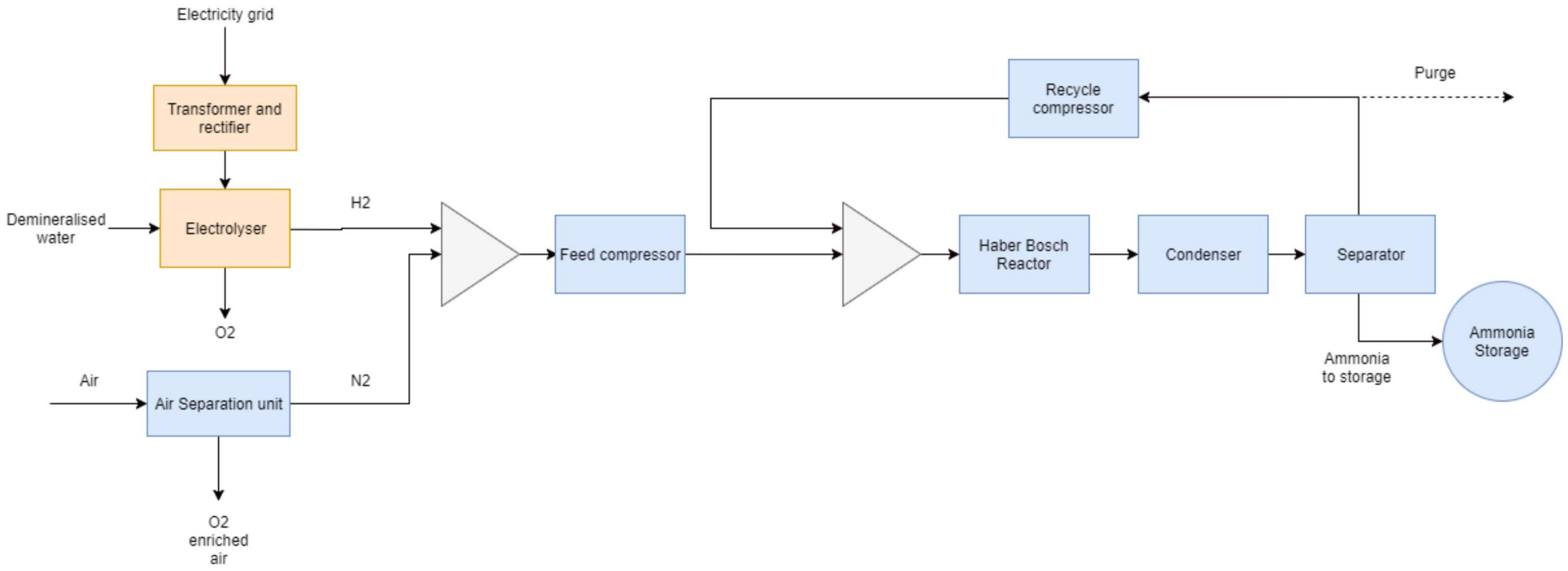


Figure 2.12: Block diagram for a power to ammonia system

ELECTROLYSER

Water electrolysis is a technology to generate hydrogen using electric power. The overall equation for water splitting is

$$H_2O \rightarrow 0.5O_2 + H_2 \tag{2.1}$$

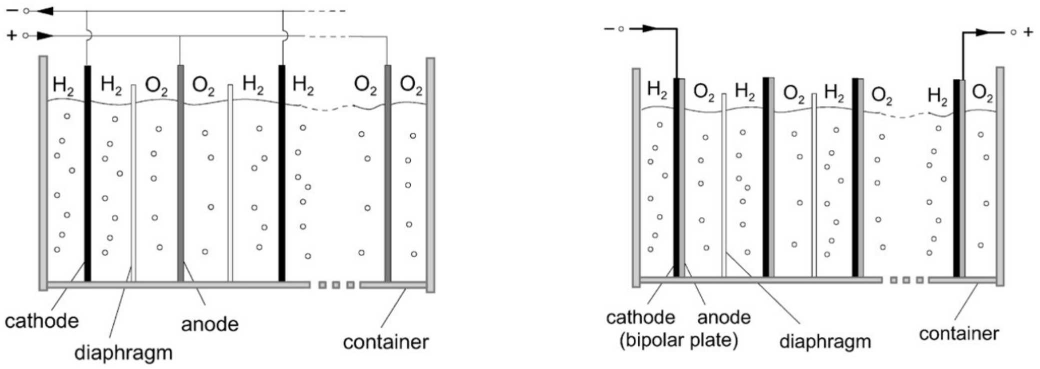
The minimum cell voltage needed for water splitting is called the reversible voltage and has a value of 1.23 V[29]. There are three types of electrolysers and all of them are governed by the theoretical energy requirement of 39.4 kWh/ kg of hydrogen[35] :

1. Alkaline electrolyser: This is the most developed water electrolyser technology available today [29]. As the name suggests, it employs an alkaline electrolyte. Anode materials are usually nickel based and cathode materials are usually stainless steel or nickel on steel[29][47]. 20-30% KOH solution is the preferred electrolyte due to its high conductivity and excellent corrosion resistance of stainless steel at this concentration. NaOH, NaCl or other electrolytes are also used in certain cases[54]. Typical operation conditions of this electrolyser are temperatures between 70-100°C and pressures between 1-30 bar [56]. Electrolysers operating at atmospheric pressure have a higher efficiency than at elevated pressures. However, the difference reduces with increasing system size. The half cell reactions at the anode and cathode are given by equations 2.2 and 2.3, respectively

$$2OH^- \rightarrow 0.5O_2 + H_2O \tag{2.2}$$

$$2H_2O + 2e^- \rightarrow H_2 + 2OH^- \tag{2.3}$$

Physical assembly of the cells can be either parallel(unipolar electrolyser) or series(bipolar electrolyser). Figures 2.13a and 2.13b represent the two configurations. Bipolar electrolysers need high precision manufacturing and is complex, but exhibit significantly lower ohmic losses. This makes it a preferred choice over unipolar electrolyser[29]. An improvement in the construction of the electrolyser is called the zero-gap design. The gap between electrode and separator is minimised to reduce ohmic losses[29][56].



(a) Unipolar alkaline electrolyser

Source: Ulleberg (2003)[56]

(b) Bipolar alkaline electrolyser

Source: Ulleberg (2003)[56]

Figure 2.13: Physical configurations of an alkaline electrolyser

Large scale alkaline electrolysers have been used around the world for hydrogen production. Most of the projects were during the period 1980s and 1990s and focused on the utilisation of hydro-electricity. Some of them are mentioned in the table 2.6[6][48].

Table 2.6: Large scale alkaline electrolyser installations

Source: Data from Bello et al.(2006)[6] and Shaltout (1998)[48]

Electrolyser manufacturer	**Installation site**	**Customer**	**Capacity ($Nm^3/hr\ H_2$)**	**Application**
Demag	Aswan, Egypt	KIMA Chemical Company	33000	Ammonia synthesis
Norsk Hydro	Kristiansand, Norway	Falconbridge Nikkelverk	1050	Nickel refining
Norsk Hydro	Reykjavik, Norway	Aburdarverksmidjan Rikisins	2600	Ammonia synthesis
Norsk Hydro	Fredrikstad, Norway	Denofa & Lilleborg Fabriker	1800	Ammonia synthesis
Norsk Hydro	Glomfjord, Norway	Norsk Hydro	6800	Ammonia synthesis

2. Proton Exchange Membrane (PEM) Electrolyser: The fundamental difference between PEM and alkaline electrolyser is the electrolyte. PEM uses a solid proton conducting membrane[35]. PEM electrolyser is not as developed as alkaline electrolyser, however it is much more compact [29].
   Most PEM electrolysers work at elevated pressures in the range of 30-60 bar and at temperatures similar to alkaline electrolyser. Hydrogen purity of 99.99+%[29] is possible due to absence of contamination by electrolyte and lower product cross over compared to alkaline electrolyser. The half cell reactions at anode and cathode are given by equations 2.4 and 2.5 respectively.

$$H_2O \rightarrow 2H^+ + 0.5O_2 + 2e^- \tag{2.4}$$

$$2H^+ + 2e^- \rightarrow H_2 \tag{2.5}$$

   Response time to variation in electric power is within 100 ms[29]. Due to expensive materials involved in construction, the cost of a PEM electrolyser is much higher compared to an alkaline one. The maximum capacity of a PEM electrolyser is about 7900 kg/year H_2. Lack of scalability is a drawback of PEM electrolyser but there is potential to improve efficiency in the future.[3].
   Stadwerke Mainz and Linde are project owners of hydrogen production plant using wind energy in Mainz, Germany. Siemens is the provider of the PEM electrolyser[1] with a peak capacity of 6MW. The electricity generation is through a 10MW wind park and the maximum hydrogen production is about 200 tonnes per year. 6-7% of the produced hydrogen is planned to be injected into the local natural gas grid and the rest will be utilised by Linde to provide their customers. Commercial testing of the plant is scheduled to be in the end of 2017[36][21].

3. Solid oxide electrolyser: This is the least mature electrolyser technology and is still in research and development stage. SOEC promises reduced electrical energy demand and is the main reason for focusing research on this technology. This technology is characterised by slow response to variation in electric power and has long startup and shut down time. A thin but dense oxide layer like Yttria stabilised zirconia (YSZ) acts as the electrolyte. Cathode material is nickel based and anode material is yttrium based. SOEC has planar and tubular configurations possible. The tubular geometry offers better mechanical strength and quicker start up and shut down, however planar geometry is easier to manufacture and displays higher electrochemical performance.
   SOEC operates at elevated temperatures of 700-100°C. This is the reason for high efficiencies achieved by SOEC. Usual operating pressure is at ambient condition, however some SOECs

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[1] Siemens Sylizer200 electrolyser - 3 nos. with 2MW each

are capable of operating at elevated pressures up to 25 bar. Due to high operating temperatures, cell degradation is rather quick and research is being focused on enhancing this limitation[29].

The performance of the three electrolysers has been compared and summarised in table 2.7

Table 2.7: Comparison of alkaline, PEM and SOEC electrolysers

Source: Data from Lehner et al.(2014)[29], Grond et al.(2013)[23] and Bertuccioli et al.(2014)[8]

Parameter	**Alkaline**		**PEM**		**SOEC**
	Present (2015)	Future (2020)	Present (2015)	Future (2020)	
Ions electrolyte	OH^-		H^+		O_2^-
Delivery pressure (bar)	40	60	60	100	<25
Operating temperature (°C)	60-80		60-80		700-1000
Max Current density (kA/m^2)	<6	<8	22	25	<3
Cell Voltage (V)	1.8-2.2	1.7-2.2	1.7-2	1.6-1.8	>1
Load density (W/cm^2)	1	2	5	5.4	NA
Cell surface max. (m2)	4	4	0.13	0.5	<0.01
Efficiency (%)	67-82	67-82	74-87	87-93	50-90
Maturity	Commercial		Precommercial		R&D
Power consumption per stack (kWh/Nm^3 H_2)	4.2-5.5	4.1-5.2	NA	NA	NA
Power consumption per system (kWh/Nm^3 H_2)	4.4-6	4.3-5.7	4.3-5.5	4.1-4.8	<3.4
Lower part load (%)	5	5	0-5	0-5	NA
Production rate H_2 per stack (Nm^3/hr)	1000	1500	120	500	NA
Capacity rate per system (kWe)	3600	5500	500	2000	NA
Lifetime (hrs)	90000	95000	50000	60000	NA
Deployment time (from stand by mode)	5 min	5 min	100 ms	100 ms	>15 min
Cold start time	20 min-hour	<10 min	5 min	5 min	hours
Annual cost improvement (%)	0.4		2.2		NA
Ramp up from min to nominal capacity (%/sec)	13	17	40	40	NA
Ramp down from nominal capacity to min (%/sec)	20	25	40	40	NA
System cost (€/kW)	930	630	1570	1000	NA
Hydrogen purity (%)	99.5+	NA	99.99+	NA	NA
Cell degradation (μV/h)	1-3	NA	<10	NA	NA

The SOEC, owing its very low stage of development and high start up and deployment time, is not considered as a practical option for this study. It is observed that for the same capacity, the cost of a PEM type electrolyser is almost 70% more than the cost of an alkaline electrolyser. Moreover, the system capacity and the life of the system is significantly higher for an alkaline electrolyser. A key advantage in favour of the PEM electrolyser is the ramp up-down rate. The ability of a PEM electrolyser to react and accommodate fluctuations in input electric power is much better than an alkaline electrolyser which gives it a strong reason to be selected as the electrolyser type for this study. However, Grond et al.(2013)[23] state that alkaline electrolysers are very much capable for power to gas applications and can satisfactorily accommodate variations in input power. A more recent study claims that modern alkaline electrolysers are capable of ramping up-down from 5% to 100% of rated capacity in a matter of seconds[40]. PEM electrolysers show good performance and have very bright possibilities for applications in the future. However, the alkaline electrolyser with its relative affordability and high lifetime coupled with satisfactory performance under fluctuating power is chosen for this study.

AIR SEPARATION UNIT

Three technologies are most popular in the industry to generate nitrogen from air.

1. Cryogenic distillation: This technology dominates the industry in air separation technology and accounts for about 90% of all commercial production. A simple block diagram of this process is shown in figure 2.14. Air is compressed to about 8 bar and cooled to ambient conditions using intercoolers. Water vapour and carbon dioxide are removed and the gas enters the distillation column through heat exchangers. Cold streams from the distillation column are used to partially condense the feed gas in these heat exchangers. High purity nitrogen is obtained at the top of the distillation column and high purity oxygen at the bottom[3][7][35]. Currently, this is the only technology commercially available to supply high purity nitrogen at large capacities[3].

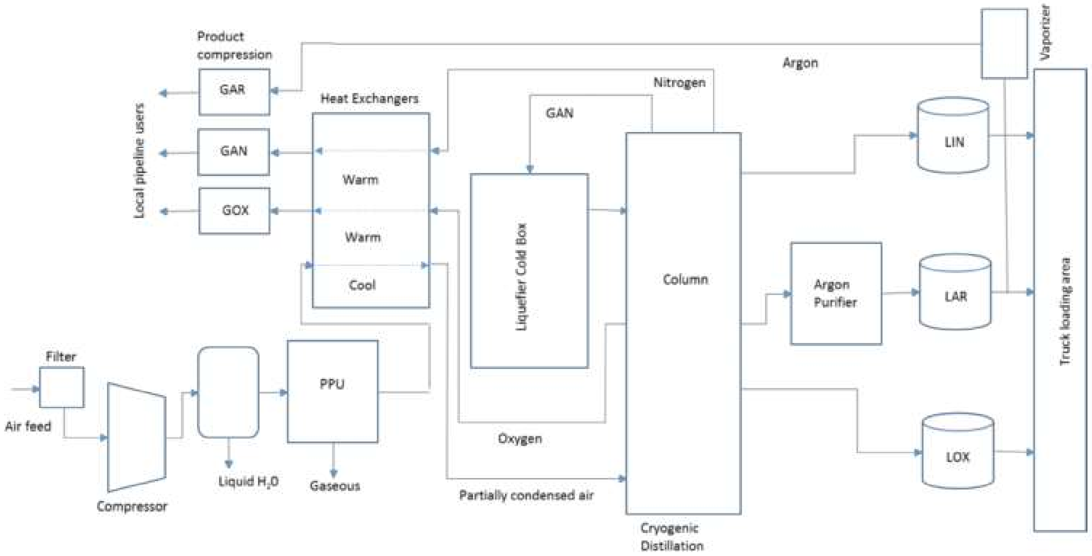

Figure 2.14: Block diagram of cryogenic distillation process [1]

Source: Bennani et al.(2016)[7]

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[1] GAR: Gaseous Argon; GAN: Gaseous Nitrogen; GOX: Gaseous Oxygen; LIN: Liquid Nitrogen; LAR: Liquid Argon; LOX: Liquid Oxygen; PPU: Pre Purification Unit

2. Pressure swing adsorption: In this process, pressurised air is filtered and passed through adsorber beds. Carbon molecular sieve is the most common adsorbant used for this application. Figure 2.15 shows a process flow diagram for a PSA system. Both adsorption towers operate in conjunction. While one column is pressurised, the other one is depressurised. Carbon molecular sieve selectively adsorbs oxygen at high pressure allowing nitrogen to pass through. When a column is fully utilised,[2] the pressure cycle is reversed to desorb oxygen and the other column now generates nitrogen. This process continues and the alternating cycle ensures uninterrupted production of nitrogen.
   Contact time of the gas with adsorbant material determines the purity of nitrogen obtained. This results in a trade off between nitrogen production capacity and purity. It is observed that purity of nitrogen produced decreases when production rates go beyond around 2000-5000 Nm^3/hr. Additional purification steps are needed to remove oxygen content from the nitrogen stream. Compared to cryogenic distillation process, PSA requires less maintenance and is much more compact[3][7][35].

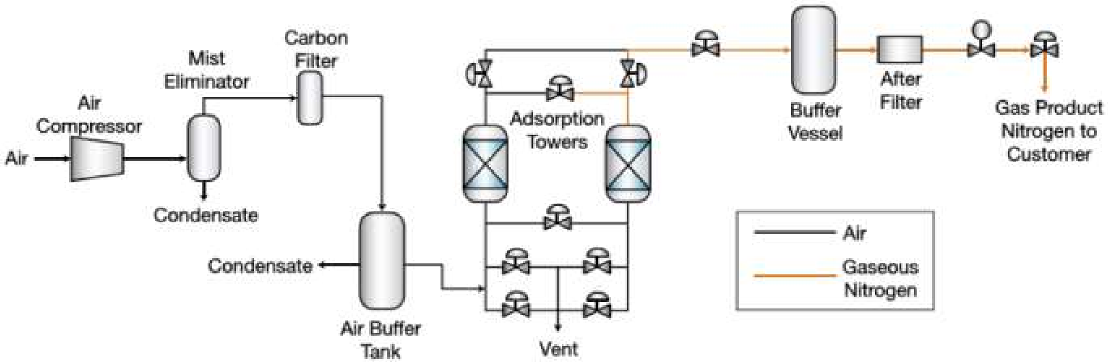

Figure 2.15: Process flow diagram of PSA process for air separation

Source: Bennani et al.(2016)[7]

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[2] State when it can no longer adsorb more oxygen

3. Membrane separation: This process utilises the principle of selective gas permeation to separate nitrogen from air. Figure 2.16 shows a process flow diagram for this process. Multiple membranes are usually employed in this process to selectively separate oxygen, carbon dioxide and water vapour. This leaves nitrogen as the retenate. Purity of nitrogen is usually limited to 99.5% and decreases with higher capacity. PSA or catalytic de-oxygenation technology is employed as an extra process step to obtain higher purity[7][35].

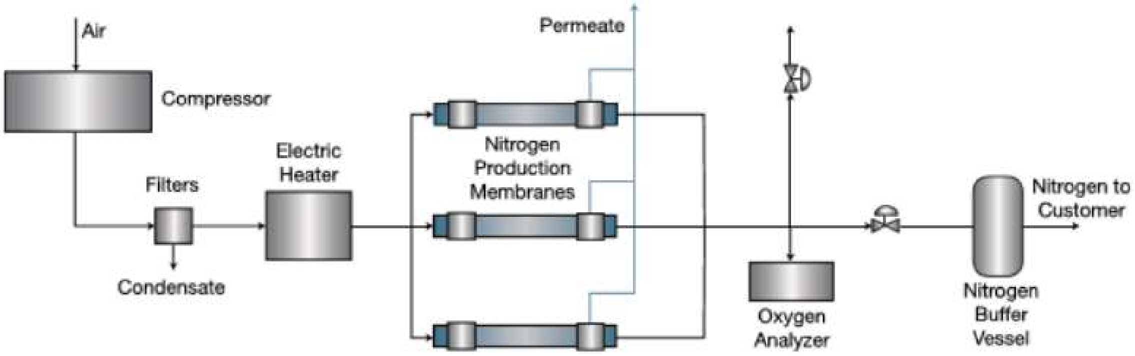

Figure 2.16: Process flow diagram of membrane separation for air separation

Source: Bennani et al.(2016)[7]

Figure 2.17 shows the operating range of the three technologies and shows how purity of nitrogen stream is affected by capacity. It helps to select the proper technology based on application.

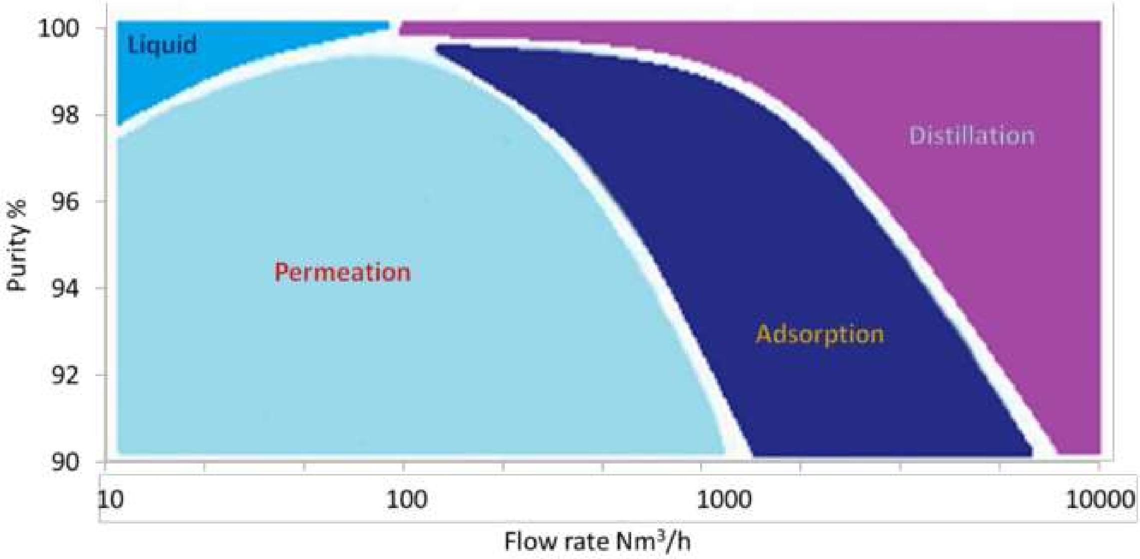

Figure 2.17: Figure regarding selection of air separation technology based on capacity and purity of nitrogen

Source: Bennani et al.(2016)[7]

AMMONIA SYNTHESIS LOOP

The ammonia synthesis reactor, recycle compressor, condenser and separator form the ammonia synthesis loop. The configuration of the loop may be unique to every plant[3]. The Haber Bosch process for synthesis of ammonia is given as[2]

$$3H_2 + N_2 \rightleftharpoons 2NH_3 \quad \Delta H = -92.44 kJ/mol_{N_2} \tag{2.6}$$

The operating conditions of the reactor are typically between 350-550°C and 100-300 bar. Iron based catalysts are usually employed in industries[7]. Equilibrium is shifted toward ammonia at higher pressure and lower temperatures[33]. However, higher temperatures aid the kinetics of reaction. The conversion per pass of reactants in a Haber Bosch loop is usually around 15-25%[3]. It is essential to have a recycle loop to improve the conversion. High purity feed is necessary for the Haber Bosch synthesis since the iron catalyst degrades in the presence of impurities like sulphur, water and oxygen[3]. The feed stream contains inerts usually from the air separation unit and this is removed using a purge stream. Figure 2.18 shows a simplified process flow diagram for the ammonia synthesis loop. An initial heating duty is needed to initiate the reaction and is shown as heater 1 in the figure. At steady state, this heating is stopped and the exothermic nature of reaction provides sufficient heat to keep the reactor running. The reactor consists of multiple catalyst beds and fresh feed in injected onto each bed. This prevents a temperature surge within the reactor. This is represented as cooler 1 in the figure and it ensures the reactor operates isothermally[3]. For industrial scale ammonia plants, ammonia is cooled to sub zero temperatures in the condenser (cooler 2 in the figure) using refrigeration. This helps improve the purity of ammonia product. Heat from the reaction is also utilised for steam and power generation. However, this is avoided for small scale plants keeping economics in mind. (personal discussion with Proton Ventures).

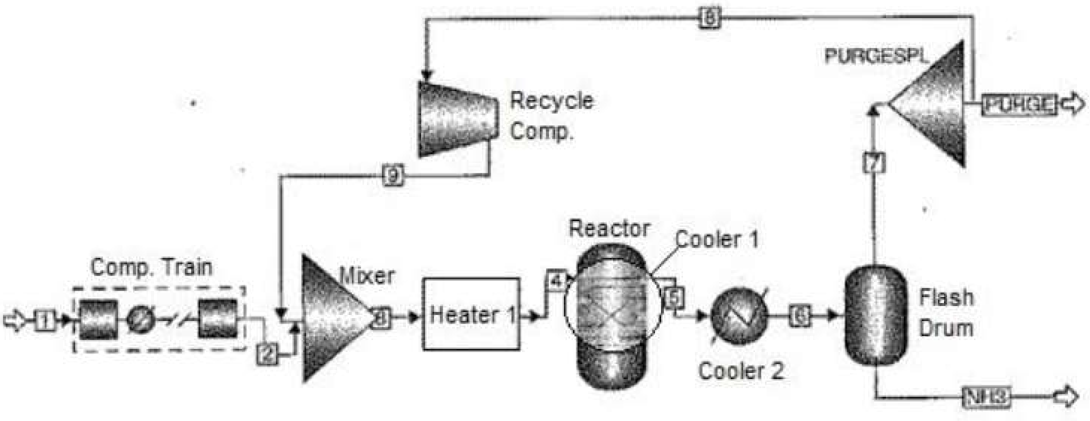

Figure 2.18: Simple process flow diagram for ammonia synthesis loop

Source: Bañares-Alcántara et al.(2014) [3]

New catalysts are being researched and developed to improve the efficiency of conversion. Ruthenium (Ru) based catalysts offer higher activity than iron based catalysts but suffer from degradation at high hydrogen pressures. Use of bimetallic catalysys like CoMoNx and FeMoNx show high ammonia concentration at exit of reactor however at the expense of reaction rate[3].

AMMONIA STORAGE

Ammonia is stored as a liquid and this is commercially done in two ways:

1. Ambient pressure and refrigerated: Ammonia is refrigerated to -33°C and stored in insulated cylindrical tanks at ambient pressure. This is usually employed for large ammonia production facilities. Each tank has storage capacity of over 10000 tonnes. Typical boil off of ammonia is 0.04% per day. Additional re-compression and flash loop is essential to prevent loss of ammonia from storage[3]. This type of storage is usually considered for storage capacities greater than 4500 tonnes[35]. Storage tanks are usually made of steel and have a secondary concrete wall. A fixed or floating roof may be employed.
   OCI Nitrogen in Geleen has two storage tanks each with a capacity of about 17000 tonnes. They own two storage tanks in the Rotterdam as well each with a capacity of 15000 tonnes[7]. Figure 2.19 shows the storage tanks in Rotterdam.

Figure 2.19: Refrigerated ammonia storage tanks at Europoort, Rotterdam

Source: Bennani et al.(2016)[7]

2. Ambient temperature and elevated pressure: Pressure vessels are used to store ammonia as a liquid at ambient temperature. Typical pressure range is from 8-17 bar. Depending on the capacity, they can be either spherical pressure vessels or skid mounted cylindrical pressure vessels. These two types are depicted in figures 2.20a and 2.20b. Spherical pressure vessels are considered when storage capacity greater than 500 tonnes is required(personal discussion with Proton Ventures).

(a) Skid mounted cylindrical pressure vessel

Source: Bennani et al.(2016)[7]

(b) Spherical pressure vessel

Source: TF Warren group[53]

Figure 2.20: Ammonia storage at ambient temperature and elevated pressure

The ammonia storage methods are compared and summarised in table 2.8. Due to refrigeration needs and large area, cost associated with refrigerated tanks is high. The spherical pressure vessels are compact but difficult to manufacture leading to high CAPEX. The skid mounted pressure vessels are bought off the shelf or custom made and is portable. Multiple units can be stacked together for larger capacity. For small scale applications, the skid mounted cylindrical pressure vessel is the best storage option.

Table 2.8: Comparison of ammonia storage methods

	Refrigerated storage tank	**Spherical pressure vessel**	**Skid mounted cylindrical pressure vessel (single unit)**
Capacity	>4000 tonnes	>500 tonnes	<210 tonnes
CAPEX	↑↑	↑↑	↓↓
OPEX	↑	↓	↓↓
Land area	↑↑	↑	↓↓

RELATED RESEARCH

Power to ammonia and using ammonia as a solution for energy storage is a trending topic among researchers. Bañares-Alcántara et al.(2014)[3] have focused on islanded ammonia production from wind power. A wind farm with a peak and average power production of 100 MW and 36.43 MW, respectively have been considered here. Surplus wind power that is available after satisfying the operational demand of the island has been utilised to produce ammonia. The peak and average power utilised for ammonia production is 36.75 MW and 18.33 MW respectively. The produced ammonia is utilised to meet the electric power demand of the island and to keep the ammonia plant operational during periods of insufficient power production by the wind turbines. Ammonia production capacity of 48 TPD to 120 TPD have been assessed for economic feasibility. Hydrogen storage has been considered in this analysis and a model has been developed to indicate optimal choice of system configuration based on variable input.

Morgan et al.(2014)[34] have presented a techno economic feasibility for a specific islanded power to ammonia case using wind power. The motivation of this study is to reduce dependency of the island on diesel and replace it with ammonia. The study assesses a range of installed capacity of wind power from 50 kW to 1.25 MW. Hydrogen storage has not been considered, but the study assumes operational capacity of ammonia plant from 0-100% of installed capacity. A difference between this study and that presented by Bañares-Alcántara et al.(2014) is that Morgan et al.(2014) do not consider ammonia to be used as a source of energy to run the ammonia plant.

Morgan (2013)[35] presents a techno-economic study of power to ammonia using offshore wind power. 100 wind turbines, each of 3 MW installed capacity has been considered for assessment with an ammonia production capacity of 300 TPD.

Wang et al.(2017)[59] have analysed a power to ammonia system focusing on energy storage using a reversible SOFC, GT and a steam turbine. Optimisation routines are performed to maximise efficiency for electricity production from ammonia and minimise investment costs. A time invariant electric power source of 100 MW has been considered in this study and a detailed energy integration strategy has been presented.

Beerbühl et al.(2015)[5] have presented a heuristic optimisation method for a grid power based ammonia production. The German electricity market data for 2013 has been used here with an ammonia production plant with capacity of 72 TPD. The study focuses on scheduling and capacity planning with respect to varying electricity price.

Bennani et al.(2016)[7] have presented feasibility studies for power to ammonia from renewable energy by creating three scenarios relevant to the Netherlands. The first scenario considers ammonia production using a stand alone wind turbine with installed capacity of 1.5 MW. The second scenario considers a residential complex with 50 kW of installed solar power capacity and 150 kW installed wind power capacity. Surplus electric power produced by the energy sources has been considered to run a power to ammonia unit. Finally, application of power to ammonia for national electrical grid balancing has been considered with a combined installed solar and wind capacity larger than 10000 MW.

ISPT(2017)[27] presents a general overview of power to ammonia technology. It gives an insight into the potential of this technology when applied to real scenarios in the Netherlands.

Siemens is involved in a demonstration project of ammonia production near Oxford, United Kingdom, using wind power and a PEM electrolyser. The produced ammonia has been planned to be combusted in a gas turbine. Cardiff University as a partner in the project is involved in research and development of utilising ammonia as a fuel in a gas turbine. The evaluation of the demonstration is scheduled to be in December 2017[49][25].

