Analysing and optimizing the value of a Hybrid renewable power plant with Green Ammonia production.

Green Ammonia formulation in Energy management system.

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Summary

Although the percentage share of renewable energy in the global energy landscape is increasing rapidly and consistently breaking records for annual installation, there is still a need for tripling up of renewable energy capacity by 2030.The costs and prices of renewable energy declining year by year, this is one of the key reasons for the shrinking of profits for renewable power developers(RPDs). Different strategies can be adopted by the renewable developers to increase revenues like improving financing costs, making multiple revenue streams for individual renewable assets etc.This creates an opportunity for P2X technologies which are becoming popular due to their ability to facilitate the integration of different energy sectors like electricity and hard-to-abate sectors.The design of a Hybrid power plant(HPP) is a complex problem that combines different assets to maximize the value of the power plant.Researchers at the Technical University of Denmark(DTU) are in the process of developing an open-source tool called HyDesign.According to desktop research, it was understood before HyDesign that no other open-source HPP sizing tool in the market could size and optimize the P2X designs.

The purpose of this thesis study is to analyze how can RPDs improve their economic value by coupling with green ammonia(GNH3) production using HyDesign.The quantitative data is collected through the literature research and qualitative data is collected through attending various conferences and industrial events.This study chooses the most prominent and proven technology which existed for more than a century now called the Haber bosch process.Haber bosch(HB) process of ammonia production is modelled in this study.Around 30+ industrial professionals were interviewed to entrepreneurially validate TUDelft's patented methodology of the Green Haber Bosch process.These interviews also provided reliable qualitative data for this study.Since there is no reference, open-source green ammonia model, modelling checks were developed in this study to verify the functioning of the model and increase confidence in the reliability of the results.Site selection hypothesis was also made for hybrid renewable power plants.For a single site data in the HyDesign data repository, evaluation results yielded that the revenue of HPP+GNH3 is more than the HPP.However, various financial metrics like LCOA, LCOE,NPV/Capex and NPV were more for the HPP than HPP+GNH3, this is due to the huge technology costs of the GNH3 plants and the lack of economies of scale of such new plants.

One-factor-at-a-time(OFAT) sensitivity analysis approach is used in this study to analyze value addition and its source for improving various financial metrics of HPP+GNH3.This sensitivity results also can be generalized for other sites.Increasing solar capacity will improve metrics like LCOE, NPV/Capex, and NPV.Increasing wind improves the LCOA and ammonia production.Increasing electrolyzer capacity will also improve NPV/Capex and ammonia production since all mass productions in the HPP+GNH3 system are dependent on the electrolyser capacity. Increasing battery will also improve a few of these 4 metrics but not to the extent of increasing solar,wind and electrolyser capacity.These results of the OFAT sensitivity analysis is also checked with HyDesign's existing surrogate-based efficient global optimization(EGO) algorithm.For a specific financial metric as an objective function in the EGO algorithm, both OFAT sensitivity analysis results and the existing EGO algorithm does the same actions.The study finds that building a large-scale HPP+GNH3 system is beneficial for RPDs and to society which yields better financial benefits and more green ammonia production which can be used in many hard-to-abate sectors.

Contents

Nomenclature

Abbreviations

Abbreviation	Definition
AEM	Anion Exchange Membrane
AI	Artificial Intelligence
Atm	Atmosphere
BESS	Battery Energy Storage System
BP	Boiling Point
BOO	Build Own Operate
BSP	Balancing Service Provider
CCUS	Carbon Capture Utilization And Storage
CSV	Comma Separated Value
CUF	Capacity Utilization Factor
DOE	Design Of Experiment
DTU	Technical University Of Denmark
EA	Environmental Assessment
EE	Electrical Energy
EGO	Efficient Global Optimization
EMS	Energy Management System
ESS	Energy Storage System
FID	Final Investment Decision
GH2	Green Hydrogen
GNH3	Green Ammonia
HB	Haber Bosch Process
HHV	Higher Heating Value
HOMER	Hybrid Optimization Model For Electric Renewables
HOPP	Hybrid Optimization Of Power Plants
HPP	Hybrid Power Plant
iHOGA	Improved Hybrid Optimization By Genetic Algorithms
IREDA	Indian Renewable Energy Development Agency
LCOE	Levelized Cost Of Energy
LHV	Lower Heating Value
MC	Modeling Check
MHOGA	Mega Watt Hybrid Optimization By Genetic Algorithms
MP	Melting Point
Mt	Million Tonnes
MTPA	Million Tonnes Per Annum
MTPD	Metric Tonnes Per Day
NASA	National Aeronautics And Space Administration
NG	Natural Gas
NREL	National Renewable Energy Laboratory
OFAT	One Factor At A Time
OpenMDAO	Open Multidisciplinary Design Analysis And Optimization
P2X	Power To X
PEM	Proton Exchange Membrane
PLF	Plant Load Factor