In March 2016, Nuon announced its plan to study the feasibility of utilising ammonia as fuel at Magnum-one of their power stations. Ammonia has been proposed to be produced using surplus electricity from wind and solar energy thereby providing a solution to seasonal storage of electricity. As part of this power to ammonia project, a new collaboration between Nuon and Gasunie and Statoil has been set up in July 2017 to investigate production of hydrogen from natural gas and utilising hydrogen directly in power production. Institute of Sustainable Process Technology (ISPT) plays an important role by bringing together research partners from all over the Netherlands like ECN, TU Delft, Proton Ventures, Akzo Nobel, OCI Nitrogen and a few others. Ammonia will play an important role in this proposed hydrogen economy as a storage medium of hydrogen[11][13].

EMERGING TECHNOLOGY

Electrochemical synthesis of ammonia from hydrogen and nitrogen is a novel ammonia production method which was first demonstrated in 1998[28]. Gaseous hydrogen was passed at the anode of a proton conducting cell. An applied voltage caused H^+ ions to migrate to the cathode where it reacted with nitrogen to form ammonia. Depending on the type of electrolyte used, the process is classified into four main categories. A detailed classification is shown in figure 2.21.

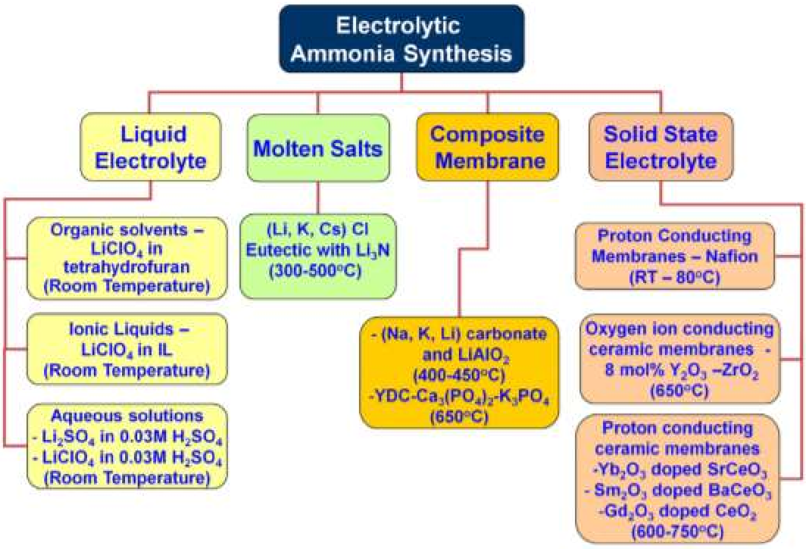

Figure 2.21: Classification of electrochemical ammonia synthesis

Source: Giddey et al. (2013)[22]

The process involving solid state electrolytes are reported to be the most promising currently because of the ease to separate hydrogen from the produced ammonia stream[3]. Apart from hydrogen as feed stream, natural gas as a substitute has also been investigated. This was done using oxide salt composite electrolyte[1] with 80% wt. YDC[2] and 20% wt. binary phosphate.
Electrochemical synthesis of ammonia is a developing technology and no commercial scale system has been developed yet. The ammonia synthesis rates are rather low from a commercial perspective. Solid state electrolyte with polymer electrolyte membrane shows the highest ammonia production rate of around 10^{-8} $molcm^{-2}s^{-1}$[22]. Commercially viable production rate is close to 4.3×10^{-7} $molcm^{-2}s^{-1}$[27]. An improvement by 1-2 orders of magnitude is necessary to make this technology suitable for commercial applications.
The technology offers ammonia synthesis at operating conditions much lower than Haber Bosch implying potential savings in material and energy costs. This system is easy to be integrated with a renewable energy network and can find applications in the future if ammonia production rates improve significantly[3].

---

[1] $(Ca_3(PO_4)_2 - K_3PO_4)$

[2] Yttrium doped ceria

3

PROJECT DESCRIPTION

This chapter helps to understand how the ammonia industry can be linked to the steel industry, by having a positive influence on both industries. Section 3.1 describes the energy network at Tata Steel IJmuiden. Section 3.2 describes the problem statement considered. Section 3.3 defines the research aim and objectives to be accomplished by this study.

3.1. TATA STEEL IJMUIDEN: ENERGY NETWORK

Steel-making is a very energy intensive process. WAG are energy rich by-product gas streams evolved during the steel making process and contain gases like hydrogen and methane in them. The composition of WAG is shown in Appendix B. Figure 3.1 shows the main processing steps in steel-making and the source of the WAG.

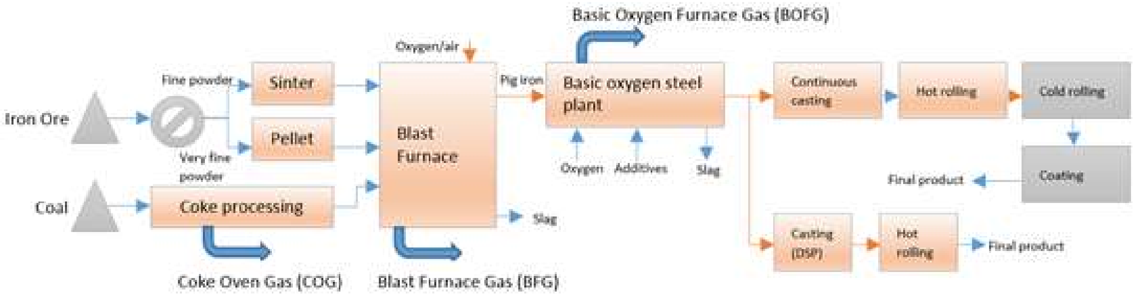

Figure 3.1: Steel-making process block diagram at Tata Steel IJmuiden

At Tata Steel IJmuiden, part of the gases is utilised to produce heat for steel making process and part of it is used to generate electricity. Two power plants owned by Nuon (IJM01 and VN24/VN25) are responsible for this. WAG are transported with pipelines to the power plants and energy is distributed back by a high voltage grid connection to the on site grid. Figure 3.2 shows the network of WAG at Tata Steel IJmuiden.

Tata Steel IJmuiden hires certain capacity[1] of the two power plants. All electricity produced within this capacity limit is owned by Tata Steel and the excess is partly owned by Nuon. About 3500 GWh of electricity is produced annually from the WAG and based on data for year 2013 it represents about 3.5% of the national electricity production. The produced electricity is utilised by Tata Steel, IJmuiden to meet its operational demand and any excess electricity is sold on the APX day ahead market.

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[1] Capacity is readjusted four times a year. It is currently 3650 GJ/hr

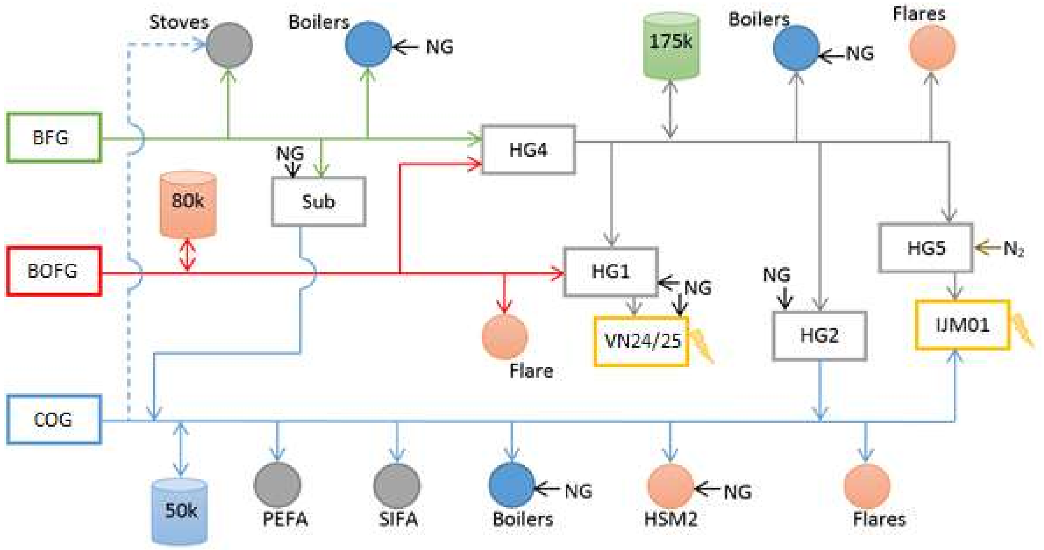

Figure 3.2: Work arising gas network at Tata Steel IJmuiden [1]

Power station VN25 is new and replaces VN24. It has a higher capacity than VN24 and can be operated at part loads. VN24 is operated only when VN25 is shut down for maintenance. IJM01 is the most efficient power station but offers no flexibility in operation. Apart from the Nuon power stations, there is a network of smaller power and steam generators within Tata Steel IJmuiden. These generators supply steam and electricity to ensure the safety of the molten-iron-route, the core control processes and other crucial devices.
Three top gas recovery turbines (TRT6, TRT7A and TRT7B) generate about 6MW each using energy from high pressure BFG stream. These generators exhibit strong fluctuations in power output.
STEG11 is a combined cycle power generator employing a gas and steam turbine. Natural gas from the local gas grid is utilised to produce a maximum of 12MW. This generator offers flexibility in operation and can be ramped down to 5MW if necessary.
TG2 is a steam turbine and the most flexible onsite generator. It is used to maintain pressure of steam in the steam network and usually produces about 5MW of power. It can be ramped up to 12-13 MW at the expense of high pressure steam.
AET is a natural gas expansion turbine and utilises energy from high pressure natural gas (60 bar) from the local grid. It produces around 1MW of electric power and natural gas at 3 bar.
The Nuon power stations and the onsite generators together make up the energy network at Tata Steel, IJmuiden.

3.2. PROBLEM DEFINITION

The energy network at Tata Steel, IJmuiden has many components and a dynamic nature of operation. This is translated into a continuous mismatch in supply and demand of electric power. Figure 3.3 displays the difference between power generation and consumption by the plant as a function of time. The figure represents a characteristic period of one week, which has a range of about -50 MW to 150 MW. This range can be as wide as -250 MW to 200 MW. During times of surplus electric power, the excess electricity is sold to the grid and during times of deficit power, electricity is purchased from the grid. The price of buying and selling is different from the usual APX day ahead market, but is similar in the sense that it varies throughout the day. The price is redetermined with 15 min time intervals, similar to the APX day ahead market. This repetitive imbalance of power de-

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[1] PEFA: Pellet Fabriek; SIFA: Sinter Fabriek; NG: Natural Gas; HG1-5, Sub: Gas mixing points; HSM: Hot Strip Mill

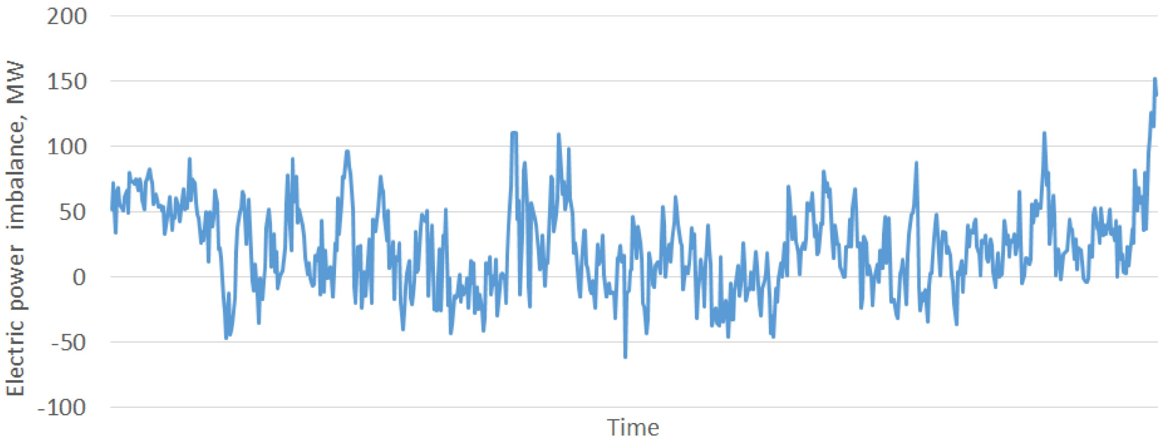

Figure 3.3: Electric power imbalance in week 1 of year 2013 at Tata Steel, IJmuiden

mand and availability and the varying electricity price are the primary motivation for investigating energy storage application. The two potential objectives of energy storage are:

- Conversion of electric power into a more valuable commodity.
- Economic gain by recovery of electric power during times of deficit when the electricity prices are too high.

The goal of this study is to assess the feasibility of a system which has the potential to address both these value addition propositions. The availability of surplus electric power and the presence of hydrogen rich gas streams help to produce ammonia in a carbon neutral manner and at the same time provide value addition to these commodities. This creates a synergistic relationship between the steel industry and the ammonia industry.

3.3. RESEARCH AIM AND OBJECTIVES

The aim of this research is to assess the techno-economic feasibility of an ammonia based energy storage system at Tata Steel, IJmuiden utilising surplus electric power
Three research objectives are distinguished:

1. To identify the major factors influencing the levelised cost of ammonia
2. To determine the optimum electrolyser capacity under conditions of varying electric power availability.
3. To investigate the influence of external hydrogen utilisation.

4

ANALYSIS OF ELECTRIC POWER IMBALANCE AT TATA STEEL IJMUIDEN

This chapter provides a statistical analysis of the electric power imbalance. It also presents a motivation for the development of a model for the techno-economic assessment of the power to ammonia system.

The first step of this case study is to understand the behaviour of electric power pattern at Tata Steel IJmuiden. Data for two consecutive years, 2013 and 2014 were made available for this study. The annual pattern for both years is shown in figure 4.1 and 4.2. The imbalance is measured with 15 minute intervals for the entire year and the corresponding unit buying and the unit selling price has been recorded at each interval.

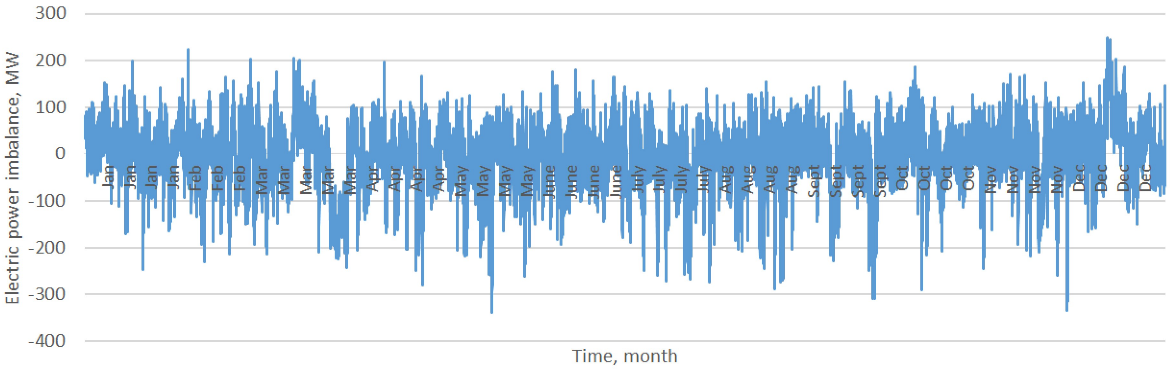

Figure 4.1: Electric power pattern at Tata Steel IJmuiden, 2013

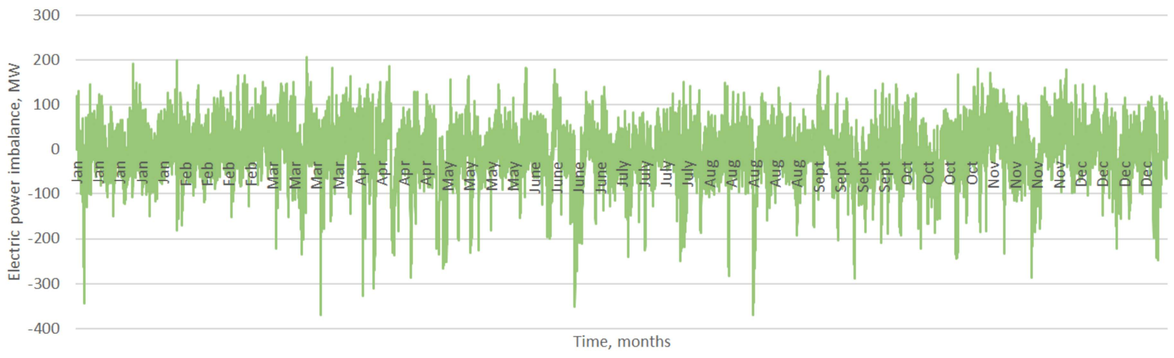

Figure 4.2: Electric power pattern at Tata Steel IJmuiden, 2014

The data set for 2013 shows a range from about -339 MW to 248 MW whereas the year 2014 data shows a range from about -370 MW to 207 MW. The two patterns are superimposed in figure 4.3.

Figure 4.3: Superimposition of electric power pattern for 2013 and 2014

By visual comparison, the patterns appear fairly similar. Several dominant inconsistencies have been marked and labelled in the figure 4.3. The reasons for these mismatches were investigated and attributed to the following causes:

1. Power plant IJM01 shut off in 2013
2. Both power plants shut down in 2014
3. Power plant IJM01 shut off in 2014
4. Power plant VN24/25 shut off in 2014

The reasons for shutdown of the power plants have not been investigated in this study. However, it does shed light on some of the major inconsistencies of the electric power pattern for both the years. For a thorough comparison, a statistical approach has been chosen. The distribution of the imbalances has been plotted for both the years as shown in figures 4.4 and 4.5. Both distributions closely fit a normal distribution curve. The mean and standard deviation are -5.94 MW and 68.33 MW respectively for year 2013 and -6.61 MW and 63.59 MW for year 2014. The difference in the coefficient of variance[1] for the two datasets is less than 17%. It is concluded that for the intent of

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[1] Coefficient of variance is a standardised measure of dispersion of a frequency distribution. It is defined as the ratio of the standard deviation to the mean.

this study, the annual pattern for electric power imbalance at Tata Steel IJmuiden is uniform, apart from the mentioned predictable inconsistencies. This allows the study to be concentrated on a single year. The data set for the year 2013 was chosen for further analysis.
During the year 2013, the imbalance is positive for 51% of the time (from actual data), implying that surplus electric power is available for almost half a year. This surplus may be utilised to feed the power to ammonia system. Import of additional electric power from the grid is required during remainder of the time.

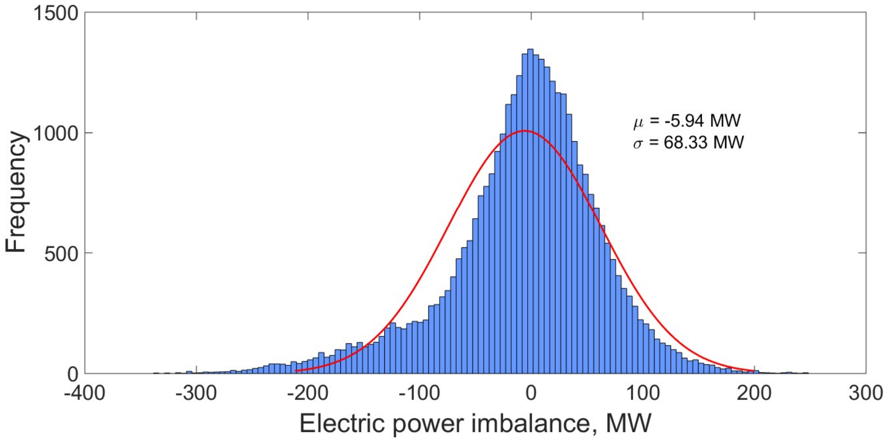

Figure 4.4: Histogram of the electric power imbalance for year 2013

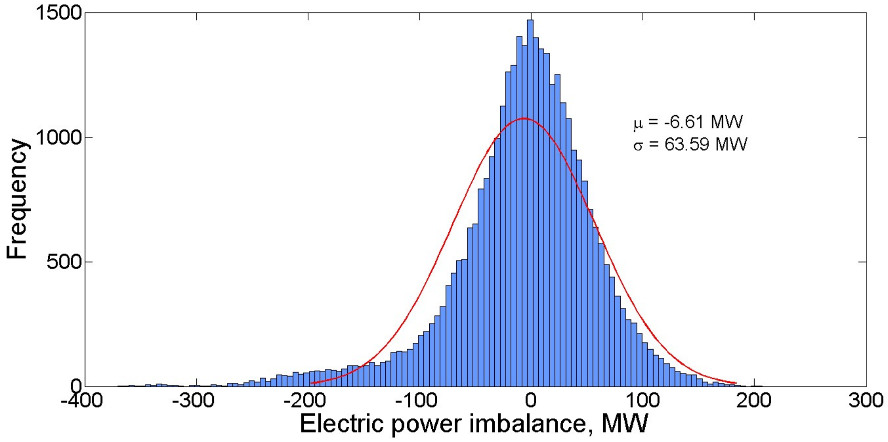

Figure 4.5: Histogram of the electric power imbalance for year 2014

A simple probability calculation (See Appendix D) of the electric power imbalance distribution for year 2013 shows that 75% of all the positive imbalances is less than 75.91 MW. It has been justified in section 5.2.1 that the rated capacity of the electrolyser corresponds to the rated capacity of the ammonia synthesis section. Hence, to maximise the operation of the system at its rated capacity with minimal import of additional power from the grid, it is to be expected that this capacity would be lower than 76 MW. However, the economic feasibility of the entire system also depends on other factors like influence of CAPEX on the capacity, actual ammonia production after considering import of additional electric power etc. This justifies the need for a model to understand the influence of factors and find the best suited capacity. It is assumed that there would be one capacity at which the costs are minimised and hence an optimum capacity exists.

5

RESEARCH APPROACH

This chapter describes the general path followed to accomplish the research objectives given in Section 3.3. Section 5.1 discusses the sources of the data sets used in this study. Section 5.2 provides a description of model developed for this study. Section 5.3 describes the various scenarios that were analysed using the model.

5.1. DATA COLLECTION

Table 5.1 shows the main data sets that were used for this study and the source from which they were obtained. Most data not provided by Tata Steel were obtained from Proton Ventures, as this company has extensive technological expertise in the field of production and storage of ammonia. These data were collected from internal company reports, discussion with experienced engineers, and process simulation models in ASPEN® HYSYS. Literature references and good engineering judgement was used where data could not be obtained from either of the participating companies.

Table 5.1: Source of main data set

Data	**Source**
Electric power imbalance	Tata Steel
Electric power price	Tata Steel
Utility prices	Tata Steel
Power to ammonia investment costs	Proton Ventures
Ammonia synthesis process specifics	Proton Ventures

5.2. DEVELOPMENT OF TECHNO ECONOMIC ASSESSMENT MODEL

5.2.1. OBJECTIVE OF MODEL

The primary objective of the model is to complete the three research objectives (See section 3.3). Figure 5.1 schematically depicts the operation principle of the model. The model accepts an electric power pattern of desired duration,the associated electric power price pattern and the utility prices as input. The main outputs provided are minimum levelised cost of ammonia along with the contribution of factors influencing it and the optimum capacity of the system to achieve this cost. Since the model is flexible in terms of input, it is a generic tool and can be used for different scenarios easily with no or very few modifications.

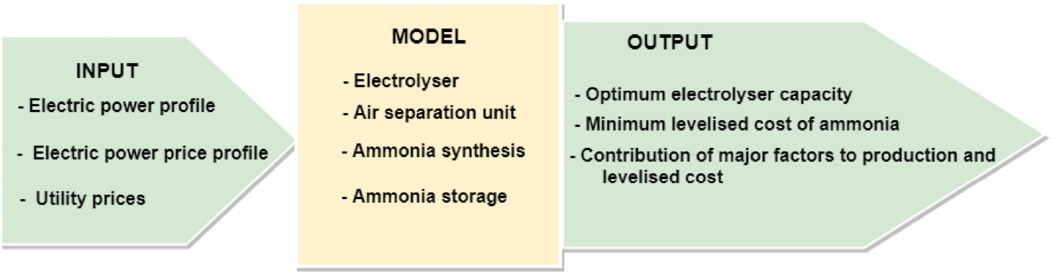

Figure 5.1: Figure showing the inputs and outputs of the power to ammonia model

A more detailed list of model outputs is given as follows:

- Plots of the electric power profile and ammonia production for a specified time period.
- Utility requirement (power and/or cooling water) for each component of the power to ammonia system.
- Ammonia storage requirement including number of storage vessels necessary.
- Plot of the utilisation of the electrolyser as a function of its installed capacity.
- Plot of the levelised[1] and unlevelised[1] production cost of ammonia as a function of the installed electrolyser capacity.
- Plot of the main factors contributing to the production cost of ammonia as a function of the installed electrolyser capacity.
- Tornado plot of the main factors contributing to minimum production cost of ammonia with a user specified sensitivity.
- Plot of the power to ammonia efficiency as a function of the installed electrolyser capacity.
- Plot of the energy storage cost as a function of the installed electrolyser capacity.

5.2.2. GUIDELINES ADOPTED FOR DEVELOPMENT OF MODEL

The following considerations have been made to develop the model:

1. For the purpose of initial allocation of power (described in subsection 5.2.3), the hydrogen compression unit, ammonia synthesis unit and the air separation unit are considered to be a single block. It has been assumed that the specific power consumption(kWh/Nm^{3}of H_2 produced by the electrolyser) of these components remains constant at all operating capacities. Hence the ratio of power demand of these units is independent of the operating capacity of the electrolyser. This simplifies the entire power to ammonia system into two blocks- the electrolyser (ELY)[2] and the ammonia synthesis section (AS)[3].

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[1] The production cost of ammonia considering the time value of money is known as the levelised cost. The production cost calculated by neglecting the time value of money is termed as unlevelised production cost. Appendix G describes levelised production cost in detail

[2] Comprises of transformer, rectifier and the electrolyser

[3] Includes hydrogen compression, feed compression, air separation, ammonia synthesis reactor, recycle compressor, separator, condenser and ammonia storage units. For cost estimation, the hydrogen compression unit is considered to be part of the electrolyser

2. Storage of hydrogen is technologically challenging and relatively expensive. Discussions with Tata Steel have resulted into exclusion of hydrogen storage from this study. This requires the hydrogen stream generated by the electrolyser to be continuously utilised by the ammonia synthesis section. As a result, the installed capacity of AS corresponds to the installed capacity of the electrolyser.

3. The electrolyser is capable to run even at part loads as low as 5%(section 2.4). However, it is not possible for the ammonia synthesis section to operate at such low loads. Thus, the minimum part load of AS determines the minimum part load of the entire system. This limit is assumed to be 25% (as indicated by Proton Ventures)

4. Continuous operation is required for AS. This means import of additional electric power during deficit is unavoidable unless some other means exist to keep the AS continuously running.

5. The system is modelled using MATLAB®.

5.2.3. LOGIC FOR POWER ALLOCATION TO THE SYSTEM

One of the most important parts of this model is to allocate electric power to the system and make a decision whether excess electric power needs to be imported for operating the system. The system has three distinct operating regions with respect to capacity.

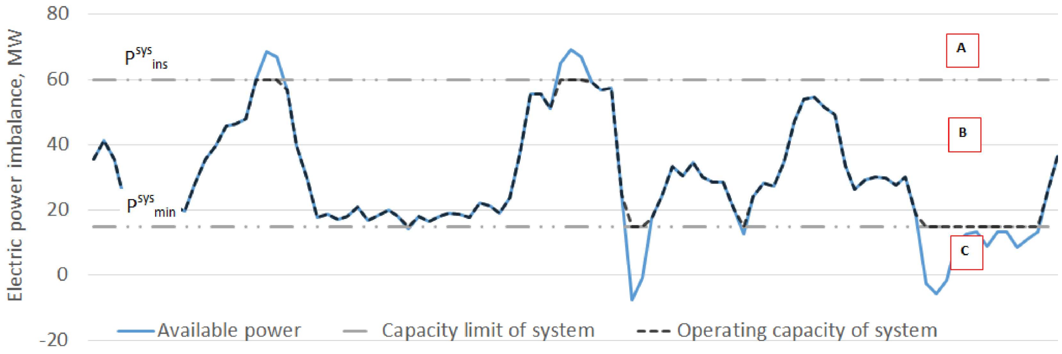

Figure 5.2: Logic for power allocation to the system

1. Region A: The available power exceeds the power consumption at the installed capacity of the system. The system will operate in this region at the installed capacity and excess power will be curtailed.

2. Region B: The available power ranges between the power consumption at the installed and minimum capacity limits of the system. The system will utilise all available power.

3. Region C: The available power is lower than the power consumption at the minimum operating capacity of the system. Electric power needs to be imported from the grid to ensure continuous operation of system.

Figure 5.2 illustrates the relation between the available electric power and the operating capacity for these three regions. P^{sys}_{ins} and P^{sys}_{min} represents the installed capacity and minimum capacity of the system. The operating capacity varies within these two limits for any variation in available power.

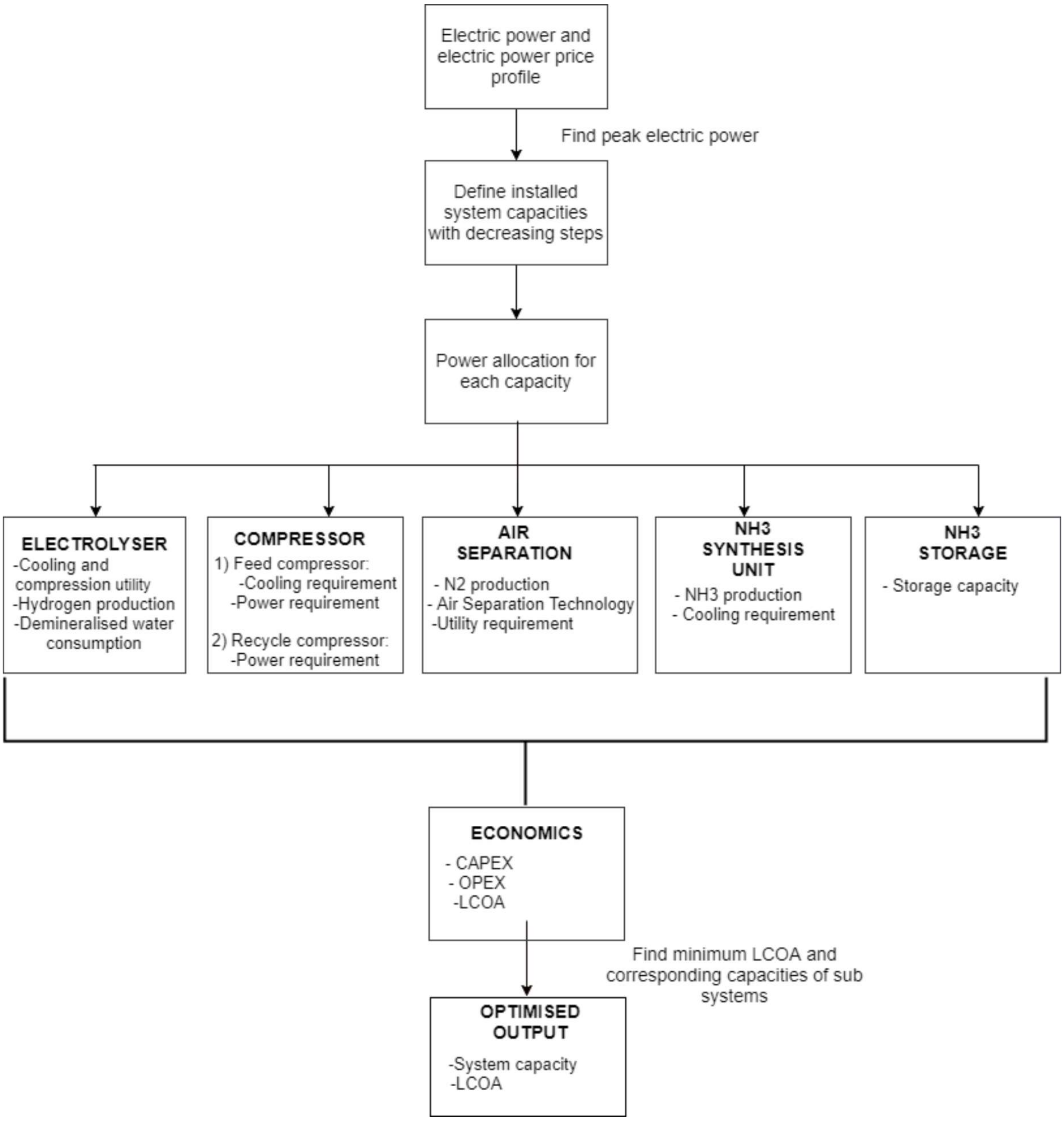

Figure 5.3: Optimisation logic of power to ammonia model

5.2.4. OPTIMISATION LOGIC OF THE MODEL

One of the objectives of the model is to find the optimum system capacity as mentioned in section 5.2.1. For this purpose an algorithm was developed that finds the installed system capacity that results into the lowest overall cost for the predetermined electric power and electricity price patterns. The algorithm is reflected schematically in figure 5.3. The optimisation mechanism is essentially formed by repetitive calculation of the total operating cost with a stepwise increase of the installed system capacity. The minimum calculated value corresponds to the optimized system capacity, within the accuracy constraint of the chosen step size.