Abbreviation	Definition
PMS	Power Management System
PPA	Power Purchase Agreement
PV	Photo Voltaic
R&D	Research And Development
RE	Renewable Energy
REDDAP	Renewable Dynamic Distributed Ammonia Plant
REOpt	Renewable Energy Optimization
RPD	Renewable Power Plant Developers
SOEC	Solid Oxide Electrolysis Cell
TPA	Tonnes Per Annum
TRL	Technology Readiness Level
TUD	Technical University Of Delft
Vol%	Volume Percentage
WT	Wind Turbine
XDSM	Extended Design Structure Matrix

Chemical Compounds	
CH_3OH	Methanol
CO	Carbon Monoxide
CO_2	Carbon Dioxide
H_2	Hydrogen
N_2	Nitrogen
NH_3	Ammonia

Units	
Bar	Unit Of Pressure
Hr	Hour
J	Joule
Kg	Kilogram
kWh	Kilowatt Hour
GWh	Gigawatt Hour
MPa	Mega Pascal
mol	Mole
MW	Mega Watt
MWh	Mega Watt Hour
Pascal	Unit Of Pressure

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Introduction

1.1. Background

The percentage share of renewable energy in the global energy landscape is increasing rapidly, consistently breaking records for the annual installation(International Energy Agency, 2024b). This change is driven by rapidly declining costs and increasingly ambitious government and multilateral policies set to grow at an increasing pace. The collective goal of the Paris Climate Agreement was to keep global warming below $2°$C while pursuing efforts to limit the warming to $1.5°$C. International Energy Agency(IEA) and International Renewable Energy Agency(IRENA) forecast that to achieve the $1.5°$C goal, the world requires at least 3 times more renewable energy at least by 2030 in comparison with 2023(COP28 UAE, 2023).

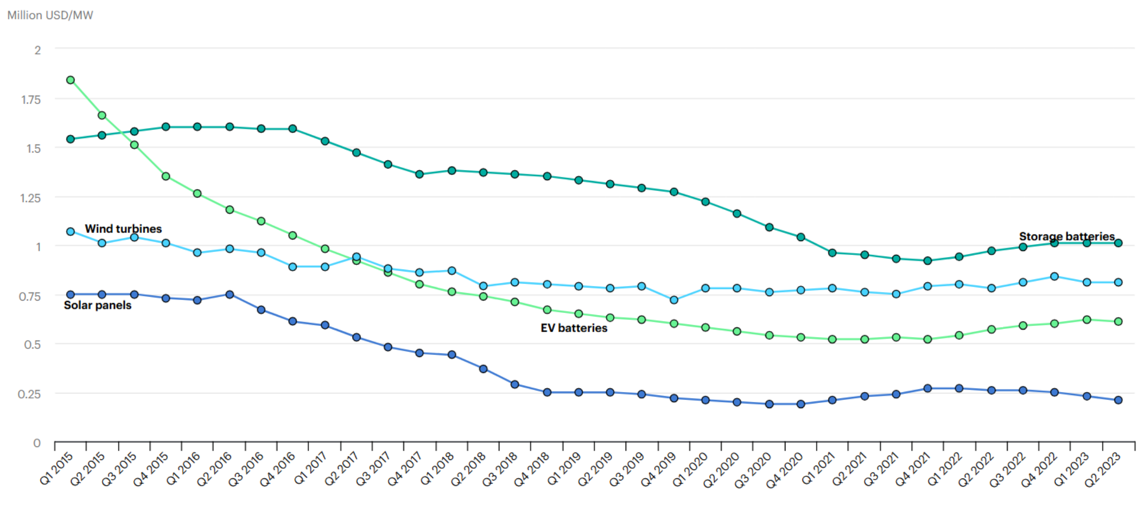


Figure 1.1: Average producer price for selected technologies from Q1 2015 to Q2 2023 (International Energy Agency (IEA), 2023)

Renewable energy developers(RPD) play a crucial role in achieving this energy transition. With the rapidly declining costs of renewable energy shown as buying price of renewable energy equipment for a RPD in Figure 1.1 and also selling price per MWh of electricity shown in Figure 1.2 the profit margins are shrinking.There are also other reasons like huge competition, rising inflation after COVID-19 and supply chain issues etc(Maloney, 2024). Different strategies can be adopted by the renewable developers to increase the revenues like improving financing costs, making multiple revenue streams for individual renewable assets, combining production outputs from different plants in the portfolio to leverage the complementarity of assets, and also entering different energy markets etc.

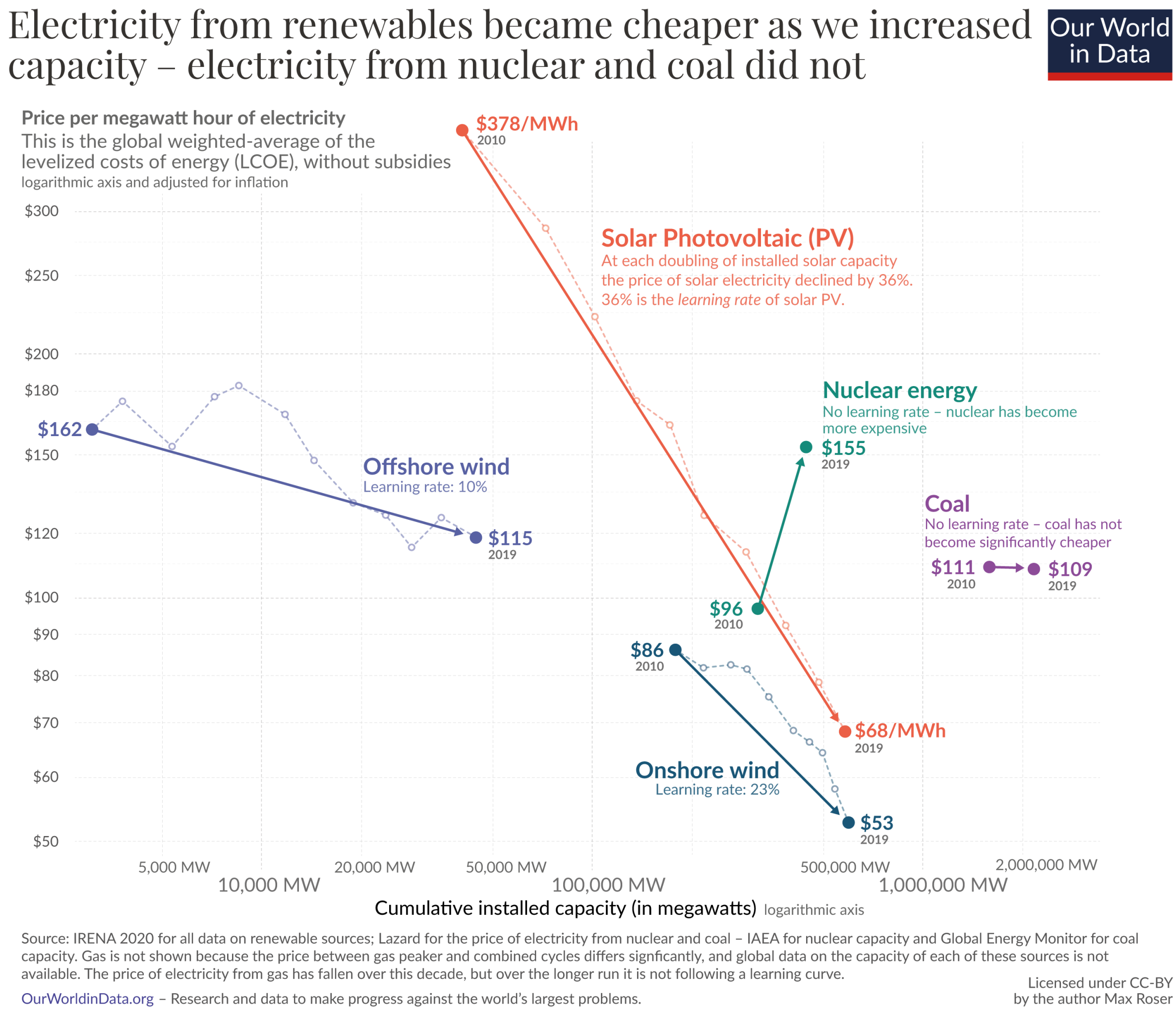


Figure 1.2: Global weighted average LCOE for different renewable technologies (Ritchie et al., 2023)

This leads to a paradigm shift in design objectives of wind and solar plants from producing energy at the lowest levelised cost of energy(LCOE), to other objectives to maximize profitability from other revenue streams associated with time-varying energy pricing, ancillary service and capacity markets. Wind, solar, and storage technologies can take part in a limited way in some of these markets today but, because of their uncertainty and variability, not to the same degree as traditional power plants. To operate these individual renewable energy plants as a traditional power plants in terms of capacity value, dispatchability, ancillary services and reliability and also to benefit from maximising their profit from different revenue streams at the asset level, developers design hybrid power plants(HPP) that combine wind, solar, storage and other renewable technologies together. This results in increasing interest in utility-scale renewable hybrid power plants(HPP)(Deign, 2023). There is a definite need for comparison of different possible hybrid renewable plants for future demanding energy markets.