5.3. SCENARIOS CONSIDERED

The following scenarios are investigated within this study:

1. Base scenario: This is the scenario which can be currently directly applied at Tata Steel IJmuiden. It considers the electric power and price pattern of the year 2013 and assesses the feasibility of a power to ammonia system, directly employing the output of the developed model as described in section 5.2.4. Sensitivity analysis is performed by varying electricity price and electrolyser CAPEX. To get a relative idea of feasibility, a sub-scenario has been considered here:
    - Complete utilisation of equipments: It is assumed that abundant electric power is available and system always operates at the installed capacity. The impact on economic feasibility has been studied with this change.
2. Hydrogen from work arising gases: In this scenario, it is considered that purified hydrogen is available from the work arising gases at Tata Steel IJmuiden and it is used to eliminate the need to import electric power from the grid to operate the electrolyser during times of deficit. This hydrogen ensures continuous operation of the ammonia synthesis section. The separation processes needed to produce high purity hydrogen and the associated costs are discussed and influence of utilising this hydrogen on the feasibility of power to ammonia system is investigated.
3. Hydrogen from external source: Tata Steel IJmuiden is involved in efforts to make a transition to a hydrogen economy and reducing its carbon footprint. This scenario assumes there is abundance of high purity hydrogen available and the minimum cost of hydrogen required to make an economically feasible ammonia production plant is evaluated. This scenario assumes sufficient hydrogen is available continuously at all capacities, thereby eliminating the need of an electrolyser to generate hydrogen. This scenario does not focus on energy storage of surplus electric power but rather energy storage of hydrogen in the form of ammonia.

6

MODELLING

This chapter describes the procedure for modelling each component of the system. Section 6.1 shows the process scheme used to model the power to ammonia system. Section 6.2 describes the assumptions and method used to model each component of the system. Section 6.3 and 6.4 describe the technical and economic modelling details of the system respectively.

6.1. PROCESS SCHEME

The block diagram of the power to ammonia scheme used in this study is shown in figure 6.1. The ammonia synthesis loop with the feed compression has been simulated using ASPEN®HYSYS. The configuration of the ammonia synthesis loop is shown in Appendix F.

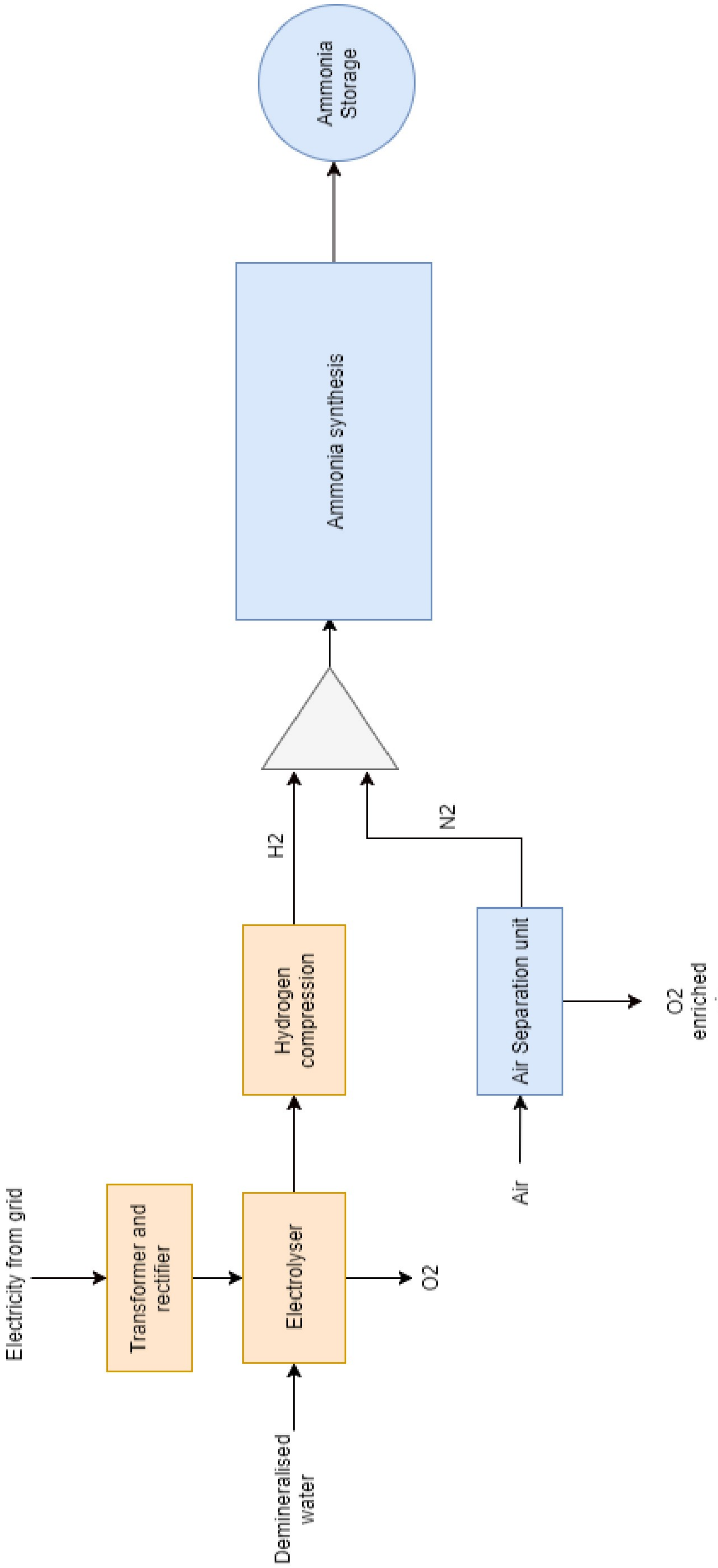

Figure 6.1: Block diagram for power to ammonia system used in this study

6.2. GENERAL ASSUMPTIONS

The major assumptions made for development of the power to ammonia model are:

1. It is assumed that the change in operating capacity of all components of the system is instantaneous with varying availability of power.
2. Oxygen from the electrolyser and the air separation unit is not considered as a valuable by-product.
3. Cooling and demineralised water are available at Tata Steel. No additional investments have been considered for these units. Prices of these utilities as available at Tata Steel have been considered.
4. Pumps for cooling water, demineralised water and final ammonia product have been neglected from this study. Similarly, electric power for the control system, lighting and other small items have been neglected.
5. Minimum electrolyser capacity is considered to be 1.2 MW which corresponds to the smallest capacity of ammonia units conceived by Proton Ventures.
6. Heat integration of components is not considered in this study.
7. It is assumed that cooling water is available at 20°C and the permissible temperature rise is 10°C.

Other assumptions are mentioned in the following subsections when modelling details of each component of the system is discussed.

6.3. COMPONENTS MODELLING

6.3.1. ELECTROLYSER BLOCK

1. Assumptions and considerations:
   - (a) The transformer and rectifier are represented in the model only by an operational power loss. A constant efficiency factor of 95% is assumed for each unit, independent of the operating capacity.
   - (b) It is assumed that the electrolyser produces hydrogen at a temperature of 80°C and atmospheric pressure. It is assumed that 0.5% of the hydrogen is lost as cross over to anode and in the purification step. 100% pure hydrogen is assumed to available after the purification step.
   - (c) Linear dependency of specific power consumption of the electrolyser on part load operation has been assumed.
   - (d) The pressure ratio of a compression stage is limited to 3.
   - (e) Stoichiometric requirement of demineralised water is assumed.
2. Hydrogen production:
   Figure 6.2 gives the relationship between operating capacities and the specific power consumption of the electrolyser. At design point, the specific consumption is 4.4 kWh/Nm^3 of hydrogen[5].

   As mentioned earlier, a linear dependency is used for this study and the corresponding equation is [5]:

$$x_{sp}^{ELY}(t) = \left[x_{design}^{ELY} - \left(1 - load^{ELY}(t)\right)\left(x_{design}^{ELY} - HHV_{H_2}\right)\right] \tag{6.1}$$

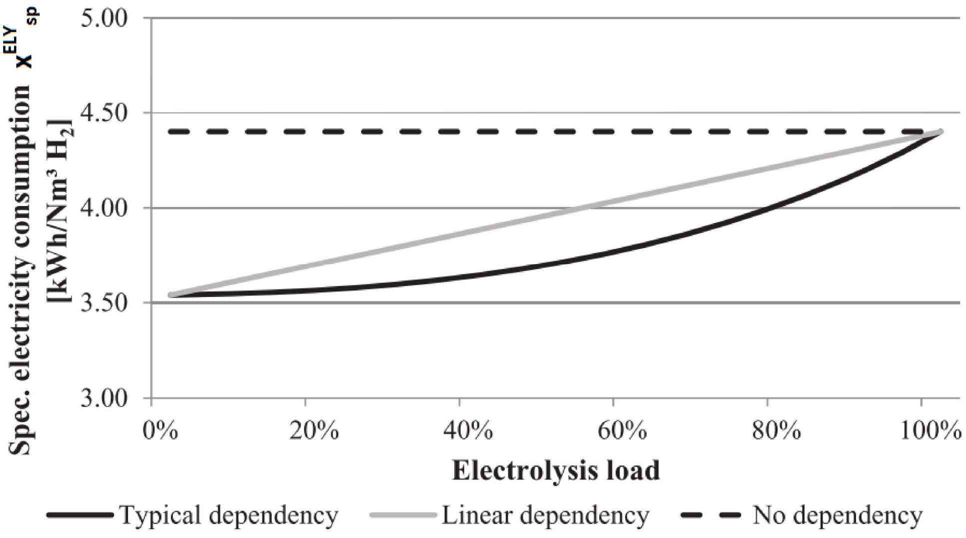

Figure 6.2: Relationship between electrolyser operating load and specific power consumption

Source: Beerbühl et al. (2015)[5]

where

$$load^{ELY}(t) = \frac{P^{ELY}(t)}{P^{ELY}_{ins}} \tag{6.2}$$

Once the specific consumption for a particular load is defined, the amount of hydrogen produced at any can be easily calculated using the relation

$$\dot{Q}_{H_2}(t) = \frac{P^{ELY}(t)}{x^{ELY}_{sp}(t)} \tag{6.3}$$

3. Heat generation:
The electrochemical reaction occurring within the electrolyser is endothermic in nature. However, due to irreversibility in the system, actual working electric potential is always higher than the reversible potential. This difference is released in the form of heat and must be removed to maintain operation of the system. The heat released is proportional to the difference between the actual cell potential and the thermoneutral voltage and is given as[41]

$$P_{h_c}(t) = I_{el}(t)\left[U_c(t) - U_{tn}\right] \tag{6.4}$$

The total heat released by the electrolyser is thus given as

$$P_h(t) = N_c I_{el}(t)\left[U_c(t) - U_{tn}\right] \tag{6.5}$$

The operating capacity of the electrolyser is calculated using the relation [41]

$$P^{ELY}(t) = I_{el}(t) N_c U_c(t) \tag{6.6}$$

Hydrogen production rate is also a function of applied electric current and is estimated using the relation [41]

$$\dot{Q}_{H_2}(t) = 80.69\,\eta_F\,\frac{N_c I_{el}(t)}{zF} \tag{6.7}$$

Combining equations 6.5, 6.6 and 6.7 a relation for heat generated by the electrolyser in known terms is obtained. The faradaic efficiency varies with current density input to the electrolyser but is close to 1[29]. Here a constant value of 0.95 has been assumed. Two electrons are transferred for every mole of hydrogen produced. Hence the value of z is 2. The heat generated by the electrolyser is given as

$$P_h(t) = P^{ELY}(t) - \frac{U_{tn}\dot{Q}_{H_2}(t)zF}{80.69\,\eta_F} \tag{6.8}$$

Cooling water requirement can be calculated using the following relation

$$m_{cw_{elec}}(t) = \frac{P_h(t)}{C_{p_{cw}}\Delta T_{cw}} \tag{6.9}$$

4. Compression of hydrogen:
   The electrolyser works under condition of ambient pressure. It is considered to be pressurised to 8 bar to match the standard outlet pressure of the nitrogen generation unit. Number of compression stages needed is estimated using the relation

$$r_p = \left(\frac{P_{final}}{P_{in}}\right)^{n_{stages}} \tag{6.10}$$

The number of stages needed is rounded up to the next whole number. The pressure ratio of the final stage is corrected to incorporate this change due to rounding up. The temperature at the outlet of a compression stage is calculated using the relation

$$T_{out} = T_{in}[r_{p_{stage}}]^{\left(\frac{\gamma_{H_2}-1}{\gamma_{H_2}}\right)} \tag{6.11}$$

The work done by a compression stage is given by the relation (adapted from [35])

$$W_{stage}(t) = T_{in}\left(\frac{\gamma_{H_2}}{\gamma_{H_2}-1}\right)R_{H_2}\dot{m}_{H_2}(t)\left[r_{p_{stage}}^{\left(\frac{\gamma_{H_2}-1}{\gamma_{H_2}}\right)} - 1\right] \tag{6.12}$$

Considering an isentropic efficiency of 75%, electric motor efficiency of 95% , the power consumption of stage is calculated as

$$P_{stage}(t) = \frac{W_{stage}(t)}{\eta_{is}\,\eta_{gen}} \tag{6.13}$$

To calculate the cooling water consumption in the intercoolers, the heat duty is estimated using the relation

$$Q_{elec_{comp}}(t) = \dot{m}_{H_2}(t)C_{p_{H_2}}(T_{out} - T_{in}) \tag{6.14}$$

$C_{p_{H_2}}$ has been estimated using Shomate's equation[35]:

$$Cp_{H_2 mol}{}^{1} = a_{H_2} + b_{H_2}T_{in} + c_{H_2}T_{in}^2 + d_{H_2}T_{in}^3 \tag{6.15}$$

$$Cp_{H_2} = \frac{Cp_{H_2 mol}}{MW_{H_2}} \tag{6.16}$$

---

[1] $a_{H_2} = 29.11; b_{H_2} = -0.1916 * 10^{-2}; c_{H_2} = 0.4003 * 10^{-5}; d_{H_2} = -0.8704 * 10^{-9};$

And cooling water consumption is calculated as

$$m_{cw_{eleccomp}}(t) = \frac{Q_{elec_{comp}}(t)}{C_{p_{cw}} \Delta T_{cw}} \tag{6.17}$$

The procedure is repeated for all stages to find the total power requirement and cooling water requirement of the compression system.

5. Demineralised water consumption:
The overall electrochemical reaction of water electrolysis is

$$2H_2O \rightarrow 2H_2 + O_2 \tag{6.18}$$

Considering complete conversion of water, under stoichiometric conditions it is clear that

$$n_{H2}(t) = n_{dw}(t) \tag{6.19}$$

$n_{dw}(t)$ is calculated by knowing $\dot{Q}_{H_2}(t)$ from equation 6.3. Mass of demineralised water required is then given as

$$m_{dw}(t) = n_{dw}(t) MW_{H_2O} \tag{6.20}$$

6.3.2. AIR SEPARATION UNIT

1. Assumptions and considerations:
   (a) Nitrogen is available at 8 bar and ambient temperature irrespective of separation technology type.
   (b) Nitrogen stream is 99.99% pure and argon is the only impurity.
   (c) Air inlet is at ambient condition.

2. ASU capacity:
The ASU capacity is determined by hydrogen production capacity of the electrolyser. For a stoichiometric production of ammonia, three moles of hydrogen are needed for every mole of nitrogen. Thus, knowing the maximum production rate of hydrogen from equation 6.3, the capacity of ASU is defined. Equations 6.21 through 6.23 are used to relate molar flow rate of hydrogen to volumetric flowrate of nitrogen.

$$n_{N_2}(t) = {}^1\!/_3\, n_{H_2}(t) \tag{6.21}$$

$$\dot{m}_{N_2}(t) = n_{N_2}(t) MW_{N_2} \tag{6.22}$$

$$\dot{Q}_{N_2}(t) = \frac{\dot{m}_{N_2}(t)}{\rho_{N_2}} \tag{6.23}$$

3. Selection of technology type:
The different technologies for air separation have been described in section 2.4 and the selection of appropriate technology as a function of nitrogen production capacity and purity is given by figure 2.17. For nitrogen production higher than 560 Nm^3/hr, cryogenic distillation is employed and for cases below this limit, PSA is selected [42].

4. Utility consumption:
   PSA type ASU:
   Power and cooling water is required for air compressors in a PSA type ASU. To estimate these requirements, the following relations, which are similar to equations 6.10 to 6.17 are used. Equations 6.10 and 6.11 are used to determine the number of stages and temperature at outlet of the compression stage. Equations 6.27 and 6.29 are used to calculate the power and cooling requirement.

$$W_{stage}(t) = T_{in}\left(\frac{\gamma_{air}}{\gamma_{air}-1}\right)R_{air}\dot{m}_{air}(t)\left[r_{p_{stage}}^{\left(\frac{\gamma_{air}-1}{\gamma_{air}}\right)} - 1\right] \tag{6.24}$$

   Where mass of air required is calculated using the relations [20]

$$\dot{Q}_{air}(t) = 6.85\dot{Q}_{N_2}(t) \tag{6.25}$$

$$\dot{m}_{air}(t) = \dot{Q}_{air}(t)\rho_{air} \tag{6.26}$$

   Assuming an isentropic efficiency of 75%, electric motor efficiency of 95% and a safety factor of 1.25[20], the power consumption of stage is calculated as

$$P_{stage}(t) = \frac{1.25\,W_{stage}(t)}{\eta_{is}\,\eta_{gen}} \tag{6.27}$$

   To calculate the cooling water consumption in the intercoolers, the heat duty is estimated using the relation

$$Q_{asu_{comp}}(t) = \dot{m}_{air}(t)C_{p_{air}}(T_{out} - T_{in}) \tag{6.28}$$

   And cooling water consumption is calculated as

$$m_{cw_{asu_{comp}}}(t) = \frac{Q_{asu_{comp}}(t)}{C_{p_{cw}}\Delta T_{cw}} \tag{6.29}$$

   Cryogenic type ASU:
   Cryogenic distillation is a more complex separation process compared to PSA. Data for utility consumption is obtained from supplier data made available by Proton Ventures (datasheet undisclosed). The specific power consumption for cryogenic systems is 0.28 kWh/Nm^3 of nitrogen. The cooling water consumption is 0.024 Nm^3 for every Nm^3 of nitrogen produced.

6.3.3. AMMONIA SYNTHESIS LOOP

The ammonia synthesis loop consists of the feed compressor, ammonia synthesis reactor, condensor, recycle compressor and ammonia separators. This loop operates at high pressures and hence utility consumption calculation using ideal gas relations would not give a good estimate. ASPEN®HYSYS model available at Proton Ventures has been modified to mimic the process conditions considered in this study. It uses Soave-Redlich-Kwong (SRK) equation of state to calculate thermodynamic properties.

1. Assumptions and considerations:

   (a) Utility consumption varies linearly with operating capacities.

   (b) Efficiency of ammonia synthesis loop is constant for all operating capacities.

2. Utility consumption: The following data has been obtained from the ASPEN®HYSYS model and used in this study:

Table 6.1: Specific utility consumption of ammonia synthesis loop

Component	**Power consumption (kWh/Nm^3 H$_2$)**	**Cooling water consumption (kg/Nm^3 H$_2$)**
Feed compressor	0.263	23.616
Recycle compressor	0.0043	-
Condenser	-	42.87

3. Ammonia production and losses: Losses in the ammonia system loop has been quantified using results from the ASPEN®HYSYS model. 1.88% of feed hydrogen is lost in the form of:

   - Purge (1.75%)
   - Dissolved in product stream (0.13%)

   Ammonia production is based on stoichiometry. 0.4% of ammonia produced in lost in purge which may be recovered using a scrubber system. The following relations are used to determine mass flow of ammonia from molar flow of hydrogen. They incorporate the effect of above mentioned losses.

$$n_{NH_3} = 0.9812(0.996)\left(1.5\, n_{H_2}\right) \tag{6.30}$$

$$\dot{m}_{NH_3} = n_{NH_3} MW_{NH_3} \tag{6.31}$$

6.3.4. AMMONIA STORAGE

1. Assumption

   (a) Short term storage is considered in this study. Storage capacity is assumed to be equal to 5 days of ammonia production at rated plant capacity.

2. Selection of storage type: The maximum scale of ammonia production considered in this study is about 50000 TPY. Compared to typical industrial ammonia plants, which have capacities greater than 100000 TPY, the capacities considered in this study are small scale. Comparing the three types of ammonia storage methods (Table 2.8), skid mounted cylindrical pressure vessels (bullet type storage) is most suitable for this study.

3. Sizing and specification: The maximum capacity of a bullet type ammonia storage is 340 m^3. This information is obtained from supplier data available at Proton Ventures. Figure 6.3 depicts the algorithm used to calculate the size and number of bullets needed for the system. Storage capacity is defined as the maximum ammonia production accumulated over 5 days. A factor of 10% is added for safety. Multiple bullets of equal capacity are considered in case the storage capacity is larger than the limit of a bullet.

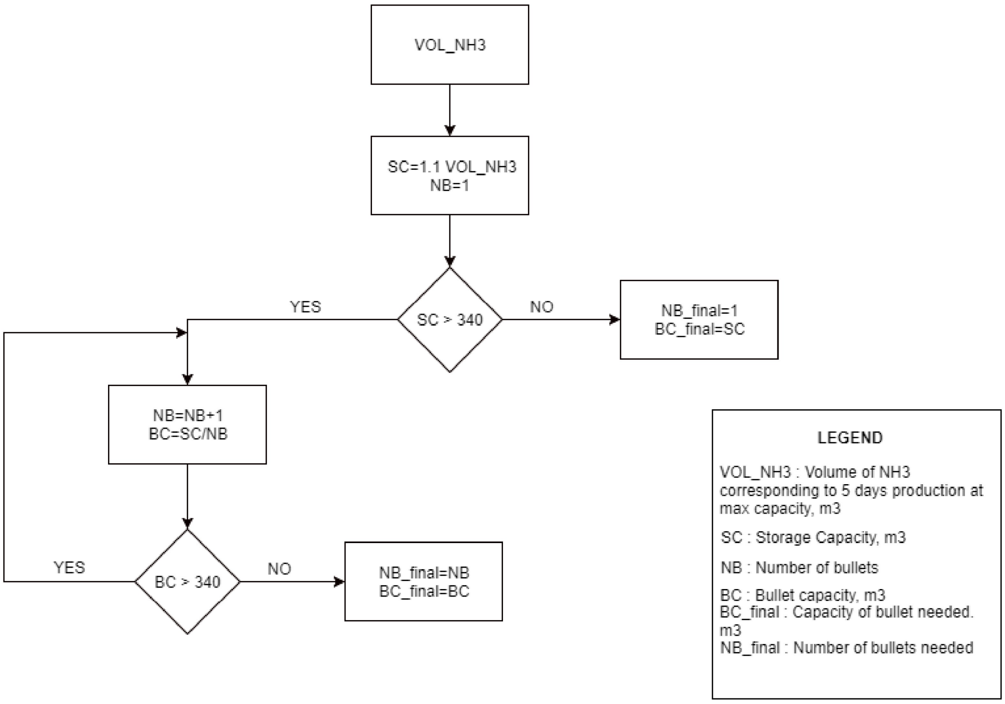

Figure 6.3: Algorithm to calculate size and quantity of bullet type ammonia storage

6.4. ECONOMIC MODELLING

1. Assumptions and considerations:
   - (a) It is assumed that the annual availability of the plant is 92%[27].
   - (b) Linear scale up of electrolyser CAPEX with capacity is considered since it employs modular units.
   - (c) The reference CAPEX of electrolyser includes the purification,transformer and rectifer costs. The cost of hydrogen compression unit is calculated separately and included in the actual CAPEX of electrolyser.
   - (d) Catalyst regeneration cost has been neglected from operating cost of ammonia synthesis section.
   - (e) Maintenance cost of electrolyser exclude stack replacement costs.
   - (f) Tata Steel currently earns revenue by exporting electricity to the grid during surplus production. This is considered to be the price of available electric power in this study.
   - (g) Life of loan period is assumed to be 15 years[35].
   - (h) Plant life is assumed to be 20 years[35].
   - (i) Annual downpayment is assumed to be 10% of total CAPEX[35].
   - (j) Interest rate on loan is assumed to be 4%[35].
   - (k) Discount rate is assumed to be 7%[35].
   - (l) Inflation rate is assumed to be 3%[35].
   - (m) Unit price of cooling water is €0.09/Nm^3
   - (n) Unit price of demineralised water is €0.44/Nm^3

2. CAPEX Estimation:

   CAPEX of each component of the system is estimated using available reference data for CAPEX and installed capacity. Suitable scaling exponents are used to estimate CAPEX for actual installed capacities. The scaling exponents are selected based on good engineering judgement for process plants[55]. Data from table 6.2 and equation 6.32 are used to estimate CAPEX of the system.

Table 6.2: Reference data for CAPEX estimation

Component	**Reference capacity** (Cap_{ref})	**Unit**	**Reference CAPEX** (Inv_{ref})	**Unit**	**Source**	**Scaling exponent** ($\mathbf{n_s}$)
Electrolyser	1.2	MW	1.7	Million €	[43]	1
Feed compression unit/ Hydrogen compression unit	65	kW	0.4	Million €	[43], For hydrogen compression unit verbal communication with Proton Ventures	0.85
Ammonia synthesis loop (excluding feed compressor)	120	kg/hr NH_3	2.2	Million €	[43]	0.67
PSA type ASU	120	Nm^3/hr N_2	0.3	Million €	[43]	0.67
Cryogenic distillation type ASU	1900	Nm^3/hr N_2	1.52	Million €	Supplier data made available by Proton Ventures (Datasheet undisclosed)	0.67
Bullet type ammonia storage	115	m^3 NH_3	47.5	1,000 €	Supplier data made available by Proton Ventures (Datasheet undisclosed)	0.67

$$Inv_{act} = Inv_{ref}\left(\frac{Cap_{act}}{Cap_{ref}}\right)^{n_s} .N_{bullets}{}^{1} \tag{6.32}$$

3. OPEX estimation:

   Figure depicts categorisation of operating costs. The operating costs of the plant are categorised as fixed and variable costs. The variable cost includes the raw material costs and the fixed cost include tax and insurance, general expense, maintenance and direct labour. In this study, it is assumed that one personnel is needed to keep the plant operational irrespective of plant capacity and hence is considered under fixed costs. Maintenance cost is a function of plant capacity, but is assumed constant for a fixed capacity and hence included under fixed costs.

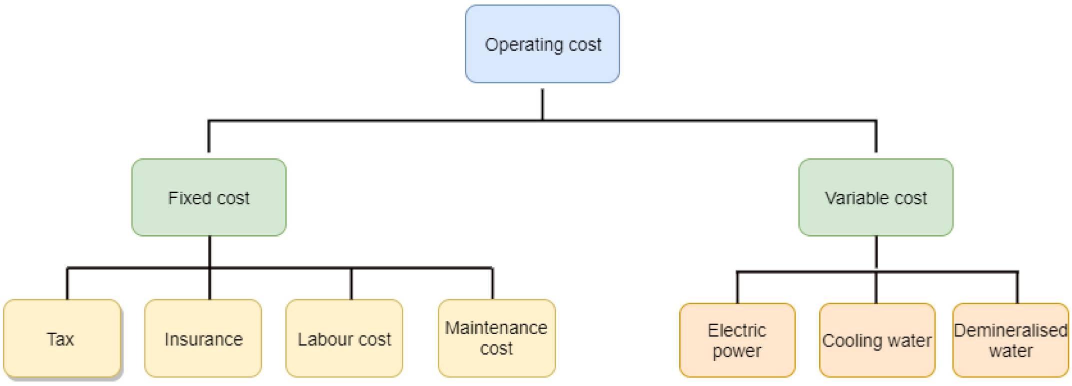

Figure 6.4: Categorisation of operating costs

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[1] $N_{bullets}$ is applicable only when estimating CAPEX of ammonia storage

(a) Variable cost:
This can be further categorised into electricity cost, cooling water cost and demineralised water cost. Appendix A describes the method that has been used to estimate total electric power consumed and the costs associated with it. Cooling water requirements are calculated using equations 6.9, 6.17, 6.29, specific cooling water requirement for cryogenic type ASU and using data from table 6.1. Demineralised water requirement is calculated using equation 6.20.

(b) Fixed cost:
Fixed cost for ELY and AS are separately calculated. The maintenance cost of ELY can be estimated as a fraction of its CAPEX. This includes the material cost for scheduled and unscheduled maintenance along with labour. With available data[8], a curve was fit to estimate maintenance costs for any given installed capacity of electrolyser. This is depicted in figure 6.5 and the equation of the fitted curve is $Y = 3.4238X^{-0.152}$.[2] Due to very dynamic operation of AS, it is considered as a complex operation. Maintenance cost for complex operations is taken as 7% of total CAPEX of AS[9]. Ammonia storage is excluded in this estimation. An additional 2% is considered as fixed cost for ammonia storage and is incorporated into the fixed cost of AS. For labour cost estimates, three shifts per day is considered with each shift having one personnel. Average salary of €40,000 per annum has been considered. Table 6.3 summarises the estimation of fixed cost for ELY and AS.