Along with adding extra capacity of renewable energy in the global energy landscape, it is also important to search for solutions to turn the hard-to-abate sectors to have a net zero or negative carbon footprint. This gives an opportunity to renewable energy developers to generate extra revenue for their renewable assets and also improve their footprints in different industrial sectors.

Power to X(P2X) technologies are becoming more and more popular for a number of reasons like their usage as a long-term energy storage option to solve the intermittency of renewable energy sources.P2X technologies facilitate the integration of different energy sectors like electricity and hard-to-abate sectors like transport, industry and heating.P2X provides an alternative to coal, oil & gas for Energy security and it also contributes to a circular economy through synthetic fuels that are converted back to electricity.

X in P2X can be anything based on end-use, but an often most preferred first step is to produce hydrogen which is called Green H2(GH2) because it comes from green power. Hydrogen is the most preferred X because of its Energy density, market maturity in industrial processes since the last few decades and its versatility as an energy carrier in various industrial sectors. The gravimetric energy density(MJ/kg) of hydrogen is almost 3 times more than gasoline, diesel and natural gas, but Volumetric energy density(MJ/L) is almost 4 times less than the rest mentioned above(Wikipedia, as accessed in e.g. 2022). There are a few infrastructure challenges in handling gaseous hydrogen. Electrolysis is the most used and matured (high-technology readiness level(TRL)) production way of GH2. The storage and transportation challenges like handling gaseous H2, expensive liquification of gaseous H2, leakage issues and lack of maturity of liquid containers and gaseous storage tanks can be solved by converting GH2 to another energy carrier which can be a feasible solution to these problems.

Hydrogen can make a key contribution to the global decarbonization target due to its capability in sector coupling. Hydrogen's role in the energy transition can be shown in Figure 1.3.In 2023 total global hydrogen production was around 97Mt(International Energy Agency, 2024a). Out of which 66.5% are from natural gas called Grey hydrogen, and 20% from coal black or brown hydrogen depending on the type of coal. Out of the remaining 13.5%, a very small share is of the GH2.

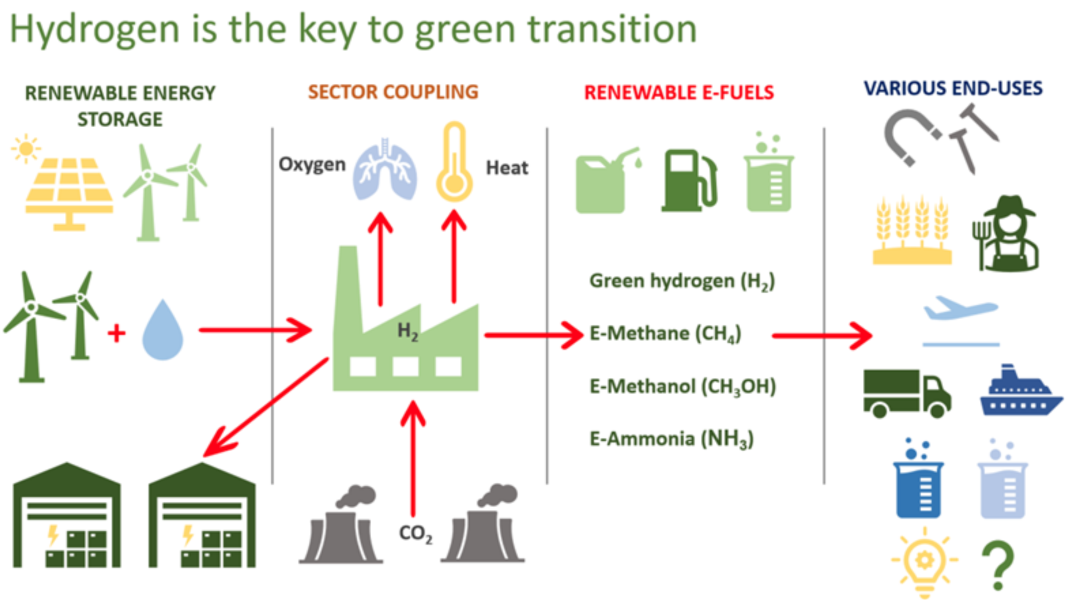


Figure 1.3: Hydrogen in energy transition (Plit, 2022)

To increase the share of Green H2 and to meet the climate goals, over the years a number of investments have been announced in the Hydrogen space and these numbers are increasing and also the number of investments which have to be turned into Financial investment decisions(FIDs) are increasing. This can be clearly seen in Figure 1.4.