Table 6.3: Estimation of fixed cost

Parameter	ELY	AS	Units	Source
Tax (T)	1	1	% of CAPEX/year	[9]
Insurance (I)	1	1	% of CAPEX/year	[9]
Labour (L)	120000		€/year	
[3] Maintenance (M)	$3.42X^{-0.152}$	7	% of CAPEX/year	[8] [9]
General expense (G)	3	3	% of CAPEX/year	[9]
Fixed cost	1.25L+T+I+M+G		€/year	[9]

Total operating cost is the sum of fixed cost and variable cost.

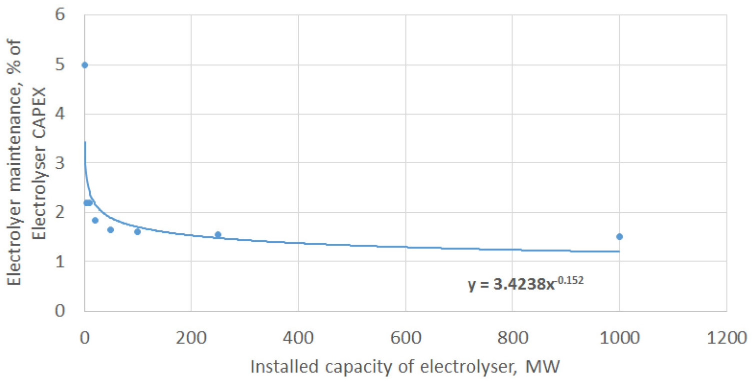

Figure 6.5: Operating cost of electrolyser as a function of its CAPEX

Source: Data from Bertuccioli et al.(2014)[8]

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[2] Y is the maintenance cost (as a fraction of CAPEX) and X is the installed capacity of electrolyser.

4. Levelised cost of ammonia:
   Levelised cost of ammonia(LCOA) is defined as the production cost of ammonia over the life of the plant normalised to a ton of ammonia[35]. A brief description of the terms in estimation of LCOA is given in appendix G. The following relation(adapted from [35]) is used to estimate LCOA :

$$LCOA = \frac{P_d + P_a\left(\frac{(\frac{1}{1+r})-(\frac{1}{1+r})^{n_{loan}+1}}{1-(\frac{1}{1+r})}\right) + OC_T\left(\frac{(\frac{1+i}{1+r})-(\frac{1+i}{1+r})^{n_{life}+1}}{1-(\frac{1+i}{1+r})}\right)}{m_{T_{NH3}}} \tag{6.33}$$

   Where

$$P_a = (C_T - P_d)\left(\frac{b}{1-(1+b)^{-n_{loan}}}\right) \tag{6.34}$$

7

RESULTS OF TECHNO ECONOMIC ASSESSMENT AND DISCUSSION

This chapter describes the validation of the developed model and discusses the key results obtained from the simulations. Section 7.2 shows the result obtained by analysis of the base case scenario. Section 7.3 describes the results from analysing scenario where hydrogen from WAG is used to minimise import of electric power. Section 7.4 discusses key findings from analysis of scenario that involves hydrogen storage in the form of ammonia. Section 7.5 provides a comparison of the results from the three scenarios.

7.1. VALIDATION OF RESULT

Literature values are used to validate the result obtained from the simulation. Literature values have been reported for ammonia plants operating continuously at their installed capacities. Table 7.1 compares the result from the techno-economic model in this analysis with reported values in literature. To make a fair comparison, results obtained from the sub-scenario (complete utilisation of equipment capacity) have been used here.

Table 7.1: Comparison of result with literature

LCOA (€/ton)	Ammonia production capacity (TPD)	Source
739	49	This study
590[1]	48	Bañares-alcántara et al.(2014)[3]
550-1000[2]	60	ISPT (2017)[27]
1028[2]	60	This study

It is seen that the LCOA obtained in this study and that by Bañares-alcántara et al.(2014) differ by less than 25% for a similar ammonia production capacity. It has been further stated that LCOA for a power to ammonia process is estimated to be 1.5-3 times higher than conventional process. On the basis of average market ammonia price for the years 2000-2013, the LCOA via electrolysis is estimated between €464/ton-€930/ton[1]. The LCOA calculated by the techno-economic model in this study varies from €693/ton - €1050/ton for ammonia production capacity of 50,000 tonnes/year to 1040 tonnes/year respectively. The values of LCOA lie within 15% of the mentioned range.

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[1] Converted from USD to Euros assuming conversion factor of 0.9

[2] Production cost and not levelised cost.

The study conducted by ISPT (2017) calculates the production cost of ammonia for several cases with several electricity prices. The production cost of ammonia calculated by the techno-economic model in this study is close to the maximum cost estimated by ISPT.
From these comparisons it is concluded that the values of LCOA calculated by the developed techno-economic model is in general agreement with the results reported for previous studies.

7.2. SCENARIO 1: BASE CASE

Figure 7.1 shows the annual utilisation of electrolyser capacity as a function of the installed electrolyser capacity. Utilisation is the ratio of actual electric power consumed by the electrolyser in a year to the electric power that the electrolyser would consume annually if run continuously at its installed capacity. The total electric power consumption of the system is a combination of available surplus and imported electric power. The utilisation decreases from over 60% to just over 25% as the installed electrolyser capacity increases from 1.2MW to 200MW. Figure 7.2 shows the fraction of available electric power consumed by the system as a function of installed electrolyser capacity. This fraction decreases from about 80% to approximately 25% with increasing installed electrolyser capacity.

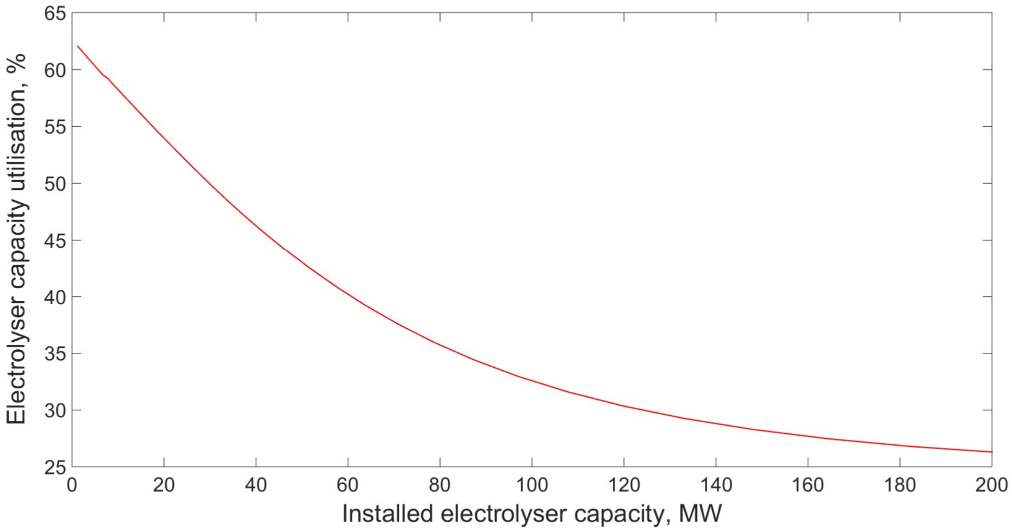


Figure 7.1: Scenario 1: Electrolyser capacity utilisation as a function of installed electrolyser capacity

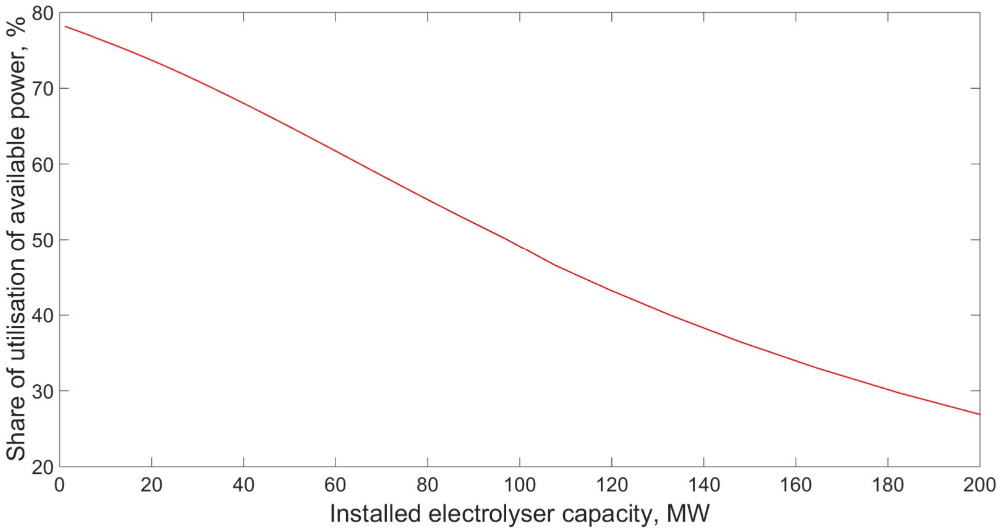


Figure 7.2: Scenario 1: Share of available electric power in total electric power consumption as a function of installed electrolyser capacity

The following parameters are distinguished as contributors to the production cost of ammonia:

1. CAPEX of ELY
2. Fixed cost of ELY
3. CAPEX of AS
4. Fixed cost of AS
5. Variable cost of the system - Utility consumption (Electricity, cooling water and demineralised water consumption)

Figure 7.3 shows the value of the aforementioned parameters as a function of the installed capacity of the electrolyser, which represents the production capacity of the plant normalised to a ton of ammonia produced. A general observation is that the cost associated with electric power consumption (OPEX electricity) is steady and dominating at nearly all plant capacities. With increase in plant capacity, costs associated with electrolyser have more influence on the production cost than AS. The trend of each contributing factor is discussed below:

1. OPEX electricity: The cost associated with electric power consumption is fairly constant and this is to be expected since electric power consumption is proportional to ammonia production. The small jump corresponding to 7.4 MW installed electrolyser capacity is because of a switch in the ASU technology from PSA to cryogenic. The specific power consumption of cryogenic system is lower than a PSA system.
2. OPEX water: Similar to OPEX electricity, water consumption is proportional to ammonia production. The relative contribution of this cost factor is small and fairly constant at all plant capacities.
3. CAPEX ELY: There is a constant rise in this factor with increasing capacity. The rise is proportional to the decrease in electrolyser utilisation.
4. CAPEX AS: The decreasing trend observed here is due to economy of scale applicable for AS. This advantage is partly compensated by decreasing equipment utilisation at higher capacities.

5. Fixed cost AS: This parameter is proportional to CAPEX of AS. It dominates at low capacities because of labour cost.

6. Fixed cost ELY: This parameter is proportional to CAPEX ELY.

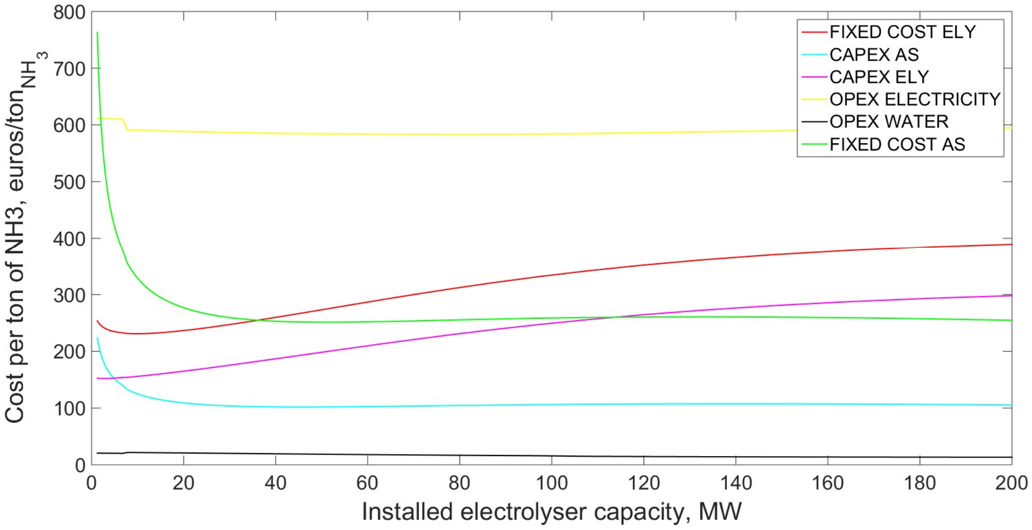


Figure 7.3: Scenario 1: Variation of main contributing parameters to production cost of ammonia with installed electrolyser capacity

Figure 7.4 shows the LCOA as a function of installed capacity of electrolyser. An optimum plant capacity exists at which production cost is minimum. The installed electrolyser capacity is 24.65 MW and the corresponding LCOA is €997/ton..

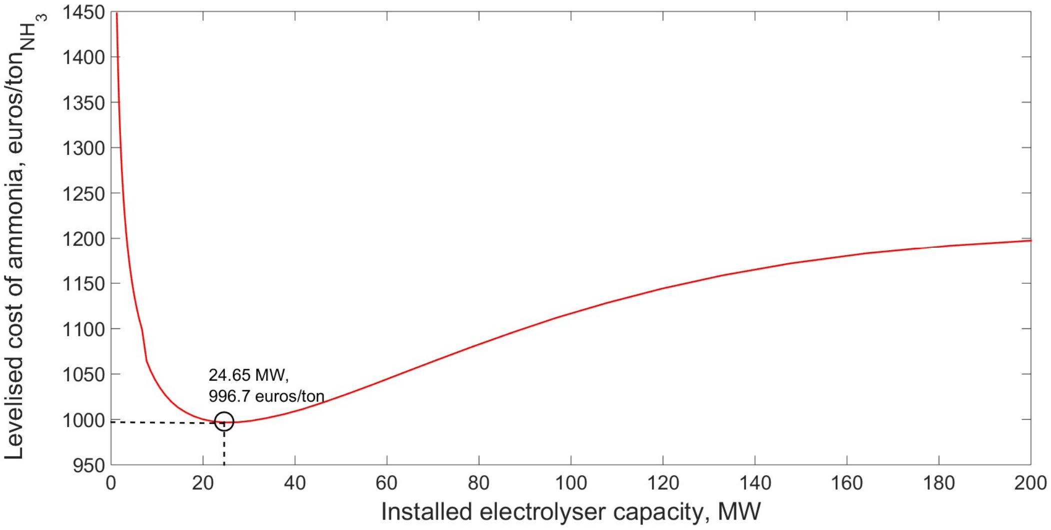


Figure 7.4: Scenario 1: Variation in levelised cost of ammonia with installed electrolyser capacity

The contributions of the individual key parameters at optimum plant capacity is depicted in figure 7.5. The two largest contributors are electric power consumption and fixed cost of AS which together represent 61% of the total costs. Costs associated with electrolyser are responsible for 29% of the production cost.

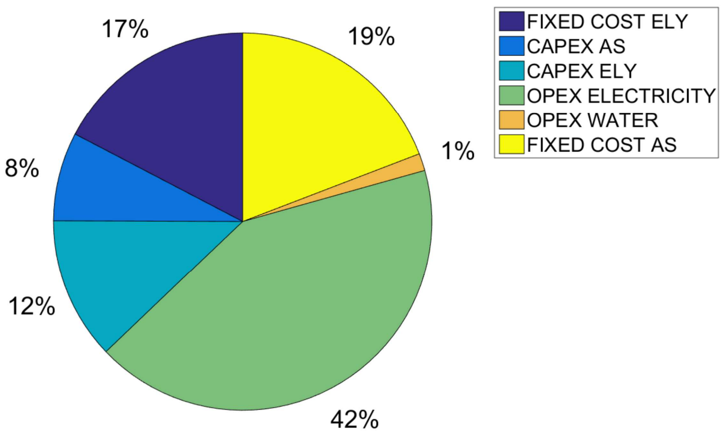


Figure 7.5: Scenario 1: Contribution of key parameters to LCOA at optimum plant capacity

The efficiency of the power to ammonia process is based on the LHV of ammonia (18.6 MJ/kg) and is defined as the ratio of total energy stored in the form of ammonia to total energy consumed in the production process. Figure 7.6 shows the variation in efficiency as a function of the installed electrolyser capacity. It is observed that efficiency increases with electrolyser capacity and varies from 47.5% to 55.2%. This increase is expected because the efficiency of the entire process is determined by the efficiency of the electrolyser and of the AS. Efficiency of electrolyser increases with decrease in its utilisation and efficiency of AS has been assumed to be constant. The overall effect is thus an increase in efficiency.

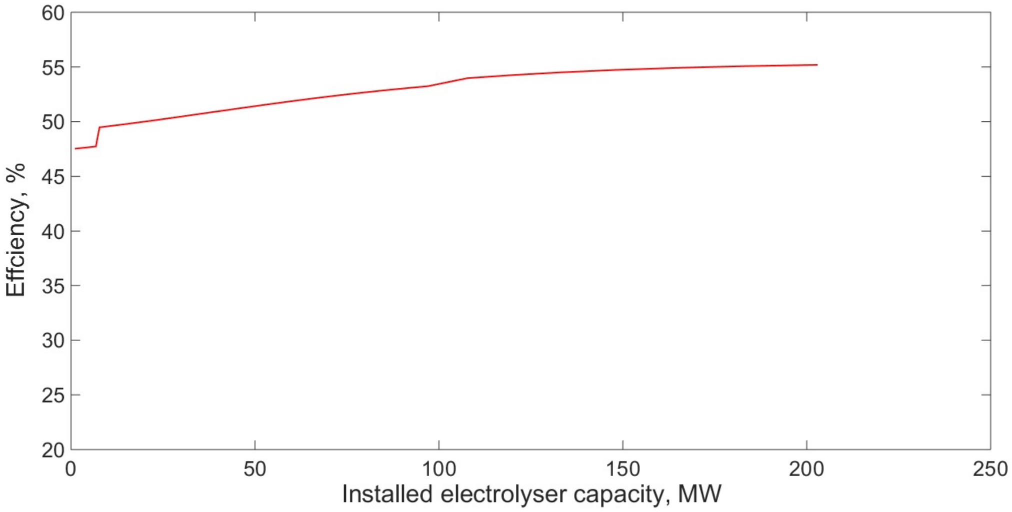


Figure 7.6: Scenario 1: Variation of power to ammonia efficiency with installed electrolyser capacity

Figure 7.7 shows the variation in the energy storage cost as a function of the installed electrolyser capacity. The energy content of ammonia is based on its LHV and is a constant. The trend of the plot is dictated by the trend of LCOA. Energy storage cost varies from €193/MWh to €281/MWh.

The main results of the analysis of scenario 1 are summarised in table 7.2

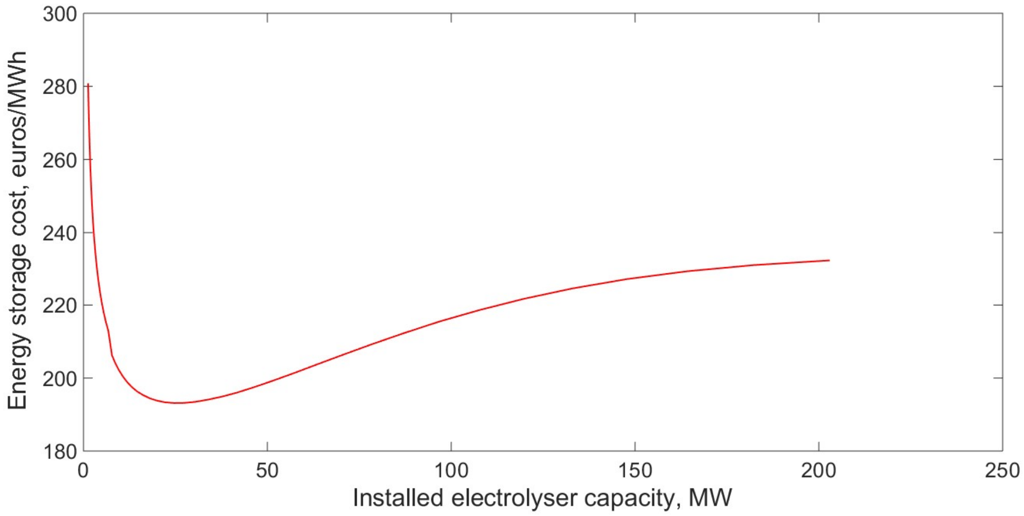


Figure 7.7: Scenario 1: Variation of energy storage cost with installed electrolyser capacity

Table 7.2: Scenario 1: Key parameters of system at optimum capacity

Parameter	**Value**	**Unit**
Ammonia production	11249	ton/year
Installed electrolyser capacity	25	MW
Type of ASU	Cryogenic distillation	-
Number of storage bullets	2	-
Capacity of unit storage bullet	274	m^3
Electric power consumed	126	GWh/year
Utilisation of available electric power	72	%
Electrolyser utilisation	52	%
Power to ammonia efficiency	50	%
Cost of energy storage	193	€/MWh
Total plant CAPEX	62	Million €
LCOA	997	€/ton

7.2.1. SENSITIVITY ANALYSIS

The following two parameters have been selected to be subjected to a sensitivity analysis:

1. CAPEX of electrolyser: The cost of the electrolyser has a significant influence on the LCOA. It is expected that electrolyser price will reduce in the future. This makes it an interesting parameter to be investigated. Sensitivity factors from 0 to 1 has been applied and its effect on the LCOA and position of optimum installed electrolyser capacity have been investigated. The average market price of ammonia in 2013 was €500/ton. The system is assumed to be economically feasible if calculated LCOA is lower than this value. The result of the analysis is depicted in figure 7.8. The dotted line represents the feasibility threshold. It is observed that reduction in electrolyser CAPEX reduces the LCOA from €997/ton to a minimum of €700/ton. The position of the optimum installed electrolyser capacity changes from 24.65 MW to 51.54 MW. Larger installed capacities are more economically attractive with drop in electrolyser cost. However, it is observed that for the current scenario, the system is not economically feasible irrespective of electrolyser CAPEX mainly caused by the limited utilisation of the electrolyser.

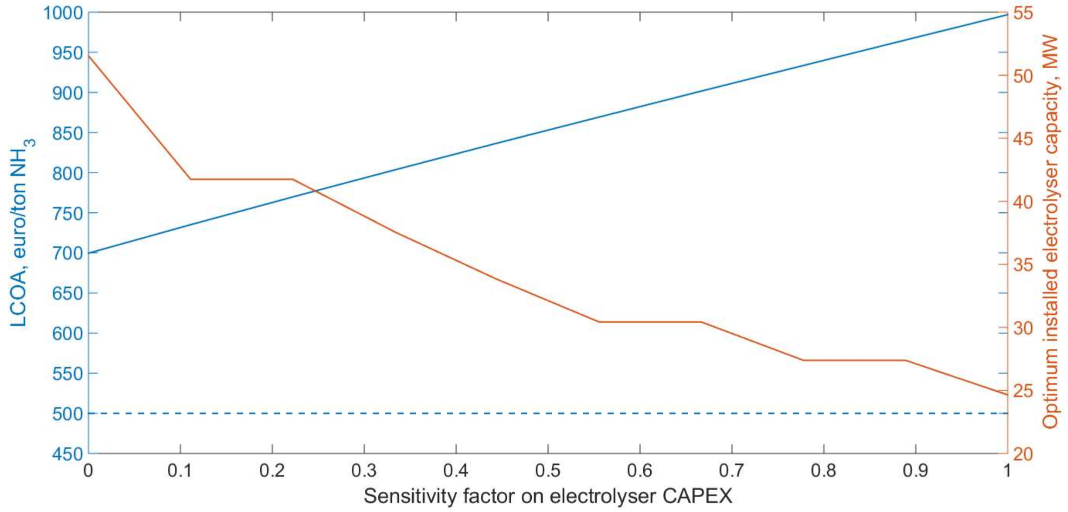


Figure 7.8: Scenario 1: Sensitivity analysis of LCOA with varying electrolyser CAPEX

2. Electricity price: Cost associated with electric power consumption has been identified as the most dominating factor to influence production cost. The same range of the sensitivity factor has been used here as for the case of electrolyser CAPEX. The result is depicted in figure 7.9. LCOA has a wide range from €997/ton to €594/ton. It is observed that the optimum plant capacity remains unchanged. Similar to the case with electrolyser CAPEX, it is observed that the plant cannot be economically feasible even if electricity is available for free mainly caused by low equipment capacity utilisation.

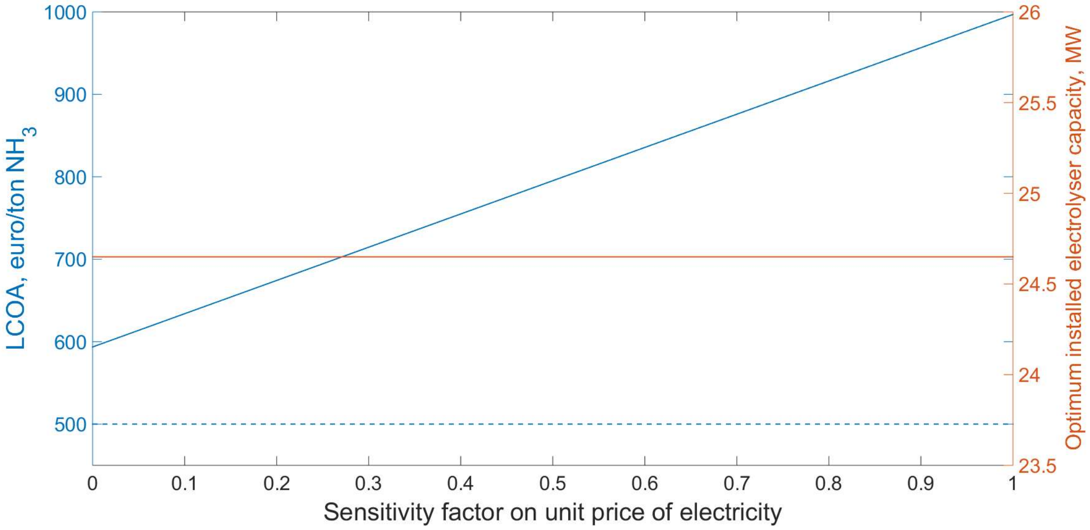


Figure 7.9: Scenario 1: Sensitivity analysis of LCOA with varying electricity price

Figure 7.10 is a snapshot of the ammonia production pattern for the system at optimum capacity for a time interval of 25 hours. The maximum and minimum power consumption of the system are indicated in the figure by black horizontal lines. It is observed that when available power exceeds the minimum part load, the ammonia production pattern is proportional to the pattern of available power. When available power is below the minimum part load, the system operates at the minimum part load by import of additional electric power and hence ammonia production is seen as a flat line during these periods. When available power is more than the installed capacity of the system, maximum ammonia production is achieved and again a flat line trend is observed.

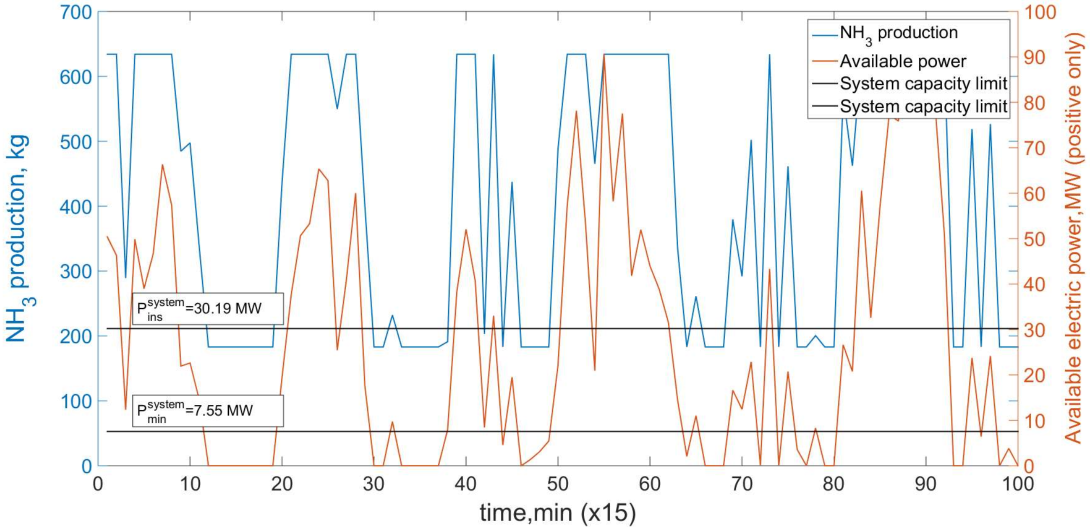


Figure 7.10: Scenario 1: Ammonia production profile at optimum capacity

7.2.2. SUB-SCENARIO 1: COMPLETE UTILISATION OF EQUIPMENTS

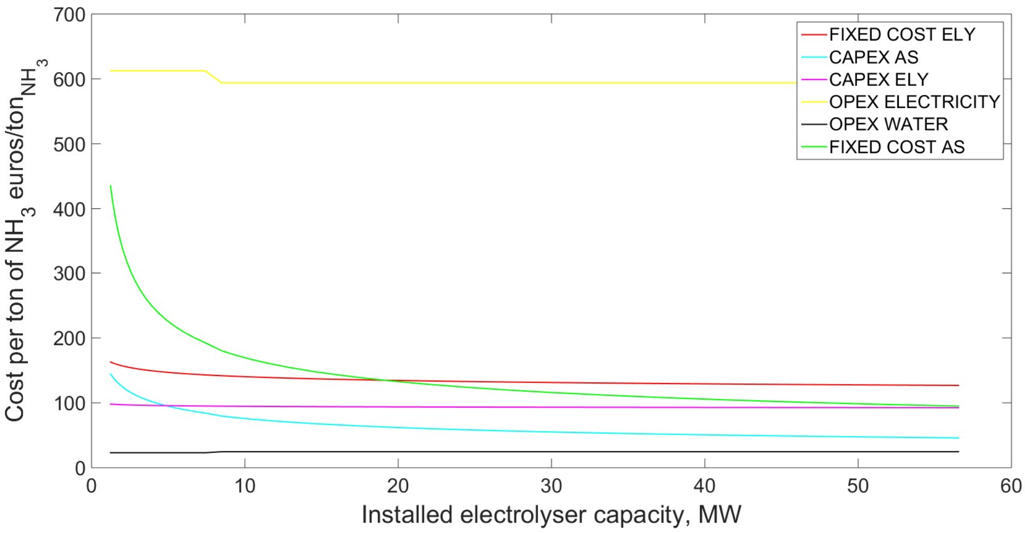


Figure 7.11: Sub-scenario 1: Variation of main contributing parameters to production cost of ammonia with installed electrolyser capacity

It is clear that low utilisation is a major reason for the system not being economically feasible in the base scenario. The effect of complete utilisation of equipments is addressed in this section. It is assumed that abundant electric power is available. The price pattern of available electric power is kept unchanged and the plant capacity is limited to 50000 ton/year of ammonia. Since the AS is operated at a constant capacity, maintenance cost of AS has been modified from 7% to 5% of

AS CAPEX. Figure 7.11 shows the variation of key parameters influencing the production cost of ammonia with the installed electrolyser capacity for this case sub-scenario 1. Full utilisation of the equipment results into a fairly flat line for CAPEX ELY and a smooth decreasing trend for CAPEX AS. Fixed costs, as expected follow the trend of CAPEX.

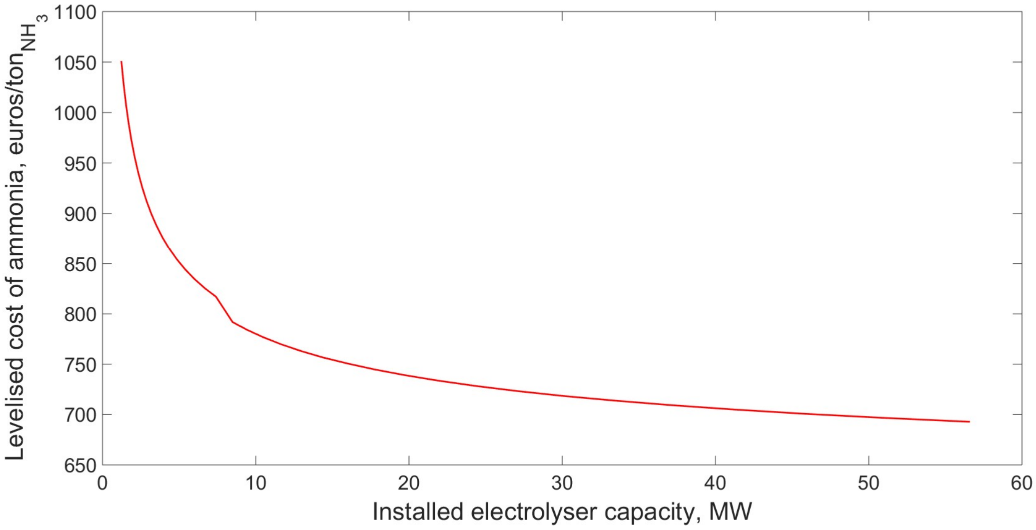


Figure 7.12: Sub-scenario 1: Variation of LCOA with installed electrolyser capacity

Figure 7.12 shows the variation on LCOA with the installed electrolyser capacity. As opposed to the base case, a continuous decrease in LCOA is observed with increasing plant capacity. Economies of scale is the main cause for this behaviour. Invariable specific costs related to electrolyser and a decreasing trend for specific costs related to AS together account for a constantly decreasing LCOA from €1050/ton to €693/ton. Figure 7.13 depicts a tornado chart that expresses the sensitivity of the system to the key parameters with a sensitivity of ±80%. It is seen that a reduction in unit electricity price by 80% leads to LCOA less than €370/ton.

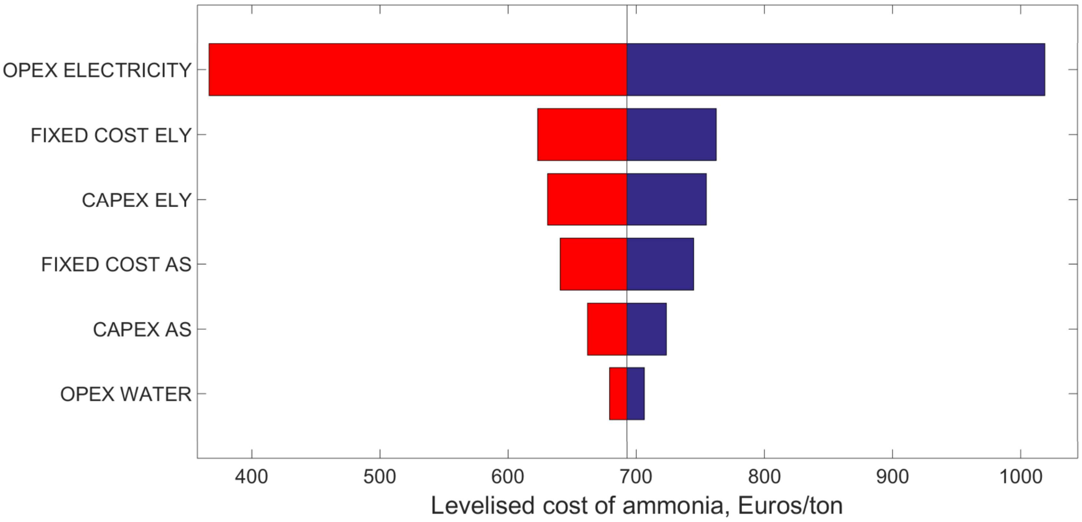


Figure 7.13: Sub-scenario 1: Tornado chart with ±80% sensitivity for scenario with equipments at full utilisation

7.3. SCENARIO 2: INCLUSION OF HYDROGEN FROM WORK ARISING GASES

Scenario 2 involves a constant supply of pure hydrogen to the AS. The amount of hydrogen supply is equal to the minimum part load of AS. This eliminates the need to import electric power from the grid to operate the electrolyser when insufficient electric power is available. COG from the WAG has been chosen as the source of hydrogen. The cleaning and separation of hydrogen and estimation of the price has been described in Appendix B. For this scenario, it has been assumed that the hydrogen generation plant is already present at Tata Steel IJmuiden and only part of the hydrogen generated is utilised. As a result, the CAPEX and OPEX of the hydrogen generation plant have been neglected and estimated hydrogen prices are conservative. The available electric power and price pattern have been kept unchanged and the system has been analysed by the same method as for scenario 1.

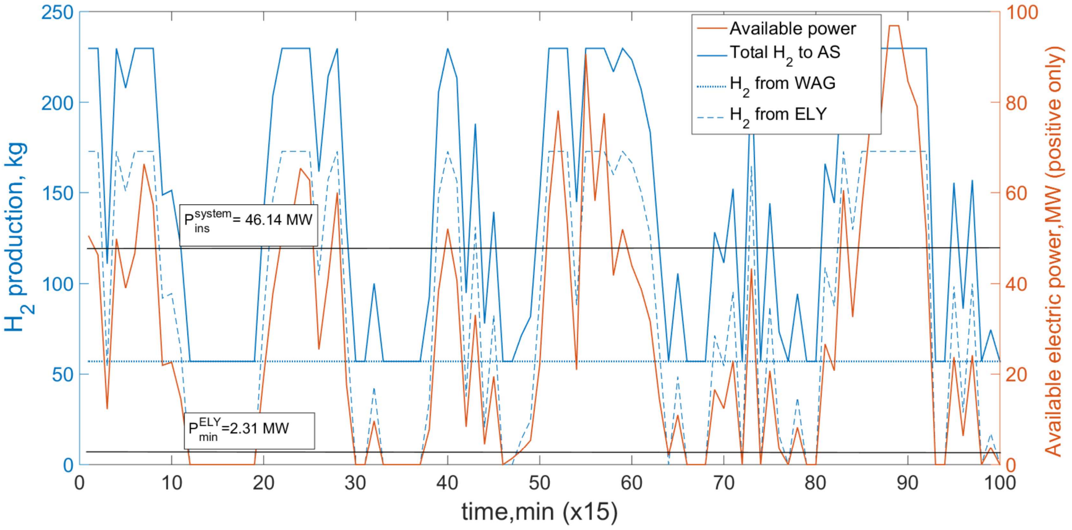


Figure 7.14: Scenario 2: Hydrogen availability to AS for optimum electrolyser capacity

Figure 7.14 shows a snapshot of hydrogen flow pattern available to the AS at the optimum electrolyser capacity. A continuous hydrogen flow is available from the WAG and corresponds to the minimum part load of the AS. This ensures that the system runs at the minimum part load when insufficient hydrogen is produced by the electrolyser. When available power exceeds the power consumption at the installed capacity of the system, hydrogen production is curtailed at maximum production seen as a flat line in hydrogen production pattern. When available power is less than minimum part load of the electrolyser, it does not consume any electric power and the hydrogen production by the electrolyser is zero. At any given point in time, the total hydrogen available to the AS is the sum of hydrogen from WAG and hydrogen produced by the electrolyser.

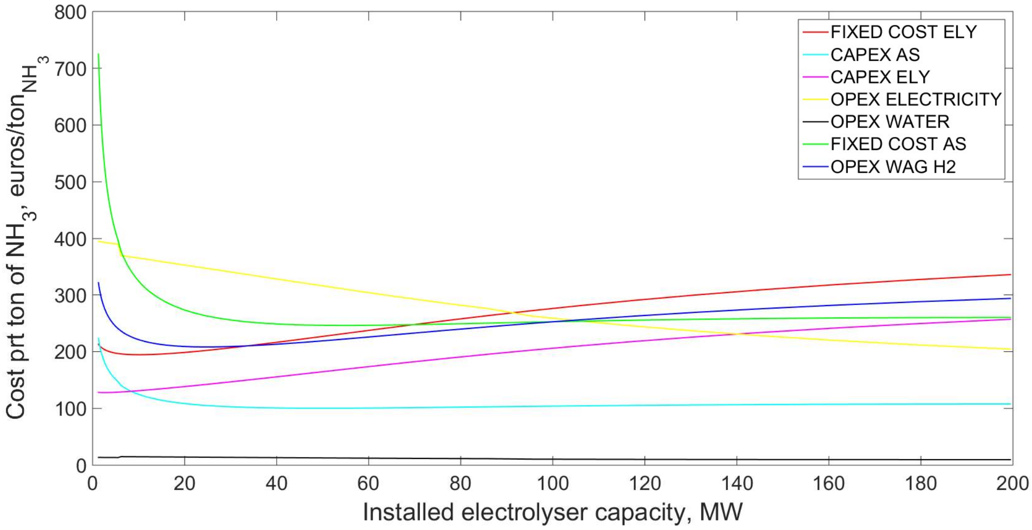


Figure 7.15: Scenario 2: Variation of main contributing parameters to production cost of ammonia with installed electrolyser capacity

Figure 7.15 shows the value of the selected key parameters as a function of the installed capacity of the electrolyser. The cost associated with electric power consumption has a decreasing trend. This is expected because import of additional electric power for the electrolyser is eliminated in this scenario. Figure 7.16 shows the utilisation of electrolyser for this scenario. Compared to scenario 1,the trend is similar, but utilisation is lower. Cost associated with the electrolyser and with hydrogen consumption from WAG show an increasing trend. This is due to lower utilisation of equipment at higher plant capacities. Costs associated with the AS show a similar trend as in scenario 1. Figure 7.17 shows the utilisation of the available electric power as a function of the installed electrolyser capacity. Compared to scenario 1, utilisation of available power is significantly higher. The only need to import electric power is to operate the AS.

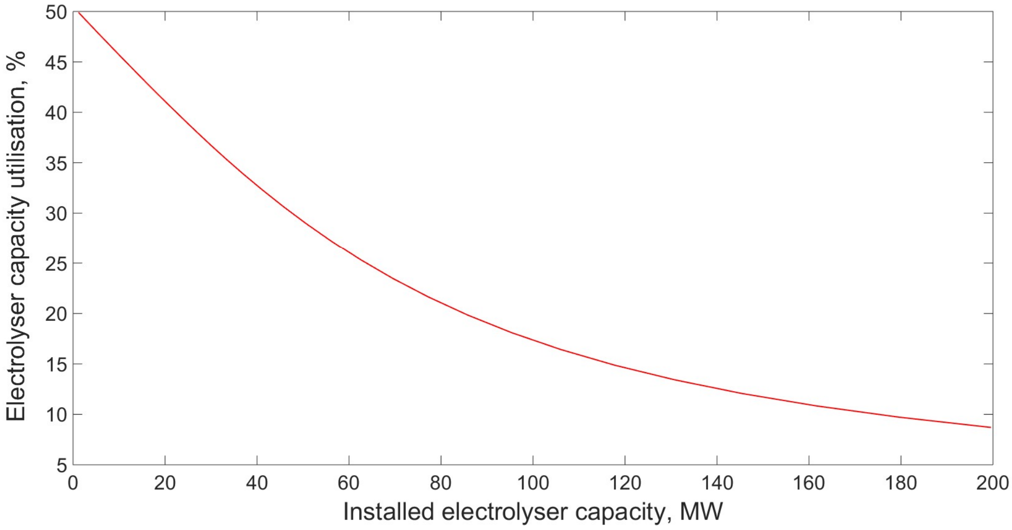


Figure 7.16: Scenario 2: Electrolyser capacity utilisation as a function on installed capacity

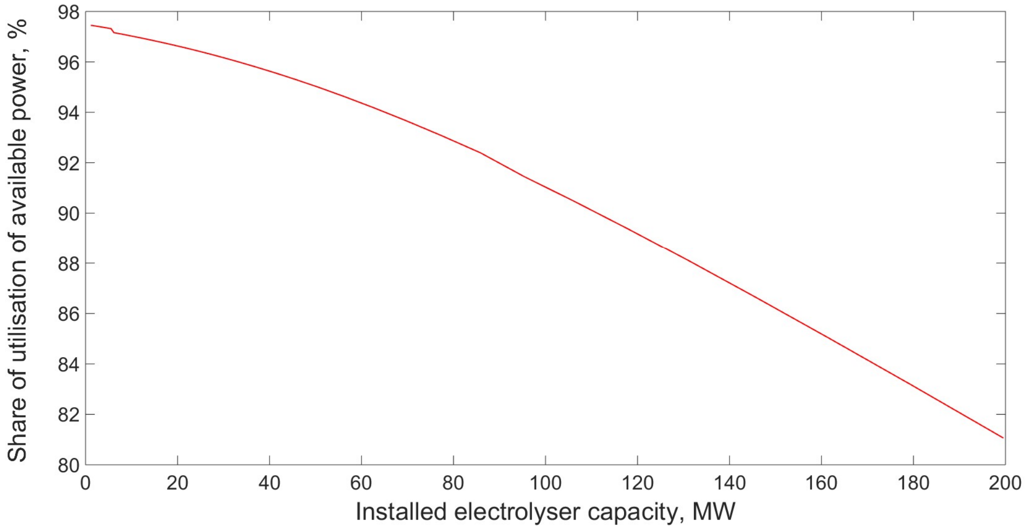


Figure 7.17: Scenario 2: Share of available electric power in total electric power consumption as a function of installed electrolyser capacity

Figure 7.18 shows the variation in LCOA with the installed electrolyser capacity. LCOA shows a range of €913/ton to €1440/ton with an optimum installed electrolyser capacity of 33.26 MW (~33 MW).

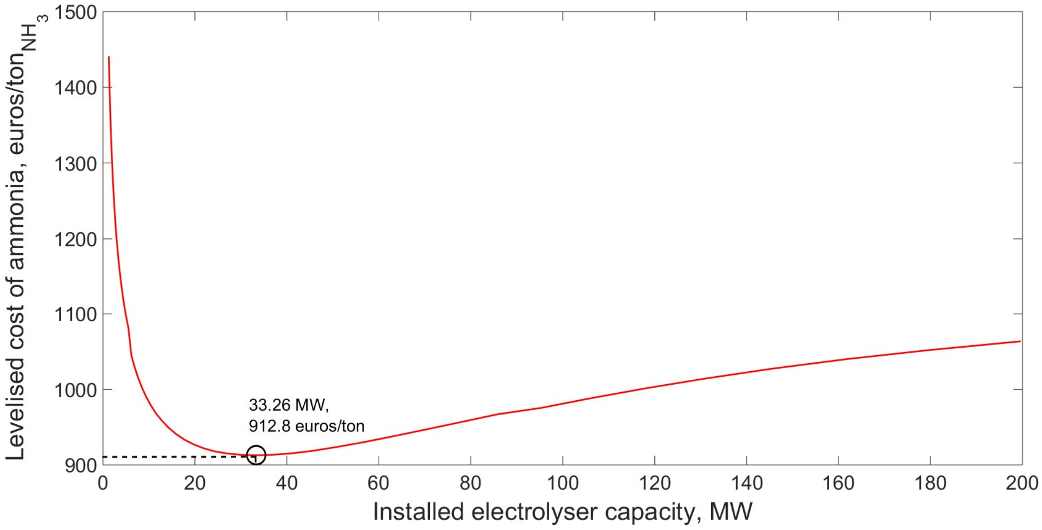


Figure 7.18: Scenario 2: Variation in levelised cost of ammonia with installed electrolyser capacity

Contribution of the main parameters to LCOA at this capacity is shown in figure 7.19. Variable cost by electric power consumption and hydrogen from work arising gas contribute 42% of total production cost while contribution of all other factors are almost same as in scenario 1.

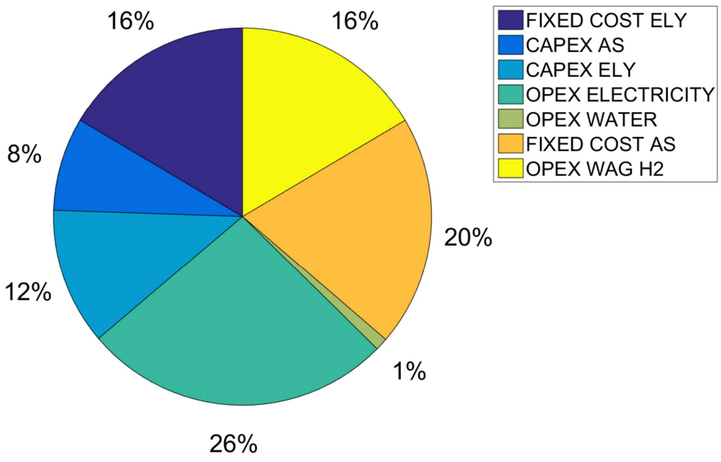


Figure 7.19: Scenario 2: Contribution of key parameters to LCOA at optimum electrolyser capacity

Main results from analysis of scenario 2 are summarised in table 7.3

Table 7.3: Scenario 2: Key parameters of system at optimum capacity

Parameter	**Value**	**Unit**
Ammonia production	16960	ton/year
Installed electrolyser capacity	33	MW
Type of ASU	Cryogenic distillation	-
Number of storage bullets	3	-
Capacity of unit storage bullet	303	m^3
Electric power consumed	120	GWh/year
Utilisation of available electric power	96	%
Electrolyser utilisation	35	%
Energy storage cost	177	€/MWh
Total plant CAPEX	85	Million €
LCOA	913	€/ton

Comparing LCOA of scenario 1 and 2, it is seen that scenario 2 shows a slightly more favourable result. This can be attributed to the hydrogen cost. Production cost of hydrogen using electrolyser with optimum capacity is €5.04/kg[1] while the production cost of hydrogen from work arising gas at the optimum capacity is €2.15/kg. Consumption of hydrogen from the electrolyser is replaced by a cheaper alternative during electric power deficits, which results into a lower LCOA.

---

[1] Calculated as $\frac{\text{Electrolyser OPEX+Electrolyser CAPEX}}{\text{Total hydrogen produced}}$ using average electricity price of €55.5/MWh

7.4. SCENARIO 3: UTILISING HYDROGEN FROM AN EXTERNAL SOURCE

Scenario 3 involves a system without an electrolyser. All hydrogen consumed is assumed to be available at site. Electric power is consumed only by AS and the availability and the price pattern have been kept unchanged. Hydrogen price has been varied between €0/kg and €1.9/kg. Figure 7.20 shows variation in LCOA with variation in both hydrogen price and plant capacity. Tables 7.4 and 7.5 represent the three-dimensional figure in the form of a matrix. Table 7.4 highlights the instances which have a LCOA less than €500/ton(Average market price of ammonia in 2013) and table 7.5 highlights instances with LCOA less than €300/ton (Current market price of ammonia). It is observed that plants with capacity greater than 6136 TPY have LCOA less than €500/ton irrespective of hydrogen price. Economic feasibility of plants with capacity lower than this limit strongly depend on price of hydrogen. Finally, it is observed that small scale plants[1] are difficult to be economically feasible unless hydrogen price is lower than €0.2/kg.

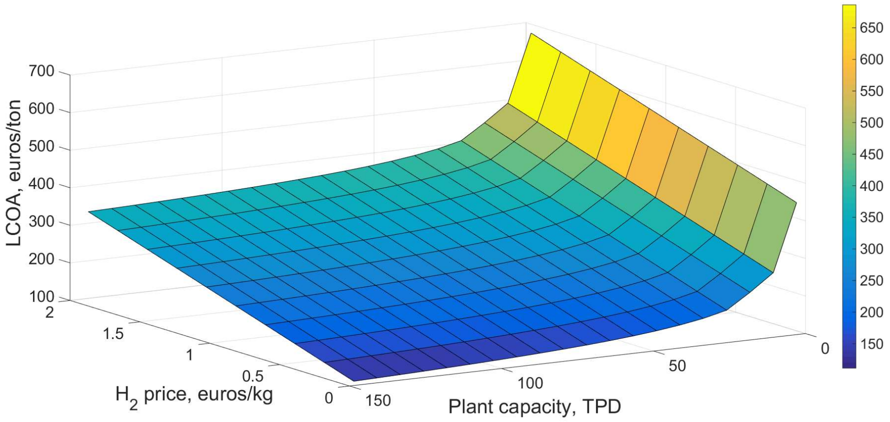
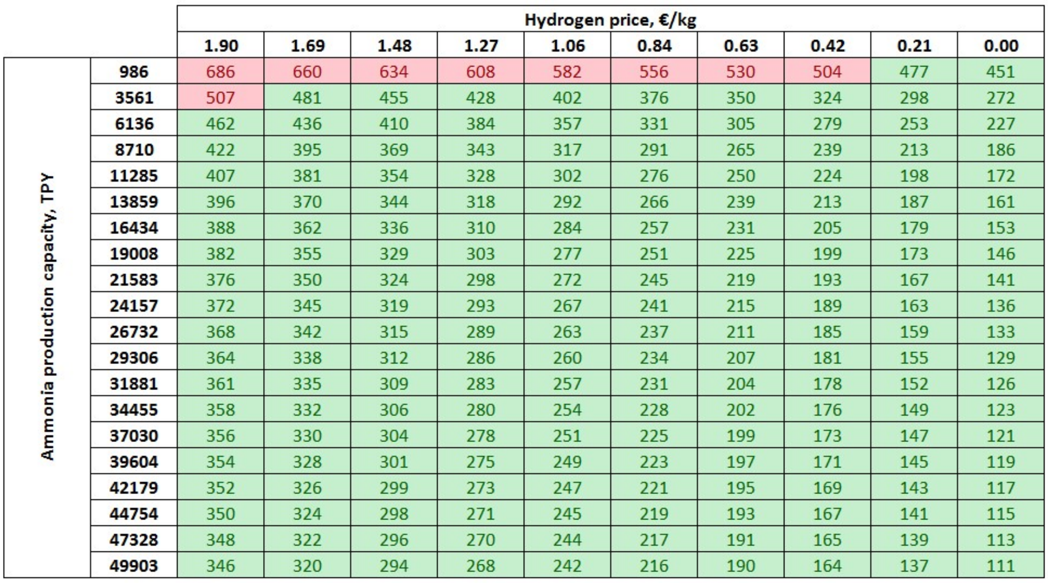


Figure 7.20: Scenario 3: Sensitivity of LCOA on hydrogen price and plant capacity

Table 7.4: Scenario 3: Feasibility of ammonia plants at market price of €500/ton



		Hydrogen price, €/kg									
		1.90	1.69	1.48	1.27	1.06	0.84	0.63	0.42	0.21	0.00
Ammonia production capacity, TPY	986	686	660	634	608	582	556	530	504	477	451
	3561	507	481	455	428	402	376	350	324	298	272
	6136	462	436	410	384	357	331	305	279	253	227
	8710	422	395	369	343	317	291	265	239	213	186
	11285	407	381	354	328	302	276	250	224	198	172
	13859	396	370	344	318	292	266	239	213	187	161
	16434	388	362	336	310	284	257	231	205	179	153
	19008	382	355	329	303	277	251	225	199	173	146
	21583	376	350	324	298	272	245	219	193	167	141
	24157	372	345	319	293	267	241	215	189	163	136
	26732	368	342	315	289	263	237	211	185	159	133
	29306	364	338	312	286	260	234	207	181	155	129
	31881	361	335	309	283	257	231	204	178	152	126
	34455	358	332	306	280	254	228	202	176	149	123
	37030	356	330	304	278	251	225	199	173	147	121
	39604	354	328	301	275	249	223	197	171	145	119
	42179	352	326	299	273	247	221	195	169	143	117
	44754	350	324	298	271	245	219	193	167	141	115
	47328	348	322	296	270	244	217	191	165	139	113
	49903	346	320	294	268	242	216	190	164	137	111

---

[1] Plants with capacity lower than 1000 TPY

Table 7.5: Scenario 3: Feasibility of ammonia plants at market price of €300/ton

		Hydrogen price, €/kg									
		1.90	1.69	1.48	1.27	1.06	0.84	0.63	0.42	0.21	0.00
Ammonia production capacity, TPY	986	686	660	634	608	582	556	530	504	477	451
	3561	507	481	455	428	402	376	350	324	298	272
	6136	462	436	410	384	357	331	305	279	253	227
	8710	422	395	369	343	317	291	265	239	213	186
	11285	407	381	354	328	302	276	250	224	198	172
	13859	396	370	344	318	292	266	239	213	187	161
	16434	388	362	336	310	284	257	231	205	179	153
	19008	382	355	329	303	277	251	225	199	173	146
	21583	376	350	324	298	272	245	219	193	167	141
	24157	372	345	319	293	267	241	215	189	163	136
	26732	368	342	315	289	263	237	211	185	159	133
	29306	364	338	312	286	260	234	207	181	155	129
	31881	361	335	309	283	257	231	204	178	152	126
	34455	358	332	306	280	254	228	202	176	149	123
	37030	356	330	304	278	251	225	199	173	147	121
	39604	354	328	301	275	249	223	197	171	145	119
	42179	352	326	299	273	247	221	195	169	143	117
	44754	350	324	298	271	245	219	193	167	141	115
	47328	348	322	296	270	244	217	191	165	139	113
	49903	346	320	294	268	242	216	190	164	137	111

7.5. COMPARISON OF SCENARIOS

The LCOA of the three scenarios are presented in figure 7.21. A hydrogen price of €1.9/kg has been used for scenario 3 in this plot.

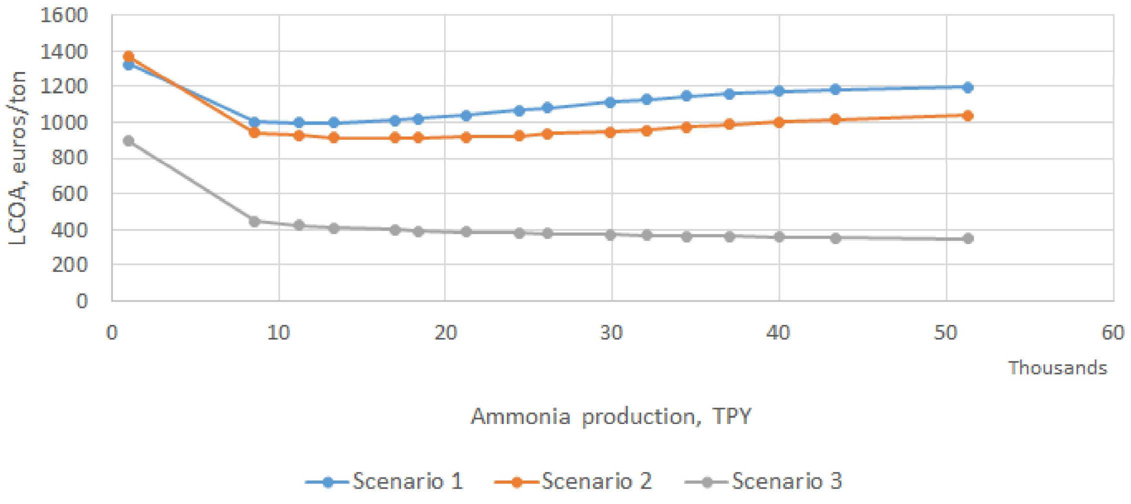


Figure 7.21: Comparison of LCOA for the three scenarios

Scenario 3, which does not employ an electrolyser appears to be the most economically attractive. For scenario 3, plant capacities larger than 8500 tonnes/year produce ammonia at competitive prices considering current market price of ammonia.

8

POWER PRODUCTION FROM AMMONIA VIA GAS TURBINE

This chapter sheds light on practicality of using ammonia as a fuel in gas turbines. Section 8.1 discusses the impact of gas turbine capacity when considered for base scenario. Section 8.2 discusses possibilities of using ammonia directly in a gas turbine by giving an update on recent developments around the world. Section 8.3 describes the process of cracking ammonia into hydrogen as an alternative to be run in gas turbines. Ammonia combustion is associated with NOx emissions and they are discussed in section 8.4.

8.1. POTENTIAL OF GAS TURBINE TO SATISFY ELECTRIC POWER DEMAND

It has been assumed that the objective of the gas turbine in this study is to provide electric power to Tata Steel, IJmuiden during periods when electric power needs to be imported from the grid to fulfil the demand (termed as 'deficit period' henceforth in this chapter). A statistical analysis of the electric power imbalance data has been conducted to understand the magnitude and durations of the deficit period. For the year 2013, approximately 68% of the magnitude of deficit period is less than 73 MW[1]. Figure 8.1 shows a probability distribution curve to understand the durations of the deficit periods.

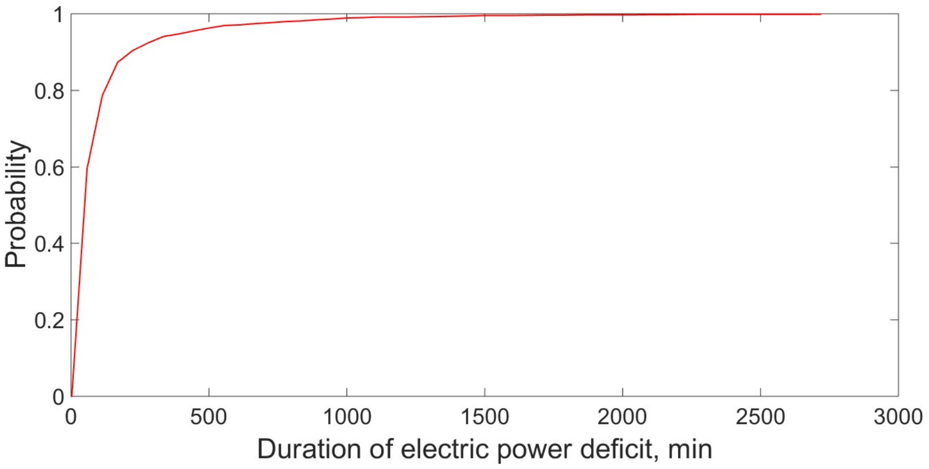


Figure 8.1: Probability distribution curve for duration of deficit period

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[1] For a normal distribution, Probability(μ-σ<X<μ+σ)≈0.6827

Table 8.1: Potential of gas turbine capacities to satisfy total electric energy deficit

Gas turbine installed capacity, MW	**NH_3 requirement[1], kg/s**	**Maximum operating time at installed capacity, hours**	**Electric power deficit duration satisfied[2], %**	**Electric power deficit magnitude satisfied[3], %**	**Total electric energy deficit satisfied, %**
200	37.7	1.2	65.5	99.6	65.2
175	33.0	1.4	69.2	98.8	68.4
150	28.3	1.7	74.0	96.8	71.7
100	18.9	2.5	82.0	84.3	69.1
75	14.2	3.4	88.0	71.1	62.5
50	9.4	5.1	90.0	51.5	46.4
40	7.6	6.5	94.7	42.7	40.4
30	5.7	8.8	96.5	32.4	31.3
25	4.7	10.8	97.4	27.4	26.7
20	3.8	13.8	98.1	21.6	21.2
10	1.9	31.1	99.7	11.2	11.2
5	0.9	83.9	100.0	5.2	5.2

It is observed that almost all of the deficit period duration is less than 1000 minutes. Almost 90% of the deficit period duration is less than 225 minutes. This implies that a gas turbine having a capacity of 73MW and capable of operating continuously for 225 minutes generates sufficient energy to satisfy almost 61% of all electric energy deficits.