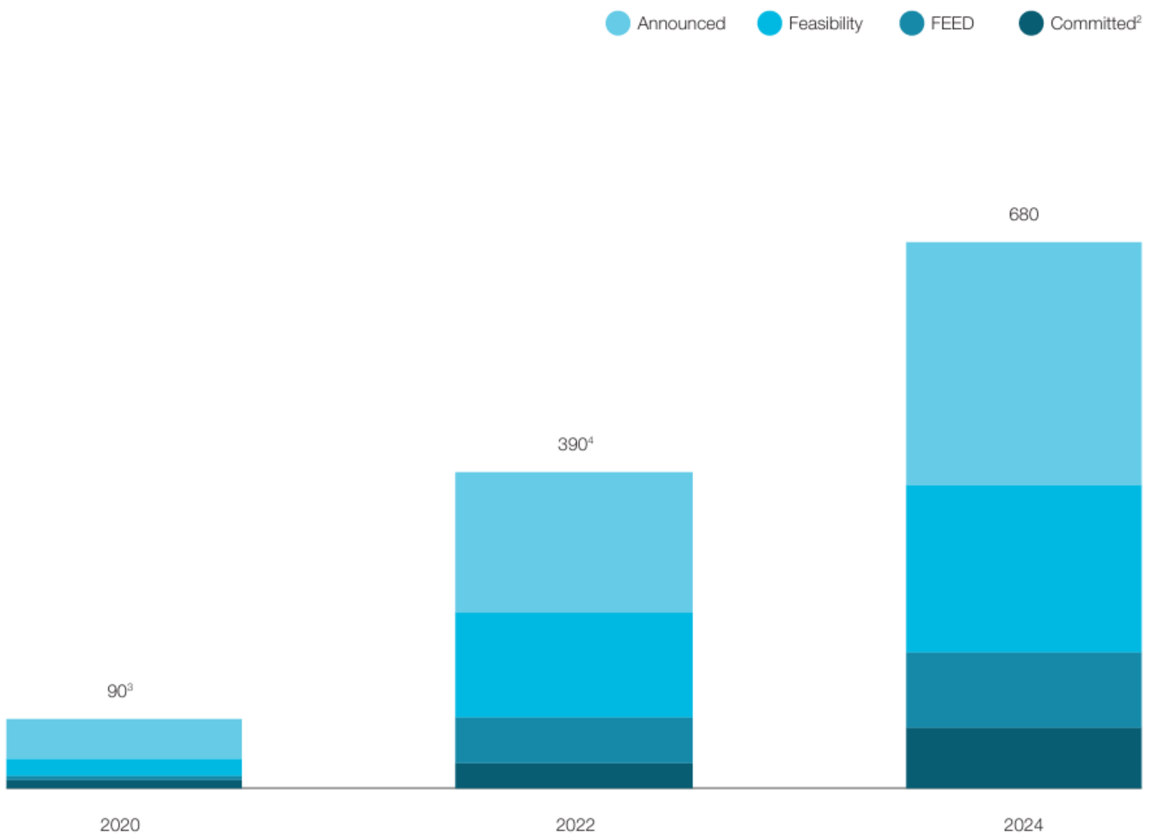


Figure 1.4: Total investments in GH2 projects in USD billion (Hydrogen Council, 2024)

Green Hydrogen can be converted or synthesized into other energy carriers, these can be referred to in Figure 1.5. GH2 when refined with either nitrogen for Green Ammonia or Carbon dioxide(CO2) for e-methanol,e-methane and e-kerosene. Green Ammonia(GNH3) and Green Methanol(GCH3OH) are predominantly becoming popular due to their growing interest in the energy market.

Green Ammonia(GNH3):- Ammonia has a high hydrogen content by weight with approximately 17.6% hydrogen by mass.Conventionally ammonia is produced by the well-established Haber Bosch(HB) process which is energy intensive. And during its green ammonia production, there is no carbon footprint. Boiling point is $-33.34°$C(Wikipedia contributors, 2023) and melting point is $-77.70°$C°C(Wikipedia contributors, 2023). Ammonia has disadvantages due to its toxic nature and risk of NOx emissions in the production process. Ammonia cracking technologies still need to become efficient and cost-effective.