Improving this value requires higher capacity and larger ammonia storage which have a direct influence on cost. In this study, storage capacity has been assumed to equal to five days of production capacity. With this constraint, gas turbine capacity has been varied to estimate the maximum operating time. The optimum plant capacity determined for scenario 1 has been chosen for this investigation. Average ammonia production for this capacity is 0.39 kg/s and average storage capacity is 168 tonnes. Table 8.1 summarises the result of the findings. The results are based on the assumption that 168 tonnes of stored ammonia is initially available. A peaking behaviour is shown by the gas turbine capacity with regard to its potential to satisfy total electric energy deficit. A gas turbine of capacity 150 MW has the peak potential to satisfy approximately 72% of all energy demand.

Roundtrip efficiency is the efficiency of the process from production of ammonia using electric power to recovering electric power from the produced ammonia. It is the product of efficiency of power to ammonia and the gas turbine cycle efficiency.

$$\eta_{rt} = \eta_{p2a} . \eta_{gt} \tag{8.1}$$

Assuming a conservative gas turbine efficiency of 30% and average power to ammonia efficiency of 50% (figure 7.6, the roundtrip efficiency using ammonia as the energy storage medium has been estimated to be about 15%. Using a combined cycle gas turbine may improve the roundtrip efficiency to 25% assuming a combined cycle efficiency of 50%.

---

[1] Calculated using energy content of ammonia based on its LHV, a conservative gas turbine cycle efficiency of 30% and generator efficiency of 95%

[2] Read from figure 8.1

[3] Calculations are shown in Appendix D under the assumption that all electric power deficit lower than its installed capacity can be satisfied by the gas turbine

8.2. DIRECT COMBUSTION OF AMMONIA IN A GAS TURBINE

8.2.1. HISTORY

General Motors Corp. in the USA conducted experiments to assess the feasibility of using ammonia as a fuel in standard gas turbines designed for hydrocarbons. Experiments were conducted using both ammonia in liquid and vapour phase using a T63-A-3 gas turbine burner[1]. The impact of several variations in fuel injector and combustion liner were investigated including variations in the distribution of primary and secondary air flow. The maximum temperature at the outlet of the burner using liquid ammonia was recorded to be just under 455°C. However, it was not possible to sustain a flame without constant ignition. High heat of vaporisation of ammonia coupled with endothermic decomposition reaction and low flame speed were the main reasons for this. Using gaseous ammonia did not change the combustion behaviour significantly. It was concluded that ammonia cannot be used as a substitute fuel for gas turbines designed for hydrocarbons without modifying burner dimensions[58].

8.2.2. RECENT DEVELOPMENTS

A collaboration project between two Japanese institutes- Tohoku University and National Institute of Advanced Industrial Science and Technology (AIST) resulted in the world's first successful demonstration of utilising an ammonia fuelled combustion turbine to generate power[14]. The experiment was carried out for a system with maximum power output of 50kW. Initial experiments were carried out by with a fuel blend of 70% wt. kerosene and 30% wt. ammonia. A prototype combustor was employed to enable a bi-fuel supply. By September 2015 successful experiments were performed with ammonia-methane co-firing (1:1 LHV ratio) and also pure ammonia combustion to produce about 42kW. For all cases, startup fuel was kerosene due to lower ignition energy needed compared to ammonia. Ammonia was introduced in the combustion chamber only after combustion was stable. The results are shown in figures 8.2a, 8.2b and 8.2c.

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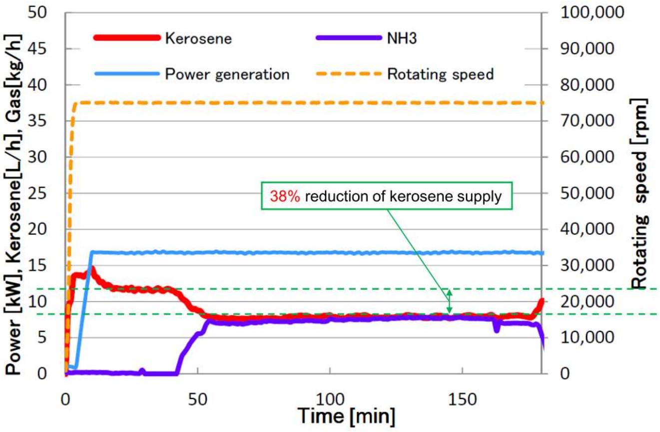
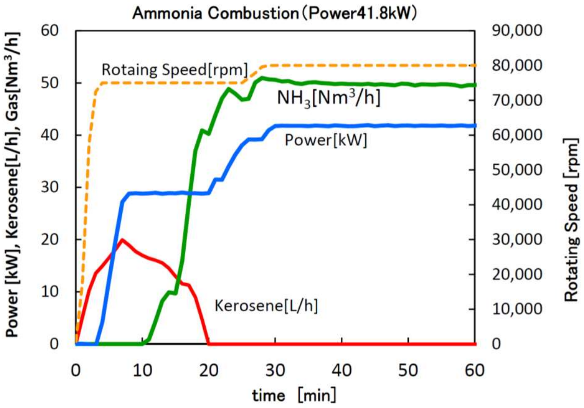
[1] Burner dimensions in the primary combustion zone area: 5.5 in diameter x 10.6 in long; Air flow distribution: Dome (13%), Primary zone (23.8%), Secondary zone (36.9%), Cooling zone (26.3%)



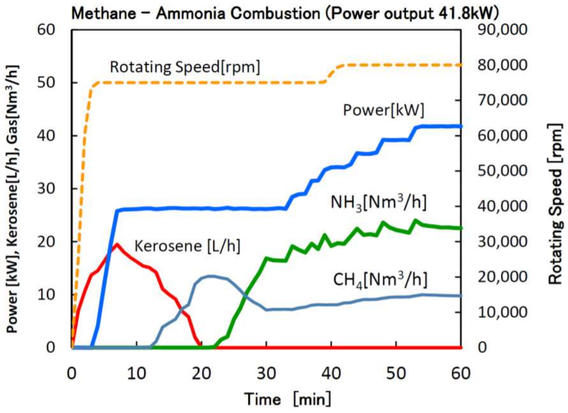
(a) Blend of kerosene and ammonia (70:30 by weight)

Source: Iki et al.(2015)[26]



(b) Pure ammonia

Source: Iki et al.(2015)[26]



(c) Blend of ammonia and methane (1:1 energy content)

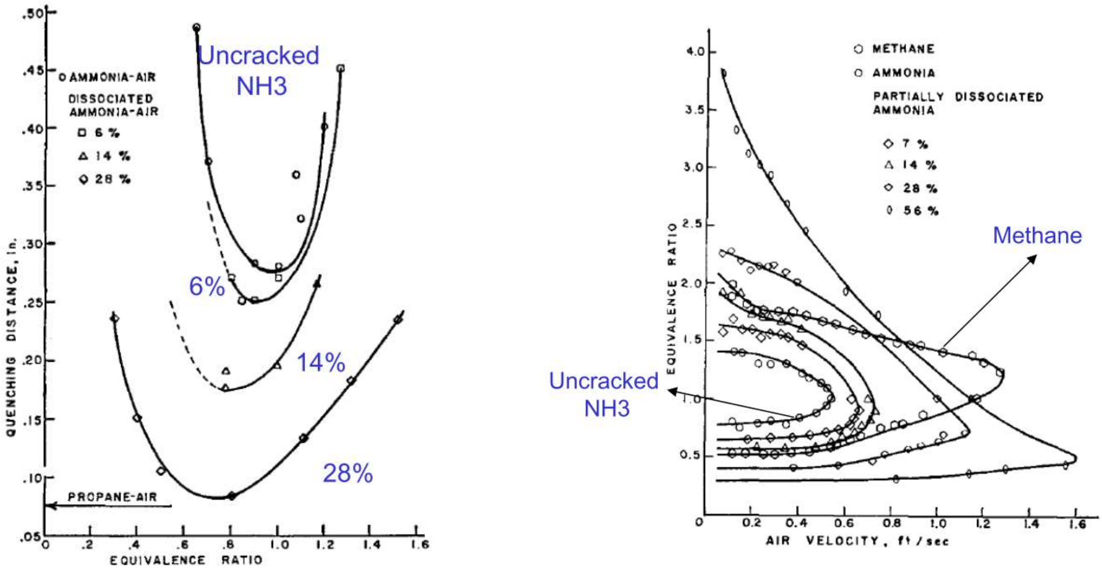
Source: Iki et al.(2015)[26]

Figure 8.2: Experimental results for power generation using several blends of ammonia in a micro gas turbine

Even though commercial gas turbines employing ammonia as fuel have not been realised yet, the recent developments show good promise for scale up in the future.

8.3. INDIRECT COMBUSTION OF AMMONIA IN A GAS TURBINE

The major drawbacks of using pure ammonia in a commercial combustion chamber are requirement of large ignition energy, large quenching distance, low flame velocity and poor flame stability[19]. To improve performance, ammonia is dissociated into hydrogen and nitrogen either fully or partly. The dissociation process is termed as cracking of ammonia. Figures 8.3a, 8.3b, 8.4a and 8.4b compare the quenching distance, flame speed and ignition energy and flame stability of uncracked ammonia with partially cracked ammonia respectively. Cracking of ammonia enhances the combustion efficiency and the flame stability[19]. Verkamp et al. (1967)[58] demonstrated that 28% dissociated ammonia exhibited combustion performance comparable to that of a hydrocarbon fuel in a gas turbine. They concluded that this composition of ammonia and hydrogen shows promise to be used as a substitute fuel for gas turbines designed for hydrocarbons.



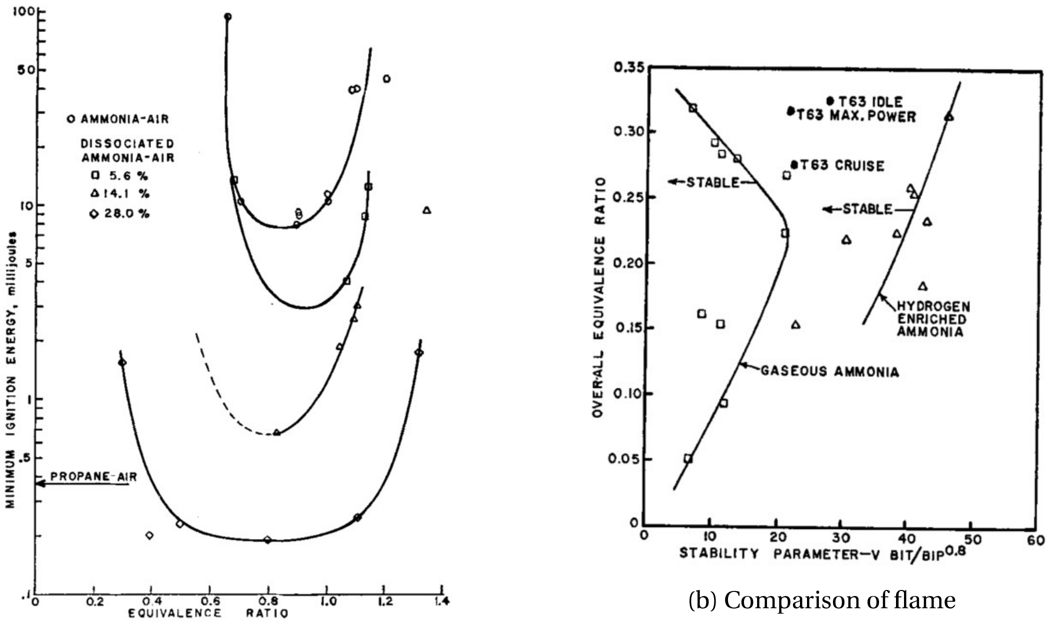
(a) Comparison of quenching distance

Source: Evans (2013)[19]

(b) Comparison of flame velocity

Source: Evans (2013)[19]

Figure 8.3: Comparison of combustion characteristics of pure ammonia with partially cracked ammonia



(a) Comparison of ignition energy

Source: Verkamp et al. (1967)[58]

(b) Comparison of flame stability

Source: Verkamp et al. (1967)[58]

Figure 8.4: Comparison of combustion characteristics of pure ammonia with partially cracked ammonia

8.3.1. METHODS OF AMMONIA CRACKING

CATALYTIC CRACKING

The most common method to crack ammonia is to pass it over a heated catalyst bed. Nickel and Ruthenium based catalysts are the usually employed[19]. Other noble metals like Rhodium, Palladium, Platinum and Iridium are also of interest for cracking ammonia[12]. A more recent development is using sodium amide[15]. This eliminates the need for use of expensive rare earth metals and is particularly attractive when high conversion is demanded. Figure 8.5 compares conversion of ammonia into hydrogen using different catalysts within a temperature range of 250-650°C. Experiments demonstrated a conversion as high as 99.2%[15].

The drawbacks of commercially available ammonia crackers are[19]:

- Limited catalyst life
- Expensive
- Significant heat loss associated with high temperature operation
- High energy demand
- Long period to reach full operation capacity

These crackers usually exhibit a cracking efficiency of about 50%[19]. A well developed heat integration network is essential to improve efficiency of the overall system.

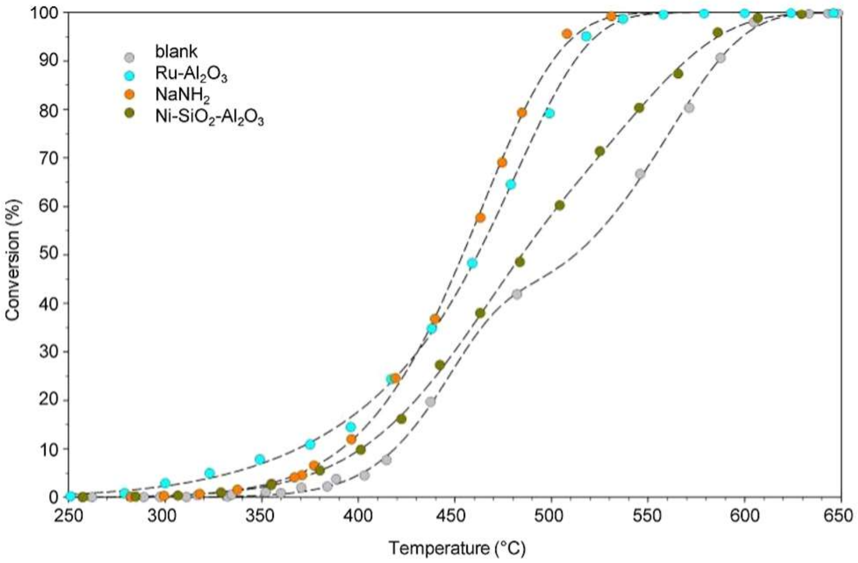


Figure 8.5: Comparison of ammonia conversion for different catalysts

Source: David et al. (2014)[15]

PARTIAL CRACKING USING A PRE BURNER

Another method employed to crack ammonia is by using a pre-burner and is specially relevant to using ammonia as a fuel in a gas turbine or combustion engine. Ammonia is partially cracked in the presence of pressurised oxygen at a temperature around 180 °C. The partially cracked ammonia mixture enters the combustion chamber of the gas turbine where it is combusted in the presence of compressed air. Figure 8.6 shows the plant configuration using a pre burner. Mixtures upto 25% cracked ammonia can be produced at relatively low temperatures. The operating temperature influences the life time of the cycle, production cost and heat loss of the system[19].

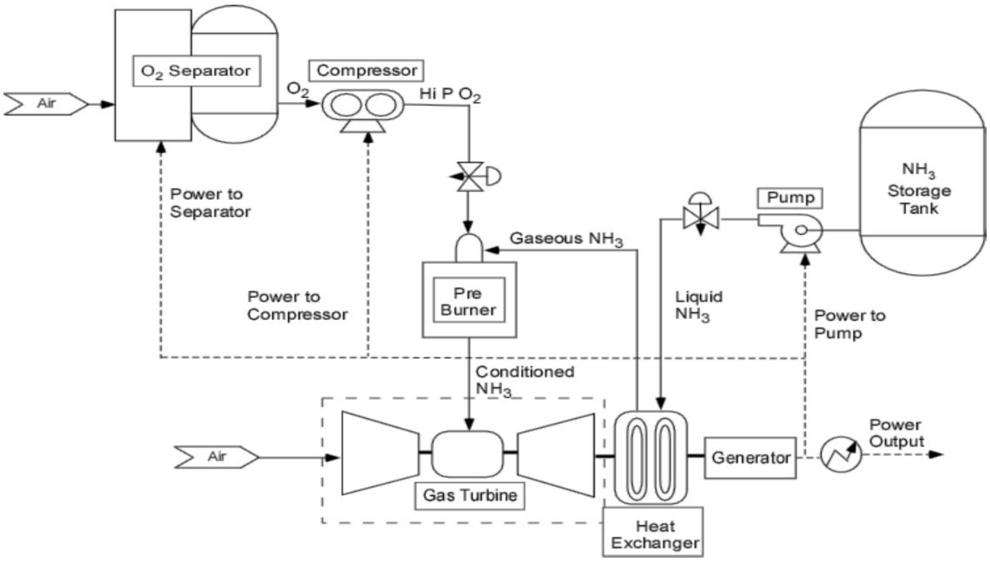


Figure 8.6: Process flow diagram for power production from ammonia using a gas turbine with a pre burner

Source: Evans (2013)[19]

The main advantages of using this method are[19]:

- No catalyst required
- Quick startup period
- Good scalability
- Pre burner can be operated using liquid or gaseous ammonia

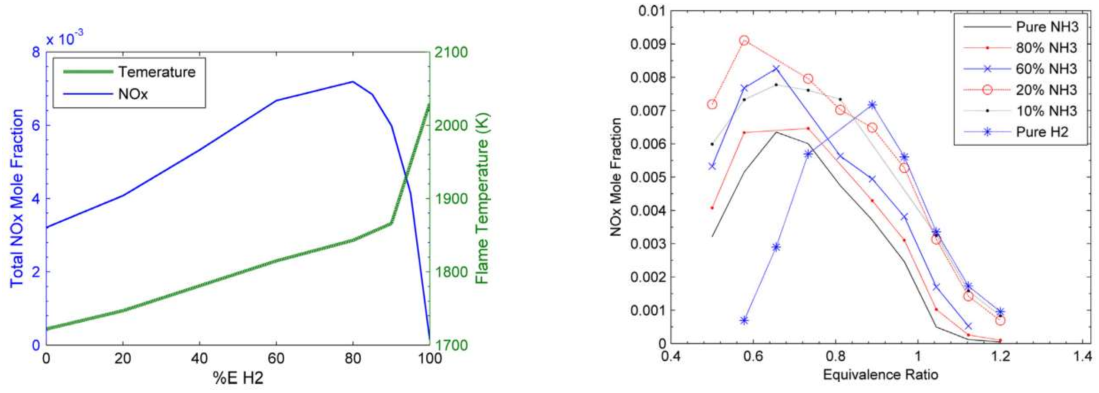
Space Propulsion Group Inc., California is involved in a project to develop a gas turbine using ammonia as a fuel by cracking. The project is funded by Montana Board of Research and Commercialisation Technology[19].

8.4. EMISSIONS

Ammonia is a carbon free fuel and is one of the main reasons for receiving much interest recently as an alternative fuel. However, ammonia is a source of nitrogen which result in formation of nitrogen oxides (NOx) during combustion. Interestingly, ammonia also finds application in selective catalytic reduction which handles NOx from industrial and automotive emissions. Nozari et al.(2015)[39] have performed a numerical study of combustion of ammonia and ammonia-hydrogen mixtures. It was observed that with increasing hydrogen content in the mixture resulted in higher NOx emissions. This trend was observed for hydrogen content upto 80% (LHV content). The reason for this was explained using two phenomena:

1. Higher hydrogen content increased the flame temperature leading to higher thermal NOx.
2. H, OH and HNO radicals formed because of hydrogen accelerate the production of fuel bound NOx.

For hydrogen content greater than 90%, fuel bound NOx, which is the major contributor to NOx emissions reduced drastically leading to a sharp drop in NOx emissions as shown by the figure 8.7a. The effect of equivalence ratio was also investigated on NOx formation for different compositions of fuel mixture. It was observed that rich mixtures have significantly lower NOx emissions. Pure ammonia showed lower NOx emissions than pure hydrogen in the rich mixture regime. This was justified due to lower adiabatic flame temperatures and oxygen content in this regime, which were identified as promoters of NOx emissions. Figures 8.7a and 8.7b show the effect of hydrogen content and equivalence ratio of the fuel mixture on NOx emissions respectively.



(a) Variation of NOx emissions with hydrogen content in fuel mixture, ϕ=0.5

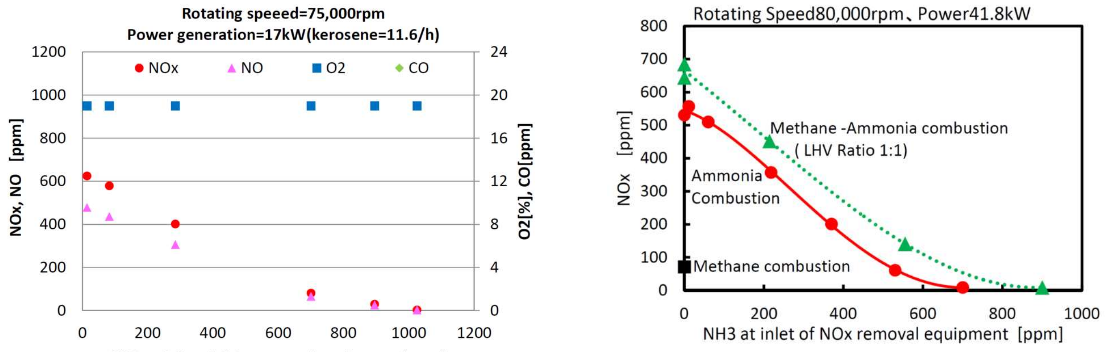
Source: Nozari et al.(2015)[39]

(b) Variation of NOx emissions with equivalence ratio in fuel mixtures, P=17 bar, T=673 K

Source: Nozari et al.(2015)[39]

Figure 8.7: Results from numerical simulation for NOx emissions at varying operating conditions

Methane is a hydrogen carrier and experiments show it has the same effect as hydrogen does when mixed with ammonia[39]. Figures 8.8a and 8.8b show the NOx emissions reported from experiments described in section 8.2.2. The NOx emissions are stated for 19% oxygen. NOx emissions from co-firing ammonia and kerosene is comparable to emissions from combustion of methane-ammonia. Combustion of pure ammonia results in lower NOx emissions compared to the other two cases.



(a) Co-firing kerosene-ammonia(70:30 by weight)

Source: Iki et al.(2015)[26]

(b) methane (pure), ammonia(pure) and methane-ammonia (1:1 energy content) co-firing

Source: Iki et al.(2015)[26]

Figure 8.8: Results from experiments for NOx emissions at varying fuel blends

NOx emissions from ammonia fired gas turbines exceed the permissible limits[39] and NOx reduction units are necessary for commercial applications. Design modifications and optimising operating parameters will help to reduce formation of NOx emissions but require more research and understanding of the combustion mechanism of ammonia.

9

CONCLUSIONS AND FUTURE WORK

This chapter summarises the most significant findings of the present study and makes some recommendations for future research work.

9.1. CONCLUSIONS

A techno-economic model for a power to ammonia plant was developed successfully. The model accepts variable availability of electric power and electric power unit price in time as input. This model was employed to assess the feasibility of using ammonia as an energy storage medium at Tata Steel, IJmuiden utilising surplus electric power from the plant operations for various operating scenarios.

1. Producing ammonia by electrolysis of water is an expensive route. For systems with installed electrolyser capacity lower than 38 MW, the variable costs for electric power consumption and fixed operation costs of the AS were identified as the main contributors to the production cost of ammonia. For systems with a higher installed capacity of the electrolyser, the variable costs for electric power consumption and costs associated with the electrolyser were found to be dominating. With a share of approximately 80%, the electric power consumption by the electrolyser dominates the electricity costs.

2. In the current scenario, the minimum levelised cost of ammonia is just under €1000/ton, which is almost three times more expensive than the current market price of ammonia. This makes competition with the open market for ammonia economically unattractive. The optimum installed electrolyser capacity was found to be 25 MW with an ammonia production capacity of 11249 tonnes/year. The main cause for the high cost involved with the base scenario was the limitation in utilisation of the equipment in conjunction with the requirement of importing electric power from the grid during periods of insufficient availability of electric power at the Tata Steel plant. Efficiency of producing ammonia lies within the range of 47.5% to 55%.
   Availability of abundant electricity at prices less than €10/MWh has the potential to make this system economically viable and produce ammonia at a competitive price. Alternatively, abundant available power coupled with reduction in electrolyser CAPEX by almost 80% and a higher market price of ammonia (~€650/ton) has the potential to produce ammonia in an economically attractive manner.

3. Utilisation of prospective excess hydrogen available at the steel plant had a positive influence on the economics of the plant. COG was identified as the most suitable source of hydrogen

and PSA the most economically attractive process for hydrogen separation with a production cost of €2.15/kg. A minimum hydrogen purity of 99.999% is required for ammonia synthesis. When excess hydrogen was utilised to eliminate electric power import for the electrolyser, the minimum levelised cost of ammonia was reduced to €913/ton.

4. In the case which assumed sufficient excess hydrogen was available to completely eliminate electrolysis, the minimum levelised cost of ammonia was found to be comparable to the current market price of ammonia (~€300/ton)[1] for capacities larger than 21000 tonnes per year and a hydrogen price lower than €1.26/kg.

5. The scale of ammonia production using surplus electric power at Tata Steel, IJmuiden was found to be limited to about 50000 tonnes per year. This limits application of produced ammonia to niche markets which need to be identified. The major markets of ammonia like urea, nitric acid, ammonium nitrate etc. are not very interesting at this scale of ammonia production.

6. The cost for ammonia as an energy storage medium for the base scenario ranges from €193/MWh to €281/MWh . This improves when abundant electric power is available. These costs are reduced to the range from €211/MWh to €137/MWh. Battery storage is currently available at costs of around €800k/MWh to €1 Million/MWh and are expected to drop to around €100k/MWh by 2020[30]. The economic advantage provide by an ammonia based energy system is clear. However, recovery of energy from ammonia through combustion technology is still under development.

Ammonia is an interesting energy storage medium which promotes green economy and offers a multitude of applications including grid stabilisation. It shows bright potential as a real game-changer in the world of energy storage and alternative fuels. However, current economic scenario and development stage makes it difficult to be considered as an immediate commercial solution.

9.2. RECOMMENDATIONS FOR FUTURE RESEARCH WORK

1. Large capacity plants modelling: The model developed for this study satisfactorily mimics a small scale ammonia plant. At industrial scale of ammonia production (>100,000 tonnes per year), the process scheme changes and heat integration plays an important role to improve efficiency of the system. Heat flows within the electrolyser unit and the ammonia synthesis unit are of special interest and needs to be looked into in detail. Moreover, significant amount of oxygen is produced to consider it as a valuable by-product. These changes play a role in the economics of the plant and should be incorporated when dealing with large scale plants.

2. Dynamic modelling of system: In this study, the system behaves under steady state conditions with varying electric power consumption. Secondly, operating capacity of the system is assumed to vary instantaneously with input electric power. Finally, it is assumed efficiency of ammonia synthesis section is constant at all operating capacities. This would not be the case in practice. A dynamic approach needs to be implemented to investigate the effect of these critical simplifications.

3. Integration with renewable energy system: Tata Steel IJmuiden has proposed setting up wind (14MW) and solar (22MW) parks in the vicinity of the plant. It would be worthwhile to investigate the effect of integrating the renewable energy system with the power to ammonia system. Using renewable energy also makes the system eligible for subsidies like SDE+ in the Netherlands. This has the potential to improve the economics of the system.

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[1] Average price of ammonia in Western Europe during October 2016 to August 2017

4. Integration with battery or battolyser: Batteries are useful components to minimise the ill effects of intermittency of available power. A battolyser is a novel invention being developed at TU Delft which acts as a battery during normal operating regime and produces hydrogen when charged beyond its full capacity. These components have the potential to utilise available electric power more efficiently and can improve the performance of the energy storage system. A study integrating these components with ammonia system is interesting and novel.

5. Simulation of ammonia fired gas turbine: The scope of the developed model in this study ends at production of ammonia. Softwares like Thermoflex, GateCycle™or Cycle-Tempo maybe used for analysing the performance of ammonia fired gas turbines. This is useful to complete the energy storage cycle from ’power to power’. Advanced numerical simulations can be performed to analyse emissions associated with ammonia combustion. A dynamic study maybe conducted to determine the optimum capacity of gas turbine and its operating behaviour to satisfy varying demand.

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A

COST OF ELECTRIC POWER CONSUMPTION

The specific power consumption of an electrolyser is a function of its operating capacity and given by equation 6.1. It has been assumed that the specific power consumption of the AS is independent of its operating capacity. However, it is dependant on the type of ASU employed. The combined effect of these three factors dictates the fraction of power consumed by the electrolyser at any operating capacity.
The specific power consumption of AS has been obtained from ASPEN® HYSYS model and the MATLAB® model. The values are normalised to Nm^3 of H_2 and depicted in table A.1.

Table A.1: Specific power consumption of AS

	Hydrogen compressor	**ASU**	**Feed compressor**	**Recycle compressor**	**Total**	**Unit**
AS with PSA ASU	0.138	0.266	0.263	0.004	0.671	kWh/Nm^3 H_2
AS with Cryogenic ASU	0.138	0.097	0.263	0.004	0.502	kWh/Nm^3 H_2

The electric power balance at any operating capacity is given as

$$\frac{P_{ELY}}{\eta_{trans}\eta_{rect}} + P_{AS} = P_{total} \tag{A.1}$$

Figure A.1 shows the fraction of power consumed by ELY and AS as a function of operating capacity of the system employing PSA type ASU and figure A.2 shows the same for a system with a cryogenic distillation unit. Data from table A.1, equations A.1 and 6.1 have been used to plot the data. The equations of the curves that fit the data in each case have been determined and used in the power allocation logic.

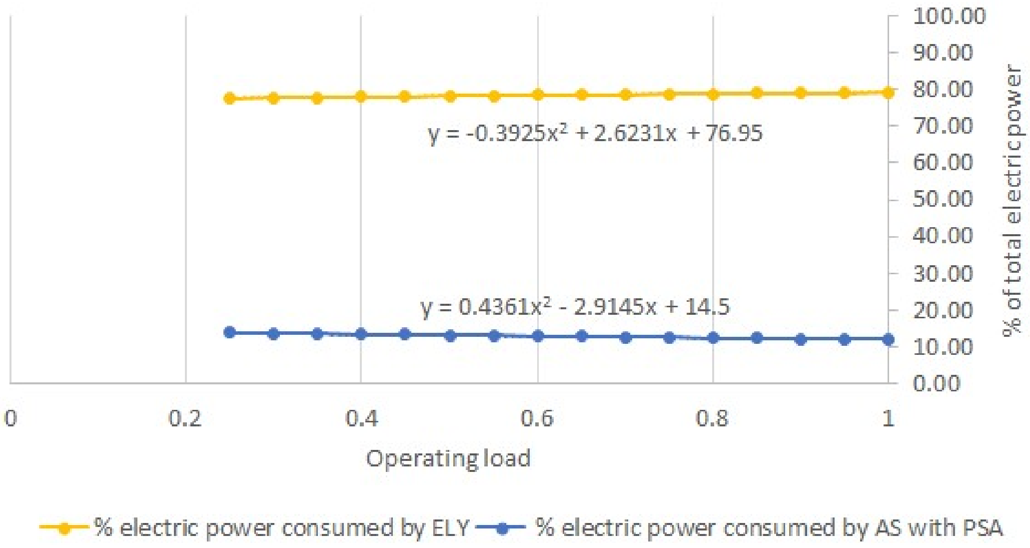

Figure A.1: Fraction pf power consumed by ELY and AS with PSA

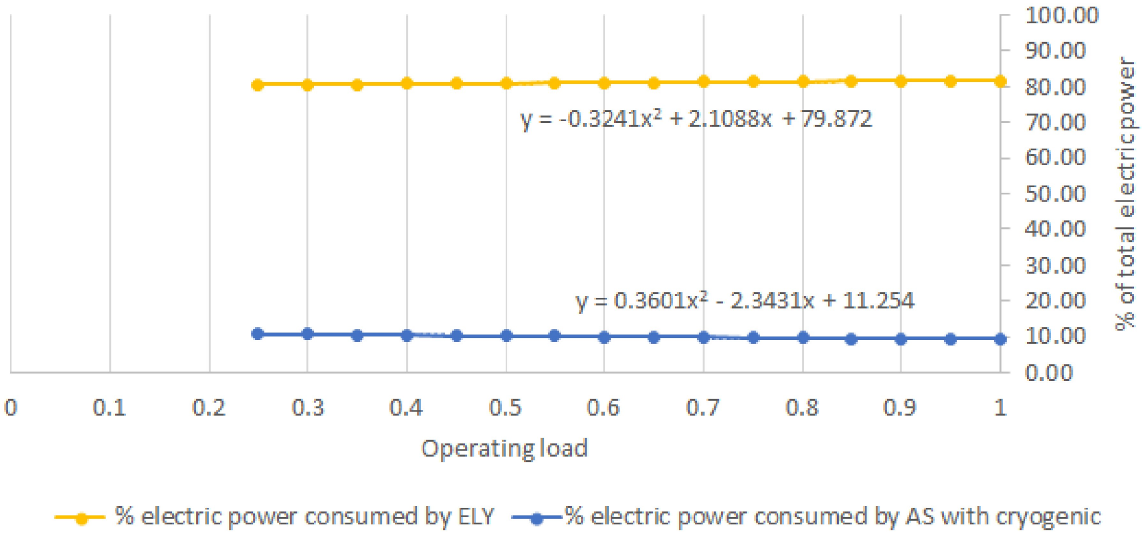

Figure A.2: Fraction pf power consumed by ELY and AS with cryogenic distillation

Figure A.3 depicts the logic used to allocate power to the system. Once peak available power is determined, an array of installed plant capacities is defined with decreasing steps (10% in this case). For an installed plant capacity P, the following terms are defined:

1. P^{ELY}_{ins}: The installed capacity of the electrolyser, and is calculated as

$$P^{ELY}_{ins} = \begin{cases} 0.817P & P \geq 9.38 \\ 0.792P & P < 9.38 \end{cases} \tag{A.2}$$

Nitrogen requirement for plants with installed capacity greater than 9.38 MW is more than 560 Nm^3 and hence fall inside cryogenic distillation ASU regime. The relation is obtained using equations in figures A.1 and A.2.

Similarly,

2. P_{ins}^{AS}: The installed capacity of AS, and is calculated as

$$P_{ins}^{AS} = \begin{cases} 0.093P & P \geq 9.38 \\ 0.12P & P < 9.38 \end{cases} \tag{A.3}$$

3. P_{min}^{AS}: The minimum capacity of AS, and is calculated as

$$P_{min}^{AS} = 0.25P_{ins}^{AS} \tag{A.4}$$

4. P_{lo}^{AS}: The working capacity of the electrolyser corresponding to minimum capacity of AS, and is calculated as

$$P_{lo}^{ELY} = 0.25P_{ins}^{ELY} \tag{A.5}$$

When available power $P_{avail}(t)$, which varies with time, is lower than 0.25P, the operating capacity of the system is below the minimum capacity. The following terms are important in this scenario:

1. $ELY\_C(t)$: Electricity consumed by the electrolyser, and is calculated as

$$ELY\_C(t) = P_{lo}^{ELY}.t \tag{A.6}$$

2. $AS\_C(t)$: Electric power consumed by AS, and is calculated as

$$AS\_C(t) = P_{min}^{AS}.t \tag{A.7}$$

3. $P\_I(t)$: Electric power needed to be imported, and is calculated as

$$P_I(t) = 0.25P - P_{avail}(t) \tag{A.8}$$

4. $SUR\_EC(t)$: Cost associated with consumption of available power, and is calculated as

$$SUR\_EC(t) = (ELY\_C(t) + AS\_C(t)).EP_{avail}(t) \tag{A.9}$$

   $EP_{avail}(t)$ is the price of available electricity at that instant.

5. $IMP\_EC(t)$: Cost associated with import of additional power, and is calculated as

$$IMP\_EC(t) = P_I(t).EP_{imp}(t) \tag{A.10}$$

   $EP_{imp}(t)$ is the price of imported electricity at that instant.

When the available power is more than the minimum limit, but less than rated capacity i.e when $0.25P < P_{avail}(t) < P$, no import of electric power is necessary and the terms defined above are calculated as

$$ELY\_C(t) = \begin{cases} \frac{-0.3241Load_{sys}(t)^2+2.1088Load_{sys}(t)+79.872}{100}P_{avail}(t).t & P \geq 9.38 \\ \frac{-0.3925Load_{sys}(t)^2+2.6231Load_{sys}(t)+76.95}{100}P_{avail}(t).t & P < 9.38 \end{cases} \tag{A.11}$$

where $Load_{sys}(t)$ is the operating load of the system at any instant and calculated as

$$Load_{sys}(t) = \frac{P_{avail}(t)}{P} \tag{A.12}$$

Similarly,

$$AS\_C(t) = \begin{cases} \frac{-0.3601Load_{sys}^2+2.3431Load_{sys}+11.254}{100}P_{avail}(t).t & P \geq 9.38 \\ \frac{-0.4361Load_{sys}^2+2.9145Load_{sys}+14.5}{100}P_{avail}(t).t & P < 9.38 \end{cases} \tag{A.13}$$

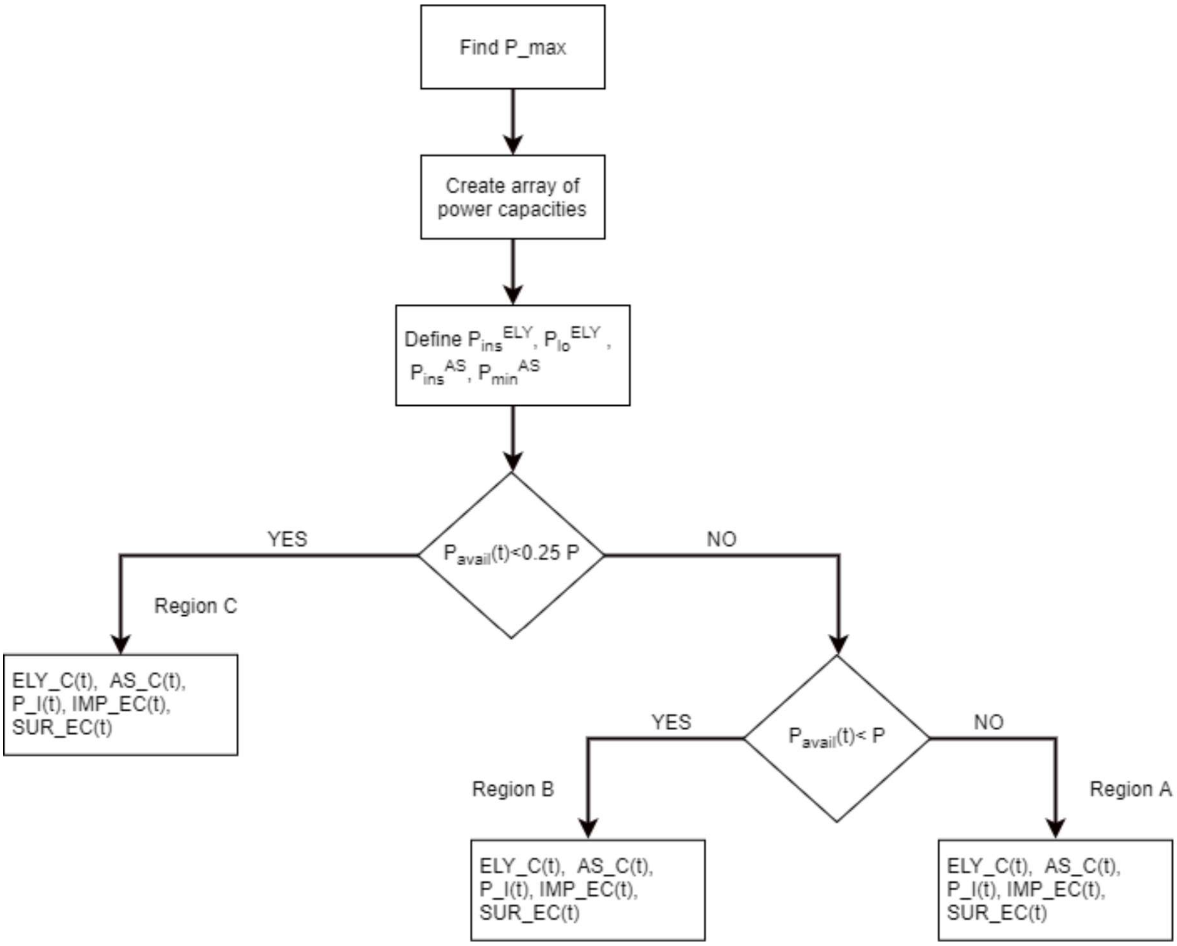

Figure A.3: Algorithm to calculate electric power consumption and associated costs

$$P\_I(t) = 0 \tag{A.14}$$

$$SUR\_EC(t) = (ELY\_C(t) + AS\_C(t)).EP_{avail}(t) \tag{A.15}$$

$$IMP\_EC(t) = 0 \tag{A.16}$$

Finally, when available power exceeds the installed capacity of the system,i.e $P_{avail}(t) > P$, both ELY and AS run at their installed capacities and no import of electric power is necessary. The excess electric power is curtailed. The relevant terms are calculated as

$$ELY\_C(t) = P_{ins}^{ELY}.t \tag{A.17}$$

$$AS\_C(t) = P_{ins}^{AS}.t \tag{A.18}$$

$$P\_I(t) = 0 \tag{A.19}$$

$$SUR\_EC(t) = (ELY\_C(t) + AS\_C(t)).EP_{avail}(t) \tag{A.20}$$

$$IMP\_EC(t) = 0 \tag{A.21}$$

The total cost of electric power consumption is calculated as

$$EC_{total} = \sum (SUR\_EC(t) + IMP\_EC(t)) \tag{A.22}$$

B

HYDROGEN PRODUCTION FROM WORK ARISING GAS

The steel industry is a source of by-product gases rich in a hydrogen, methane, carbon dioxide and some other compounds. These gases, known as work arising gases, are categorised into three types depending on their source:

1. Coke oven gas (COG)
2. Blast furnace gas (BFG)
3. Basic oxygen steelmaking furnace gas (BOFG)

The composition[1] of the three gas streams are depicted in figures B.1a, B.1b and B.1c.

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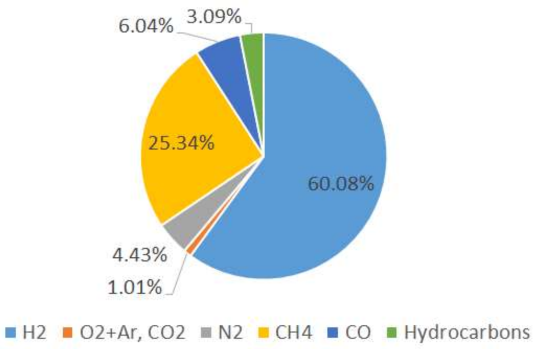
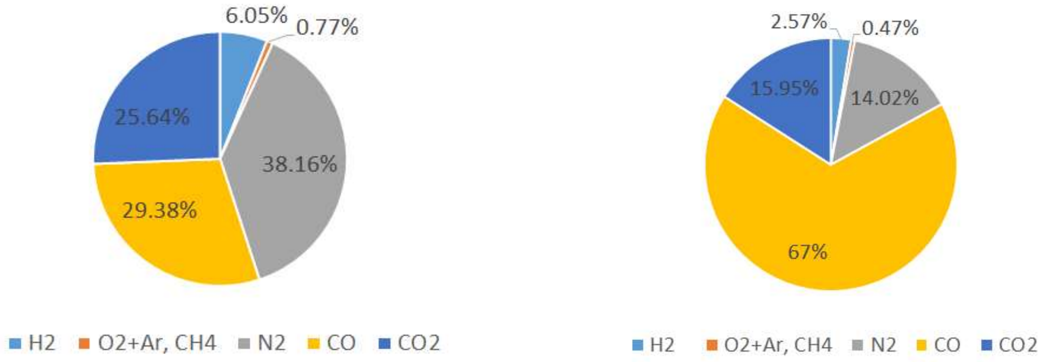
[1] Data made available by Tata Steel IJmuiden for year 2015. Percentages are volume based



(a) Composition of COG



(b) Composition of BFG

(c) Composition of BOFG

Figure B.1: Composition of WAG at Tata Steel, IJmuiden

Due to very low hydrogen concentration and mediocre carbon monoxide content, BFG has not been considered as a potential hydrogen source. The following technologies are suitable to obtain hydrogen from COG and BOFG:

1. Pressure swing adsorption: High hydrogen content in COG makes PSA an attractive technology to be considered for hydrogen separation.

2. Pressure swing adsorption + Steam methane reforming: The by product stream of COG obtained after separation of hydrogen using PSA is highly concentrated with methane. This makes steam methane reforming a suitable technology to be considered to extract more hydrogen from COG.

3. Water gas shift reaction: High concentration of carbon monoxide in BOFG makes this technology a possible solution to produce hydrogen from BOFG.

Figures B.2, B.3 and B.4 are used to represent the above mentioned technologies as process block diagrams

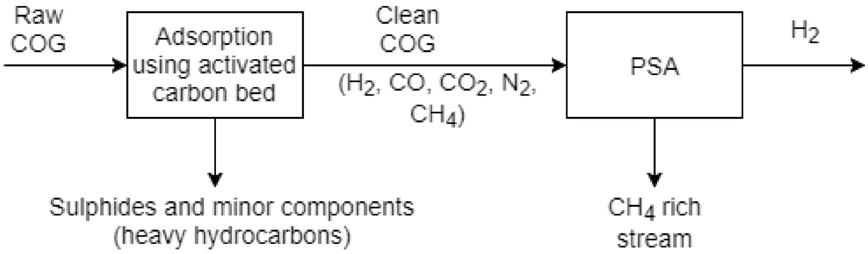


Figure B.2: Separation of hydrogen from COG via PSA

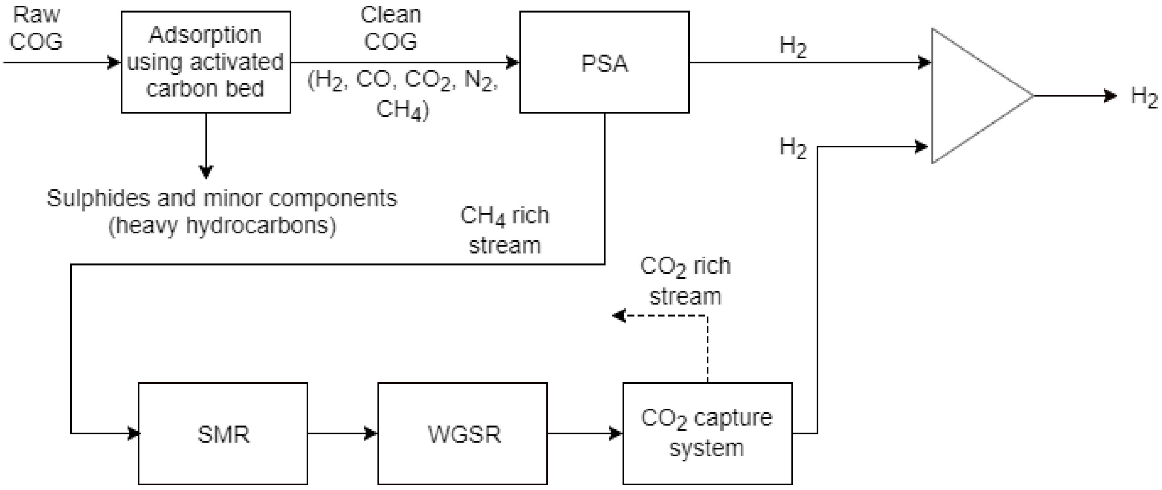


Figure B.3: Hydrogen production from COG via PSA and SMR[1]

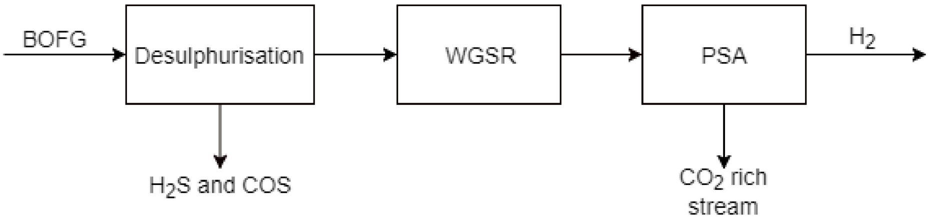


Figure B.4: Hydrogen production from BOFG via WGSR

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[1] SMR: Steam Methane Reforming; WGSR: Water Gas Shift Reaction

The three process routes are compared and summarised in table B.1.

Table B.1: Economic comparison of hydrogen production routes from WAG

Route	**H_2 capacity**[1] **(TPD)**	**Capital cost**[2] **(M \$), 2016**	**Integral cost**[3] **of H_2 production (\$/T), 2016**	**Remark**
PSA COG	72	57	769	Desulphurisation unit not included in cost estimate. Additional column needed to remove H_2S, COS and hydrocarbons from COG
PSA+SMR COG	194	245	1226	CH_4 rich stream is obtained with a PSA used to separate H_2. Direct usage of COG in SMR not recommended due to high H_2 content (reverse reaction preferred)
WGS BOFG	85	93	1067	Desulphurisation unit not included in cost estimate.

Although there is high hydrogen production potential using steam methane reforming, it involves additional investments and is energy intensive, specially due to requirement of carbon capture system. For the intent of this study, due to relatively low capital investment and simpler process route, hydrogen separation from COG using PSA has been selected for estimation of production cost.

Tata Steel IJmuiden indicates that the capital cost of a 12 TPD hydrogen production unit using PSA is around €7 million to €13 million. The variable cost varies from €1100/ton to €1284/ton. Average values are used for this study. Table B.2 shows the reference economic data for hydrogen separation from COG using PSA.

Table B.2: Reference economics data for hydrogen separation from COG using PSA

Parameter	**Value**	**Units**	**Symbol**
Reference capacity	4088	ton/year	Cap_{ref}
Reference CAPEX	10	Million €	Inv_{ref}
Reference variable cost	1192	€/ton	VC_{ref}

Economy of scale is utilised in the estimation of CAPEX for any capacity using an exponential factor of 0.67[55].

$$Inv_{act} = Inv_{ref}\left(\frac{Cap_{act}}{Cap_{ref}}\right)^{0.67} \tag{B.1}$$

Fixed cost is assumed to be 20% of CAPEX[45][4] and is calculated as

$$FC_{act} = 0.2\frac{Inv_{act}}{Cap_{act}} \tag{B.2}$$

Variable cost includes raw material cost for PSA system and is linearly proportional to the system capacity. Hence variable cost per ton of hydrogen produced remains constant irrespective of capacity. Assuming a 10% depreciation, the production cost of hydrogen is calculated as [45]

$$PC_{H_2} = FC_{act} + VC_{ref} + 0.1\frac{Inv_{act}}{Cap_{act}} \tag{B.3}$$

---

[1] This is the total hydrogen production potential for the selected stream

[2] Reference capital cost data from L.Basye et al.(1997)[4] and M. Mann(1995)[32] have been scaled to required capacity using an exponential factor of 0.67. Figures have been converted to value in 2016 using Nelson Farrer indices for refinery inflation.

[3] Operating cost has been assumed to be 25% of total capital and an annual depreciation of 10% has been assumed.

[4] Please note that written permission needs to be obtained from Tata Steel, IJmuiden to access B. Ramani(2016)[45] due to confidentiality clause

C

POWER TO GAS DEMONSTRATION PLANTS

Table C.1: List of power to gas demonstration plants in Europe, March 2013

Source: Grond et al.(2013)[23]

Project owner	**Location**	**Installed capacity (kW)**	**Electrolysis technology**	**Product**	**Application**
Audi AG	Werlte, Germany	6.000	Alkaline	Methane	Gas grid - mobility
ITHER	Aragon, Sweden	4.000 + 70	Alkaline + PEM	Hydrogen	Mobility
E.ON AG	Falkenhagen, Germany	2.000	PEM	Hydrogen	Unknown
INGRID Project	Puglia region, Italy	1.200	Alkaline	Hydrogen	Gas grid
RH2 WIND Project Gruppe	Grapzow, Germany	1.000	Alkaline	Hydrogen	CHP & gas grid
Vattenfall	Hamburg, Germany	900	Alkaline	Hydrogen	Mobility
Enetrag AG	Prenzlau, Germany	500	Alkaline	Hydrogen	Unknown
Thuga & ITM Power	Frankfurt, Germany	360	PEM	Hydrogen	Gas grid
Electrochaea	Foulum, Denmark	250	PEM	Methane	Gas grid
DVGW & KIT	Karlsruhe, Germany	200	unknown	Methane	Gas grid
Sotavento Project	Xermade, Spain	200	Alkaline	Hydrogen	Engine
Stadt Herten & Evonic Industries	Herten, Germany	165	PEM	Hydrogen	Mobility
Unknown	Utsira, Norway	50	Alkaline	Hydrogen	Fuel cell & hydrogen turbine
Hidrolica Project	Tahivilla, Spain	40	PEM	Hydrogen	Fuel cell
Solar Fuel & Fraunhofer ZWS	Stuttgart, Germany	25	PEM	Methane	Gas grid
DNV KEMA	Groningen, The Netherlands	7	PEM	Methane	Gas grid

D

PROBABILITY CALCULATION

When dealing with normally distributed data, the probability of an occurrence can be estimated using a standard normal distribution table.

The following part is most relevant to Chapter 4.

The probability that electric power is available (imbalance is positive) at any given instant is given as

$$P(EP_{Imbal} > 0) = 1 - P(EP_{Imbal} < 0) \tag{D.1}$$

The Z value for any occurrence is given as

$$Z = \frac{x - \mu}{\sigma} \tag{D.2}$$

For the case considered in this study, μ=-5.94 MW and σ=68.33 MW. To find Z score for imbalance less than zero, equation D.2 is used with x=0 This gives Z score of 0.087. The probability of Z=0.087 is read from figure D.2 and corresponds to 53.59%. This is the probability of an imbalance being less than 0 ($P(EP_{Imbal} < 0)$). Using this value in equation D.1, we get $P(EP_{Imbal} > 0)$=46.41% To estimate the magnitude of positive imbalance lying within 75% of its range, the following equation is used

$$P(X) - P(EP_{Imbal} < 0) = 0.75(0.4641) \tag{D.3}$$

Substituting $P(EP_{Imbal} < 0)$=0.5359, value for P(X) is obtained as 0.8839. The corresponding Z value for this probability is read from D.2 as 1.19
The value of imbalance corresponding to this Z value is obtained using equation D.2 as 75.91 MW.

The following part is most relevant to section 8.1 The fraction of total electric power deficit that can be satisfied using a 100 MW gas turbine can be calculated as

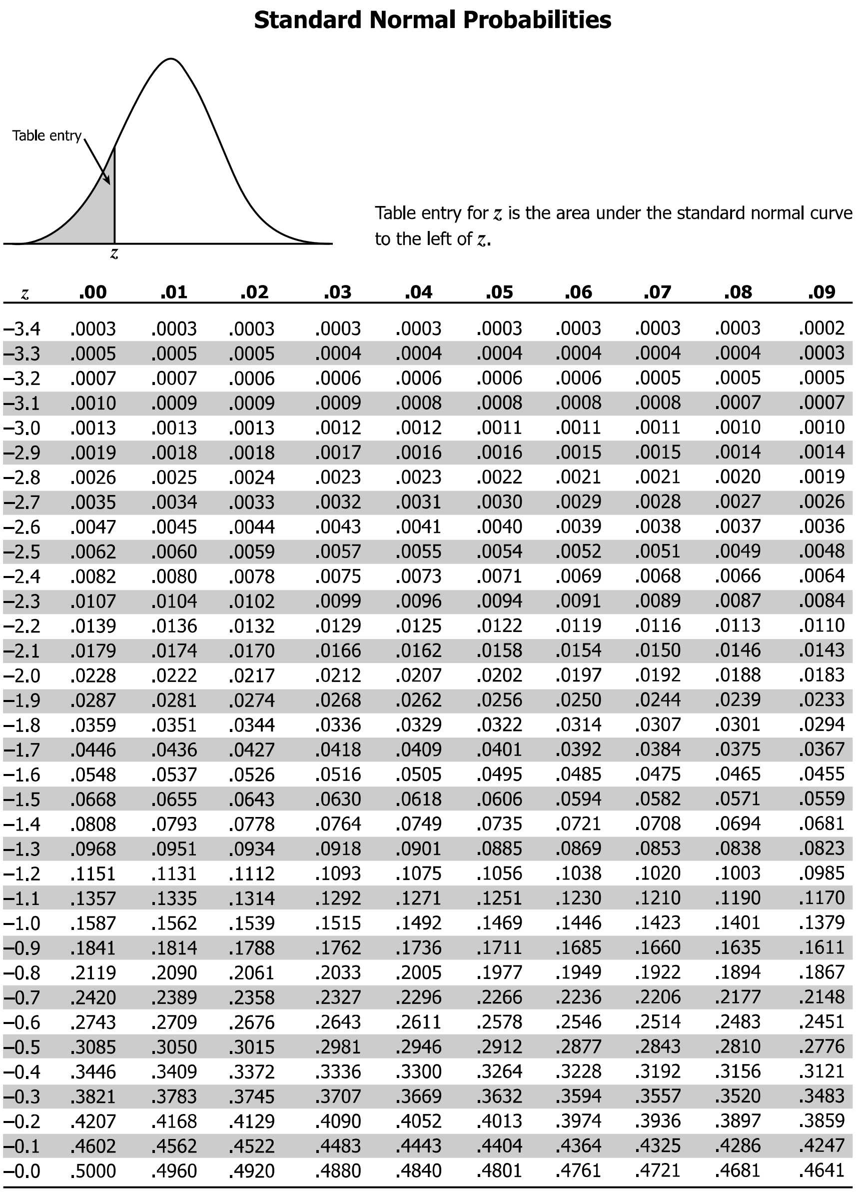
$$P(-100 < EP_{imbal} < 0) = \frac{P(EP_{imbal} < 0) - P(EP_{imbal} < -100)}{P(EP_{imbal} < 0))} \tag{D.4}$$

Z value to calculate $P(EP_{imbal} < -100)$ has been obtained by substituting x=-100, μ=-5.94 and σ=68.33 in equation D.2. The value of Z is -1.38 and the corresponding probability is read from figure D.1 as 0.0838. Substituting $P(EP_{imbal} < -100) = 0.0838$ and $P(EP_{imbal} < 0) = 0.5359$ (as calculated previously) in equation D.4,
$P(-100 < EP_{imbal} < 0) = 84.36\%$
This is the percentage of magnitude of deficit that can be satisfied using a 100 MW gas turbine.