Out of various energy carriers of hydrogen shown in Figure 1.5, GNH3 is chosen for this study since it has favourable physical properties, liquid ammonia's volumetric energy density is 50% greater than that of liquid hydrogen and it is already traded globally.Consequently, 87% of planned hydrogen export capacity aims to ship hydrogen in the form of ammonia(Bloomberg Carbon Transition Coalition, 2023).

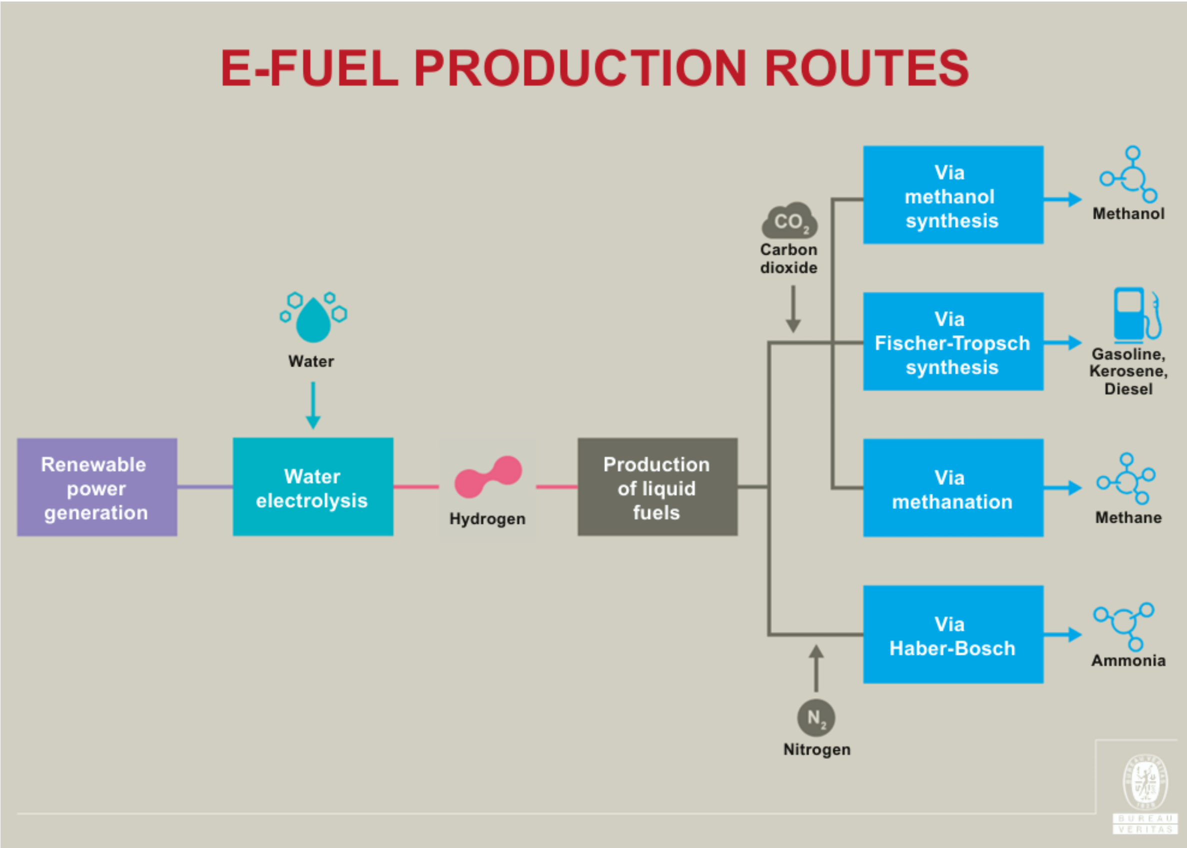


Figure 1.5: E-fuel production routes (Bureau Veritas Marine & Offshore, 2023)

1.2. Problem analysis

Investments in GH2 developments, including further conversion into ammonia, require tools for detailed analysis. Such tools also help renewable energy developers to assess their own benefit in such projects for better decision-making.

Existing HPP design tools are analysed based on the information available openly on their websites.Table 1.1 is a summary of all analyzed tools. It can be clearly seen that most of the tools do not have the capability of analysing the technical and economic aspects of chemical plants for P2X evaluation. In the Table 1.1 all the commercial software like GE FLEXIQ,DNV Solar farmer,DNV Wind farmer, Homer-Pro, Homer-Front and Univeristy of Zaragoza's iHoga/Mhoga are not open source software, which restricts the effective contribution to them by general public.Out of the open source software, NREL's HOPPand REOpt does not have the capability to work on multiple time frames and to do P2X analysis.

This creates a requirement to develop tools that are capable of analyzing, designing and optimizing the HPP interaction with Green NH3, to better understand the value addition of the Green NH3 to the HPP developers and also in the Global energy investments ecosystem.

HyDesign

The design of an HPP is a complex problem that combines different assets to maximize the value of the power plant. The design and operational aspects of such a system have been the subject of numerous research. Sizing, physical design, and operational strategies are the main aspects that should be included in a tool for the design and operation of HPPs(Das et al., 2022).

The design of HPPs starts with the sizing of different components like PVs, WTs, ESS, etc, followed by physical interactions between these assets and electrical collection systems. Lastly, Operation and control of the HPP consist of an Energy management system(EMS) and a Power management system(PMS). Along with these 3 steps, the design must be capable of handling the non-linearities of different technologies, forecasting uncertainties at all levels, and also scalable to different energy markets(Das et al., 2022). Although many tools have been developed for either larger hybrid systems, microgrid applications or individual technology plants shown in Table 1.1 there is definitely a requirement for new tools with capabilities which that are specific to utility-scale hybrid power plants.

The researchers at the **Technical University of Denmark(DTU)** are in the process of developing an open-source tool called "**HyDesign**" for the design and operation of utility-scale renewable hybrid plants to meet the unmet needs. The latest version of the HyDesign(V1.4.1) tool has Solar, Wind, BESS(Li-ion), and basic Green H2 models in it.

Features	NREL HOPP	FLEXIQ	DNV Solar & Wind farmer	REopt REOpt	Homer-PRO	Homer-Front	iHOGA / MHOGA	HyDesign
Physical & Electrical Infrastructure Design	✔	✔	✔	✘	✔	✔	✔	✔
Interactions between multiple technologies	✔	✔	✘	✔	✔	✔	✔	✔
Opensource software	✔	✘	✘	✔	✘	✘	✘	✔
Microgrids	✔	✔	✔	✔	✔	✘	✔	✔
Enhanced by AI	✘	✘	✘	✘	✘	✘	✘	✘
Different Electricity markets	✘	✔	✘	✘	✘	✔	✔	✔
Forecast Uncertainties	✘	✔	✘	✘	✔	✔	✘	✔
Multiple timeframes	✘	✔	✔	✘	✔	✔	✔	✔
P2X	✘	✘	✘	✘	✘	✘	✔	✔

Table 1.1: Comparison of a few HPP Design Softwares[1].

1.3. Research questions

After understanding the capabilities of the HyDesign platform and analyzing the needs for P2X in the energy transition, particularly in the case of hybrid renewable plants and renewable plant developers, research objectives are formulated for this study are listed below.

Main research question:

How can the value(economic benefits) of utility-scale HPP be optimized by coupling with the production of energy carrier Green NH3.

[1] HPP design tools are analysed based on the information openly available on their websites

Sub- research questions:

To deduce a scientific answer with logical reasoning for the main research question many intermediate questions to be answered through many steps over the period of this study. These need the sub-research questions and are listed below.

1. How to model and integrate the production of green ammonia in the hybrid renewable power plant design of HyDesign?

   It was understood that the production of energy carriers like Green NH3 is currently missing in the tool which will lead to a gap in the analysis and optimization of possible extra revenue streams of HPP. Energy flow through the system is mainly controlled by EMS.So, it is essential to integrate the GNH3 production functionality in EMS of the HPP system.

2. How does the value(economic benefits) of utility-scale hybrid renewable power plant change with this HPP+GNH3 system design?

   Understanding whether there will be any value in producing GNH3 is important for a renewable energy developer before making a financial and design decision. if there is any value then how can it be changed using changes in system design?

3. What can be the possible Modelling checks(MC) to verify the model and what sensitivity framework be made on a model for this HPP+GNH3 system design?

   After drafting a set of EMS equations, a way to verify the proper functioning of the EMS can be done through the necessary verification checks these are called as Modelling checks.what are those modelling checks for the HPP+GNH3 model? Observing the dependencies of the different system parameters based on each other is important how can sensitivity analysis be performed in this HPP+GNH3 system?

The aim of this thesis study is to analyze the HPP plant's interaction and added with GNH3 through developing and integrating Green NH3 model in existing EMS of HyDesign.