Following a similar routine, the potential of several gas turbine capacities have been determined and summarised in table D.1

Table D.1: Potential of gas turbine capacity to satisfy electric power deficit

Gas turbine capacity, MW	**Z value**	**Magnitude of electric power deficit satisfied, %**
200	-2.84	99.57
175	-2.47	98.76
150	-2.11	96.80
100	-1.38	84.25
75	-1.01	71.07
50	-0.64	51.53
40	-0.50	42.66
30	-0.35	32.43
25	-0.28	27.45
20	-0.21	21.64
10	-0.06	11.24
5	0.01	5.25

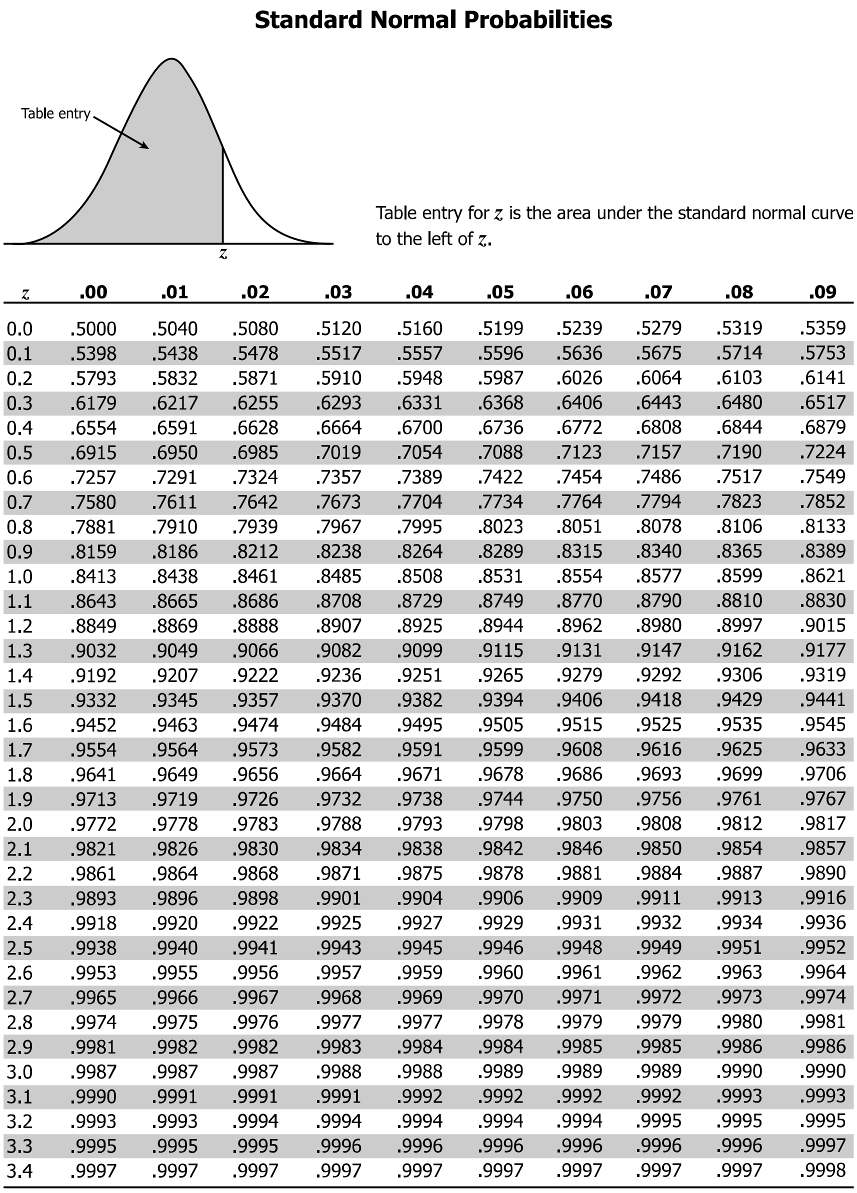


Standard Normal Probabilities

Table entry for z is the area under the standard normal curve to the left of z.

z	.00	.01	.02	.03	.04	.05	.06	.07	.08	.09
–3.4	.0003	.0003	.0003	.0003	.0003	.0003	.0003	.0003	.0003	.0002
–3.3	.0005	.0005	.0005	.0004	.0004	.0004	.0004	.0004	.0004	.0003
–3.2	.0007	.0007	.0006	.0006	.0006	.0006	.0006	.0005	.0005	.0005
–3.1	.0010	.0009	.0009	.0009	.0008	.0008	.0008	.0008	.0007	.0007
–3.0	.0013	.0013	.0013	.0012	.0012	.0011	.0011	.0011	.0010	.0010
–2.9	.0019	.0018	.0018	.0017	.0016	.0016	.0015	.0015	.0014	.0014
–2.8	.0026	.0025	.0024	.0023	.0023	.0022	.0021	.0021	.0020	.0019
–2.7	.0035	.0034	.0033	.0032	.0031	.0030	.0029	.0028	.0027	.0026
–2.6	.0047	.0045	.0044	.0043	.0041	.0040	.0039	.0038	.0037	.0036
–2.5	.0062	.0060	.0059	.0057	.0055	.0054	.0052	.0051	.0049	.0048
–2.4	.0082	.0080	.0078	.0075	.0073	.0071	.0069	.0068	.0066	.0064
–2.3	.0107	.0104	.0102	.0099	.0096	.0094	.0091	.0089	.0087	.0084
–2.2	.0139	.0136	.0132	.0129	.0125	.0122	.0119	.0116	.0113	.0110
–2.1	.0179	.0174	.0170	.0166	.0162	.0158	.0154	.0150	.0146	.0143
–2.0	.0228	.0222	.0217	.0212	.0207	.0202	.0197	.0192	.0188	.0183
–1.9	.0287	.0281	.0274	.0268	.0262	.0256	.0250	.0244	.0239	.0233
–1.8	.0359	.0351	.0344	.0336	.0329	.0322	.0314	.0307	.0301	.0294
–1.7	.0446	.0436	.0427	.0418	.0409	.0401	.0392	.0384	.0375	.0367
–1.6	.0548	.0537	.0526	.0516	.0505	.0495	.0485	.0475	.0465	.0455
–1.5	.0668	.0655	.0643	.0630	.0618	.0606	.0594	.0582	.0571	.0559
–1.4	.0808	.0793	.0778	.0764	.0749	.0735	.0721	.0708	.0694	.0681
–1.3	.0968	.0951	.0934	.0918	.0901	.0885	.0869	.0853	.0838	.0823
–1.2	.1151	.1131	.1112	.1093	.1075	.1056	.1038	.1020	.1003	.0985
–1.1	.1357	.1335	.1314	.1292	.1271	.1251	.1230	.1210	.1190	.1170
–1.0	.1587	.1562	.1539	.1515	.1492	.1469	.1446	.1423	.1401	.1379
–0.9	.1841	.1814	.1788	.1762	.1736	.1711	.1685	.1660	.1635	.1611
–0.8	.2119	.2090	.2061	.2033	.2005	.1977	.1949	.1922	.1894	.1867
–0.7	.2420	.2389	.2358	.2327	.2296	.2266	.2236	.2206	.2177	.2148
–0.6	.2743	.2709	.2676	.2643	.2611	.2578	.2546	.2514	.2483	.2451
–0.5	.3085	.3050	.3015	.2981	.2946	.2912	.2877	.2843	.2810	.2776
–0.4	.3446	.3409	.3372	.3336	.3300	.3264	.3228	.3192	.3156	.3121
–0.3	.3821	.3783	.3745	.3707	.3669	.3632	.3594	.3557	.3520	.3483
–0.2	.4207	.4168	.4129	.4090	.4052	.4013	.3974	.3936	.3897	.3859
–0.1	.4602	.4562	.4522	.4483	.4443	.4404	.4364	.4325	.4286	.4247
–0.0	.5000	.4960	.4920	.4880	.4840	.4801	.4761	.4721	.4681	.4641

Figure D.1: Standard normal probabilities



Standard Normal Probabilities

Table entry for z is the area under the standard normal curve to the left of z.

z	.00	.01	.02	.03	.04	.05	.06	.07	.08	.09
0.0	.5000	.5040	.5080	.5120	.5160	.5199	.5239	.5279	.5319	.5359
0.1	.5398	.5438	.5478	.5517	.5557	.5596	.5636	.5675	.5714	.5753
0.2	.5793	.5832	.5871	.5910	.5948	.5987	.6026	.6064	.6103	.6141
0.3	.6179	.6217	.6255	.6293	.6331	.6368	.6406	.6443	.6480	.6517
0.4	.6554	.6591	.6628	.6664	.6700	.6736	.6772	.6808	.6844	.6879
0.5	.6915	.6950	.6985	.7019	.7054	.7088	.7123	.7157	.7190	.7224
0.6	.7257	.7291	.7324	.7357	.7389	.7422	.7454	.7486	.7517	.7549
0.7	.7580	.7611	.7642	.7673	.7704	.7734	.7764	.7794	.7823	.7852
0.8	.7881	.7910	.7939	.7967	.7995	.8023	.8051	.8078	.8106	.8133
0.9	.8159	.8186	.8212	.8238	.8264	.8289	.8315	.8340	.8365	.8389
1.0	.8413	.8438	.8461	.8485	.8508	.8531	.8554	.8577	.8599	.8621
1.1	.8643	.8665	.8686	.8708	.8729	.8749	.8770	.8790	.8810	.8830
1.2	.8849	.8869	.8888	.8907	.8925	.8944	.8962	.8980	.8997	.9015
1.3	.9032	.9049	.9066	.9082	.9099	.9115	.9131	.9147	.9162	.9177
1.4	.9192	.9207	.9222	.9236	.9251	.9265	.9279	.9292	.9306	.9319
1.5	.9332	.9345	.9357	.9370	.9382	.9394	.9406	.9418	.9429	.9441
1.6	.9452	.9463	.9474	.9484	.9495	.9505	.9515	.9525	.9535	.9545
1.7	.9554	.9564	.9573	.9582	.9591	.9599	.9608	.9616	.9625	.9633
1.8	.9641	.9649	.9656	.9664	.9671	.9678	.9686	.9693	.9699	.9706
1.9	.9713	.9719	.9726	.9732	.9738	.9744	.9750	.9756	.9761	.9767
2.0	.9772	.9778	.9783	.9788	.9793	.9798	.9803	.9808	.9812	.9817
2.1	.9821	.9826	.9830	.9834	.9838	.9842	.9846	.9850	.9854	.9857
2.2	.9861	.9864	.9868	.9871	.9875	.9878	.9881	.9884	.9887	.9890
2.3	.9893	.9896	.9898	.9901	.9904	.9906	.9909	.9911	.9913	.9916
2.4	.9918	.9920	.9922	.9925	.9927	.9929	.9931	.9932	.9934	.9936
2.5	.9938	.9940	.9941	.9943	.9945	.9946	.9948	.9949	.9951	.9952
2.6	.9953	.9955	.9956	.9957	.9959	.9960	.9961	.9962	.9963	.9964
2.7	.9965	.9966	.9967	.9968	.9969	.9970	.9971	.9972	.9973	.9974
2.8	.9974	.9975	.9976	.9977	.9977	.9978	.9979	.9979	.9980	.9981
2.9	.9981	.9982	.9982	.9983	.9984	.9984	.9985	.9985	.9986	.9986
3.0	.9987	.9987	.9987	.9988	.9988	.9989	.9989	.9989	.9990	.9990
3.1	.9990	.9991	.9991	.9991	.9992	.9992	.9992	.9992	.9993	.9993
3.2	.9993	.9993	.9994	.9994	.9994	.9994	.9994	.9995	.9995	.9995
3.3	.9995	.9995	.9995	.9996	.9996	.9996	.9996	.9996	.9996	.9997
3.4	.9997	.9997	.9997	.9997	.9997	.9997	.9997	.9997	.9997	.9998

Figure D.2: Standard normal probabilities

E

EVALUATION OF DERIVED PRODUCTS FROM AMMONIA

Products derived from ammonia have been evaluated using relative scores ranging from 1 to 5. This evaluation helps to determine the apt product from Tata Steel's perspective. It should be noted that the scoring is relative. The following parameters are identified as key to evaluate products:

(a) Local consumption of ammonia for product: This parameter gives an indication of quantity of direct consumption of ammonia to obtain the final product. Data from Malveda et al.(2014)[31] has been used as a reference scale and it focuses on ammonia consumption in Western Europe. For cases where data was unavailable, a score of 2 has been set as default. A weight of 50% has been assigned to this parameter as it directly translates into ammonia production capacity.

(b) Technical maturity: This parameter compares the technological readiness level for producing the end product. All commercially available technologies are given a score of 5. Weight for this parameters is set to be low(5%) since almost all processes considered here are commercially available and no process has a significant advantage to offer in this field.

(c) Potential for utilisation of chemicals available at Tata Steel, IJmuiden: This parameter indicates the availability of chemical feedstock required to produce the end product. A score of 5 indicates all chemical feedstock needed for production is available at Tata Steel, IJmuiden. Lower score implies chemical feedstock from an external source is needed for production. A weight of 10% has been assigned to this parameter.

(d) Ease of regenerating ammonia: This parameter gives an indication of the reversibility of the production process. A higher score implies ammonia can be regenerated with fewer steps from the product. A weight of 5% has been set to this parameter. A higher flexibility ensures an easier transition of business focus from one product to another.

(e) Potential for carbon capture and utilisation (CCU) application: A higher score in this parameter implies more CO_2 is utilised per unit of ammonia. A score of 1 implies no CCU is possible. A weight of 5% has been assigned to this parameter.

(f) Process route simplicity: This parameter gives an indication of the number of process steps involved in production of the end product. Longer process steps are usually associated with higher equipment and energy costs. A higher score implies fewer process steps and a weight of 10% has been assigned here.

(g) Ease of storage, transport and handling: This parameter gives an indication of the phase of end product and its toxicity to human life and environment. A higher score implies product is easier to handle and transport and safer in general. A weight of 15% has been assigned here.

Each product has been evaluated using the mentioned weighted score. The result is summarised in table E.1. Products are arranged in descending order of scores. It is observed that urea, nitric acid and ammonium nitrate are the three most suitable products derived from ammonia and apt for Tata Steel IJmuiden. However, it should be noted that results are sensitive to the assigned weights. Secondly, selection of an application also depends heavily on the production capacity of ammonia. Products like urea, nitric acid and ammonium nitrate dominate the ammonia market and entering this competitive market would mean requirement of an industrial scale of ammonia plant. Niche applications of ammonia or derived products need to be identified for small scale ammonia production as in this study.

Table E.1: Evaluation of products derived from ammonia

		(a)	**(b)**	**(c)**	**(d)**	**(e)**	**(f)**	**(g)**	**Weighted average score**
	Weight assigned	0.5	0.05	0.1	0.05	0.05	0.1	0.15	
Sr no	Product								
1	Urea	4	5	5	4	3	4	5	4.3
2	Nitric acid	5	5	5	1	1	4	3	4.2
3	Ammonium nitrate	4	5	5	1	1	4	5	4.0
4	Ammonium sulphate	3	5	5	5	1	4	5	3.7
5	Ammonium (bi) carbonate	2	5	5	5	5	5	5	3.5
6	Formamide	2	5	5	5	5	5	4	3.4
7	Ammonium chloride	2	5	4	5	5	5	4	3.3
8	Sodium carbonate	2	5	4	1	5	5	5	3.2
9	Melamine	2	5	4	1	2	3	5	2.9
10	Hydrogen cyanide	2	5	5	2	5	4	1	2.7
11	Ammonium phosphates	1	5	4	5	1	4	5	2.6
12	Sulphonamides	2	5	2	1	1	2	5	2.5
13	Guanidine	2	3	4	1	2	2	4	2.5
14	Acrylonitrile	2	5	3	1	1	3	3	2.4
15	Caprolactum	2	5	2	1	1	1	5	2.4
16	Hexamethylenediamine	2	5	2	1	1	2	4	2.4
17	Polyurethane	2	5	1	1	1	1	5	2.3
18	Pyridines	2	5	2	1	1	2	3	2.2
19	Amines	1	5	4	1	1	3	3	2.0

As a supplementary study, the CCU potential using WAG has been evaluated for several derived products of ammonia. Table E.2 summarises the results. All numbers are based on stoichiometry.

Table E.2: CCU potential of products derived from ammonia via WAG

Sr no	Product	Source of H2	H2 potential (TPH)	NH3 potential (TPH)	Product potential (TPH)	CO2 generated in H2 production (TPH)	CO2 utilised (TPH)	CCU potential (%)
1	Urea	H2 in COG	3.0	17.1	30.1	0.0	22.1	1.6
		CH4 in COG	5.1	28.7	50.7	27.9	37.2	2.7
		BOFG via WGSR	3.5	20.0	35.3	77.8	25.9	1.9
2	Ammonium bicarbonate	H2 in COG	3.0	17.1	79.3	0.0	44.2	3.2
		CH4 in COG	5.1	28.7	133.5	27.9	74.4	5.4
		BOFG via WGSR	3.5	20.0	93.1	77.8	51.8	3.7
3	Sodium bicarbonate	H2 in COG	3.0	17.1	84.3	0.0	44.2	3.2
		CH4 in COG	5.1	28.7	142.0	27.9	74.4	5.4
		BOFG via WGSR	3.5	20.0	99.0	77.8	51.8	3.7
4	Ammonium chloride	H2 in COG	3.0	17.1	53.7	0.0	44.2	3.2
		CH4 in COG	5.1	28.7	90.4	27.9	74.4	5.4
		BOFG via WGSR	3.5	20.0	63.0	77.8	51.8	3.7
5	Hydrogen cyanide	H2 in COG	3.0	17.1	27.1	0.0	44.2	3.2
		CH4 in COG	5.1	28.7	45.6	27.9	74.4	5.4
		BOFG via WGSR	3.5	20.0	31.8	77.8	51.8	3.7
6	Melamine	H2 in COG	3.0	17.1	10.5	0.0	11.0	0.8
		CH4 in COG	5.1	28.7	17.8	27.9	18.6	1.3
		BOFG via WGSR	3.5	20.0	27.3	77.8	13.0	0.9
7	Guanidine nitrate	H2 in COG	3.0	17.1	30.6	0.0	11.0	0.8
		CH4 in COG	5.1	28.7	51.6	27.9	18.6	1.3

Table E.2: CCU potential of products derived from ammonia via WAG

Sr no	**Product**	**Source of H2**	**H2 potential (TPH)**	**NH3 potential (TPH)**	**Product potential (TPH)**	**CO2 generated in H2 production (TPH)**	**CO2 utilised (TPH)**	**CCU potential (%)**
		BOFG via WGSR	3.5	20.0	36.0	77.8	13.0	0.9
8	Formamide	H2 in COG	3.0	17.1	45.2	0.0	44.2	3.2
		CH4 in COG	5.1	28.7	76.1	27.9	74.4	5.4
		BOFG via WGSR	3.5	20.0	53.0	77.8	51.8	3.7

F

ASPEN HYSYS MODEL FOR AMMONIA SYNTHESIS LOOP

The process scheme for ammonia synthesis used in this study is obtained from the ASPEN®HYSYS model shown in figure F.1. This particular process scheme is for an ammonia production of about 2 tonnes per hour. The scope of this process scheme begins from the mixed feed stream of hydrogen and nitrogen and ends at final ammonia product to storage. Table F.1 indicates the main components used in the ASPEN®HYSYS model. Some key stream data is shown in table F.2.

Feed hydrogen and nitrogen streams from the electrolyser and air separation unit respectively are mixed and compressed from 8 bar(a) to 296.5 bar(a). It passes through the recycle compressor C-101 along with unreacted feed from the reactor and unseparated ammonia from the high pressure separator V-101 to the ammonia synthesis reactor CRV-100. This is designed as a fixed conversion reactor with a single pass conversion of 22.5%. Due to the exothermic nature of ammonia synthesis, the condenser E-101 is required to operate with a heat load of about 2210 kW to cool the reactor outlet stream to 40 °C. The purge to recycle ratio employed in this process scheme is 0.005. The purge stream has about 68% of hydrogen content and 10% ammonia (mole basis). Usually a scrubber system is employed to absorb ammonia leaving behind a high hydrogen content stream. This may be used as a fuel in an application in the vicinity of the ammonia synthesis plant or purified further to be used as feedstock for ammonia synthesis again. Ammonia separators operate at two pressure levels of 293.5 bar(a) and 41 bar(a) to ensure maximum separation of ammonia. The recycle compressor C-101 has a mass flow rate which is almost 5.3 times higher than feed compressor C-100 and compensates for the pressure drop across the reactor, condenser and the high pressure separators. This is estimated to be close to 3 bar. The final ammonia product is obtained at the outlet of the low pressure separator V-102 with a purity of 99.69% (mole basis). Hydrogen and nitrogen are the impurities in dissolved state.

Table F.1: Main equipments in ammonia synthesis loop

Tag	**Equipment**
Compressor C100	Feed compressor
CRV-100	Ammonia synthesis reactor
E-101	Condenser
C-101	Recycle compressor
V-100/V-101	High pressure separator
V-102	Low pressure separator

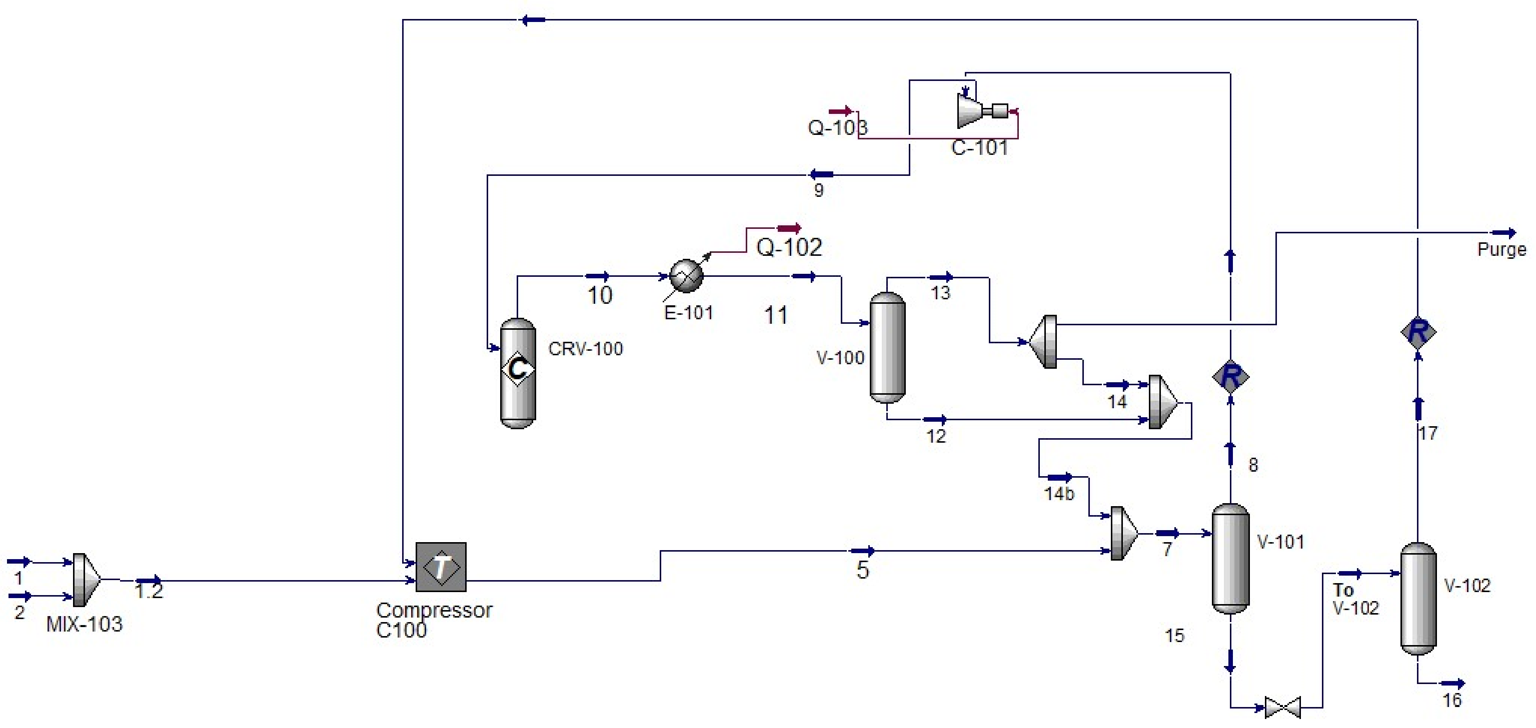
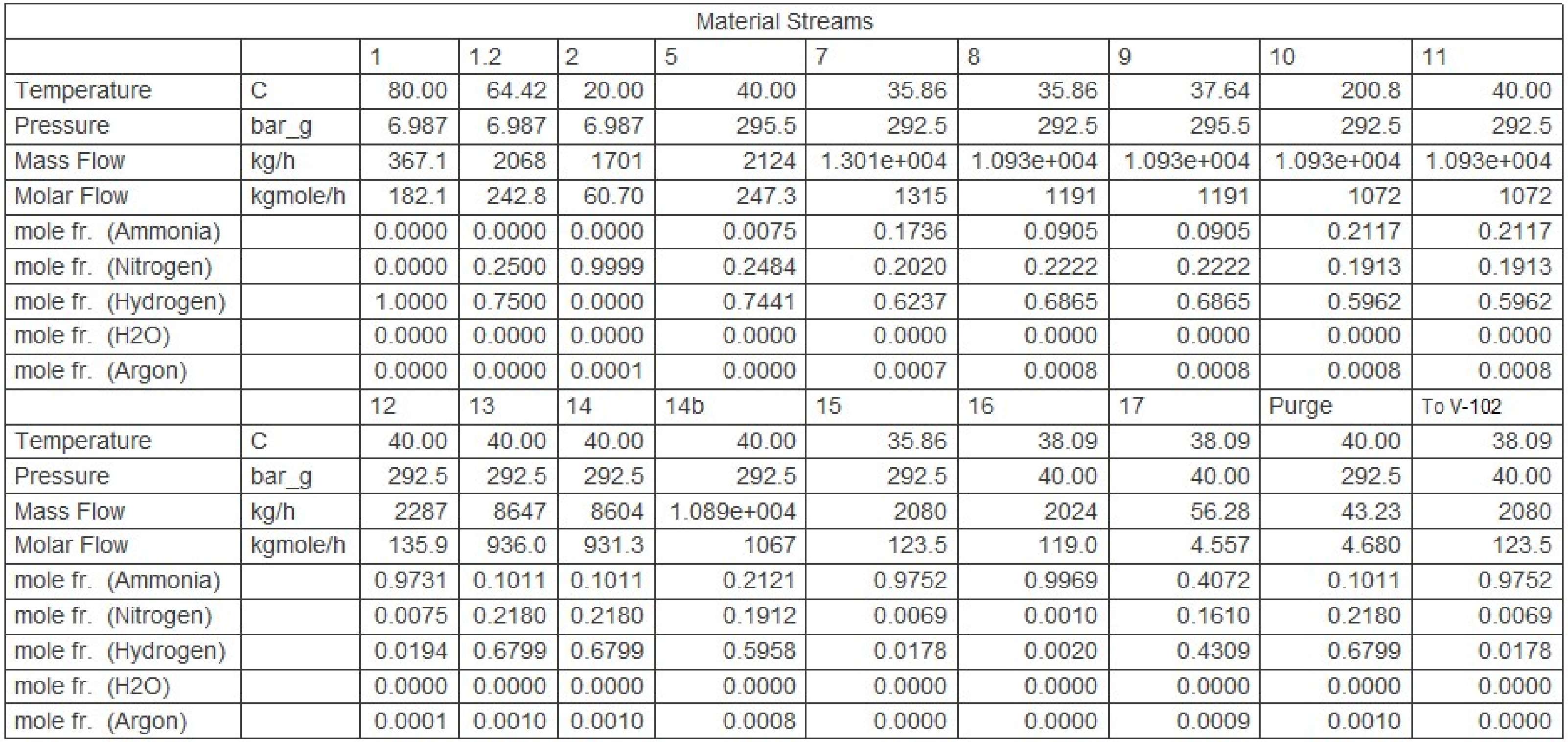


Figure F.1: Process scheme for ammonia synthesis loop

Table F.2: Stream data in ammonia synthesis loop



		Material Streams								
		1	1.2	2	5	7	8	9	10	11
Temperature	C	80.00	64.42	20.00	40.00	35.86	35.86	37.64	200.8	40.00
Pressure	bar_g	6.987	6.987	6.987	295.5	292.5	292.5	295.5	292.5	292.5
Mass Flow	kg/h	367.1	2068	1701	2124	1.301e+004	1.093e+004	1.093e+004	1.093e+004	1.093e+004
Molar Flow	kgmole/h	182.1	242.8	60.70	247.3	1315	1191	1191	1072	1072
mole fr. (Ammonia)		0.0000	0.0000	0.0000	0.0075	0.1736	0.0905	0.0905	0.2117	0.2117
mole fr. (Nitrogen)		0.0000	0.2500	0.9999	0.2484	0.2020	0.2222	0.2222	0.1913	0.1913
mole fr. (Hydrogen)		1.0000	0.7500	0.0000	0.7441	0.6237	0.6865	0.6865	0.5962	0.5962
mole fr. (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
mole fr. (Argon)		0.0000	0.0000	0.0001	0.0000	0.0007	0.0008	0.0008	0.0008	0.0008
		12	13	14	14b	15	16	17	Purge	To V-102
Temperature	C	40.00	40.00	40.00	40.00	35.86	38.09	38.09	40.00	38.09
Pressure	bar_g	292.5	292.5	292.5	292.5	292.5	40.00	40.00	292.5	40.00
Mass Flow	kg/h	2287	8647	8604	1.089e+004	2080	2024	56.28	43.23	2080
Molar Flow	kgmole/h	135.9	936.0	931.3	1067	123.5	119.0	4.557	4.680	123.5
mole fr. (Ammonia)		0.9731	0.1011	0.1011	0.2121	0.9752	0.9969	0.4072	0.1011	0.9752
mole fr. (Nitrogen)		0.0075	0.2180	0.2180	0.1912	0.0069	0.0010	0.1610	0.2180	0.0069
mole fr. (Hydrogen)		0.0194	0.6799	0.6799	0.5958	0.0178	0.0020	0.4309	0.6799	0.0178
mole fr. (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
mole fr. (Argon)		0.0001	0.0010	0.0010	0.0008	0.0000	0.0000	0.0009	0.0010	0.0000

G

LEVELISED COST OF AMMONIA

Levelised cost is a term used frequently to compare alternative forms of energy generation. Levelised cost of production and levelised cost of energy are the two variants used when used in connection to the energy industry. In this study, levelised cost of production is more relevant and is coined as levelised cost of ammonia(LCOA).

LCOA takes into account the time value of money. This is the advantage LCOA has over basic production cost. LCOA can be understood as the average cost of ammonia that would be needed to break even at the end of plant lifetime. Comparing LCOA with market price of ammonia provides an indication of the economic feasibility of the plant. A simplified equation to calculate LCOA is:

$$LCOA = \frac{NPV_{system}}{\text{Total ammonia produced in plant lifetime}} \tag{G.1}$$

The Net Positive Value (NPV) of the system is calculated using the relation[34]:

$$NPV_{System} = P_d + P_a.Y\left(\frac{1}{1+r}, N\right) + OC_T.Y\left(\frac{1+i}{1+r}, L\right) \tag{G.2}$$

Where

$$Y(k,l) = \sum_{j=1}^{l} k^j = \begin{cases} \frac{k-k^{l+1}}{1-k} & k \neq 1 \\ l & k = 1 \end{cases} \tag{G.3}$$

N is the loan life period,
L is the plant life period,
P_d is the downpayment on the system,
OC_T is the total operating cost of the system,
r is the discount rate. Unlike the interest rate, the discount rate not only takes into account the time value of money, but also the uncertainty of future cash flows.
i is the inflation rate,
P_a is the annual payment. This term is calculated using the following relation[34]:

$$P_a = (C_c - P_d)CRF \tag{G.4}$$

Where C_c is the total capital cost of the system, CRF is the Capital Recovery Factor and calculated using the equation[34]

$$CRF = \begin{cases} \frac{b}{(1-(1+b)^{-N})} & b \neq 0 \\ \frac{1}{N} & b = 0 \end{cases} \tag{G.5}$$

Where b is the interest rate for the loan

H

CLASSIFICATION OF ENERGY STORAGE TECHNOLOGIES

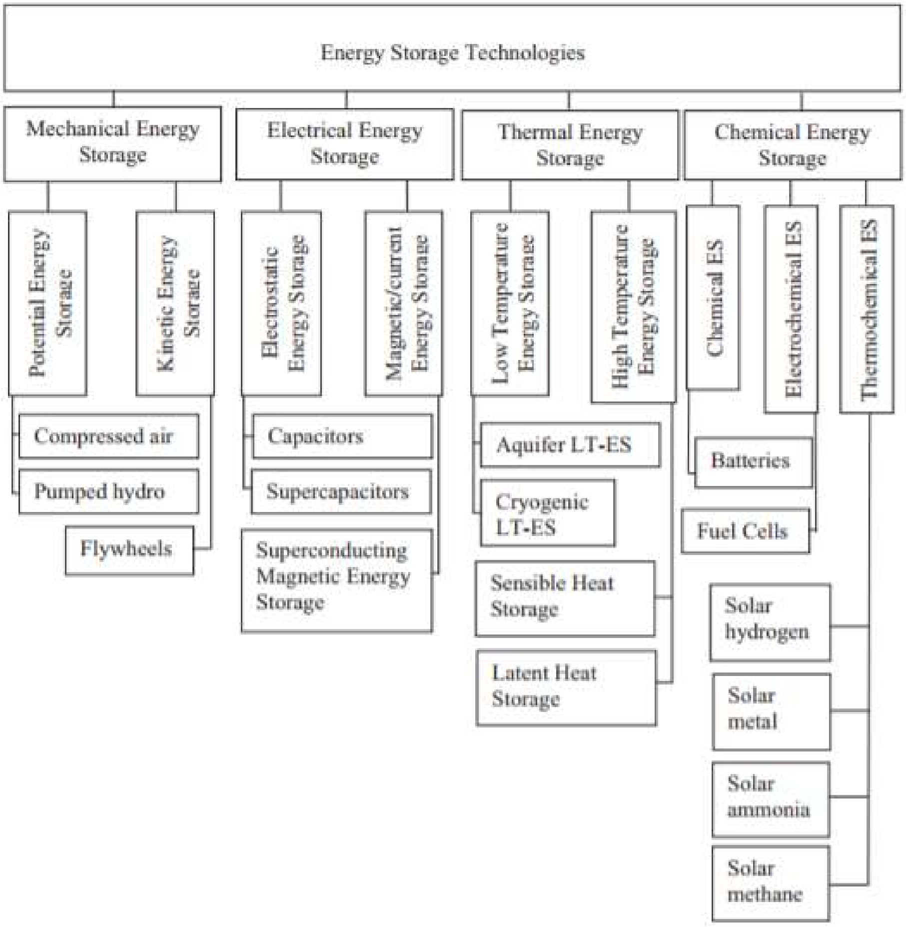


Figure H.1: Classification of energy storage technologies

Source: A.Evans et al. (2012)[18]