1.4. Structure of the report

The report is structured as follows: chapter 2 contains the definition of Hybrid power plants and their benefits and provides information about the Green Ammonia production processes and methodology adopted in this study. In chapter 3 the architecture of the HyDesign is illustrated and a modelling approach for Green NH3 integration in EMS is presented. The following chapter, chapter 4 has the site selection hypothesis for the HPP power plants along with technical and resource details of the base case site of this study.it also has a detailed list of modelling checks for EMS model of HPP + Green NH3. After that, in chapter 5 Results of the EMS model and optimization are presented for a particular case study.Detailed Sensitivity analysis is also carried in this chapter.Finally, chapter 6 summarizes the main outcomes of this study and describes the findings related to all the research objectives of this thesis study.

2

Methodology and Technology Description

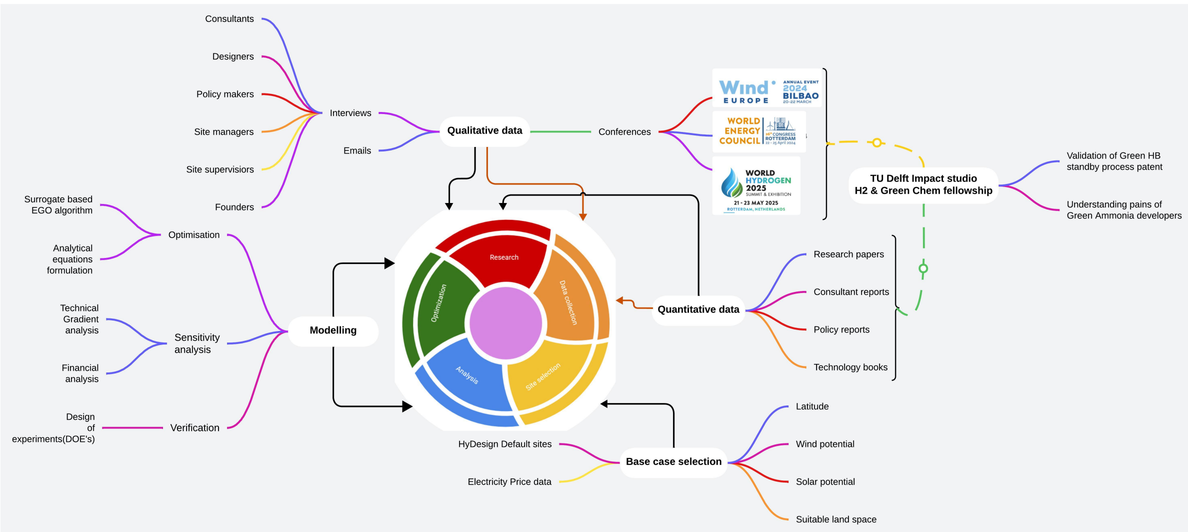


Figure 2.1: Research process flow map

2.1. Methodology

This study has been carried out in many steps using different ways.A pictorial illustration of all such ways is shown in Figure 2.1.The initial problem analysis and research questions are drafted with thorough literature research and after the discussion with research supervisors. Understanding of the technologies is developed during thorough desktop research through several academic research papers, consultant reports, policy reports and technology book chapters.This exercise gave enough information for quantitative data collection.

Qualitative data collection was made while speaking with several industrial professionals at recent 2024 conferences in Europe and also by interviewing different stakeholders of the Green ammonia ecosystem. Enough clarity and confidence are developed during those interviews on ambiguous topics like costs, Potential benefits of Hybrid renewable power plants,Green Ammonia plants, operational modes of Green Ammonia processes, etc. Along with this current research study, entrepreneurial validation of the potential standby mode of the green ammonia process is conducted as a part of H2 & Green Fellowship program of TUdelft Impact studio.TUdelft Impact Studio is the pre-startup program of TU Delft for researchers and students who want to bring their impactful innovations or research to the market.Team of experts are ready to support in exploring the market and the commercial potential of the technology.

Site selection was conducted based on various aspects like Wind potential, solar potential, suitable land space, and geographical location. Base case selection was made using the available data files in Hydesign. A sensitivity study was done for the base case to analyze the technical gradients and financial metric interdependencies. Finally study concludes with optimized configurations for the base case scenario using surrogate-based Efficient Global optimization (EGO) algorithm along with some analytical equation formulations for optimization of the financial value.

The green ammonia industry is still nascent and a lot of research is currently going on in this domain. Very few pilots are up and running in the world at present. This clearly results in uncertainty in information about costs, technological challenges, and design aspects. Because of such uncertainty, qualitative data was collected using interviewers, emails, and visiting conferences.

Research outputs and coded EMS files are stored in the Hydesign repository in GitHub.This report will be made available in TUdelft research repository.

2.2. Hybrid renewable plants

As per the draft version of work package 1 of IEA Wind TCP task 50(IEA Wind TCP 50, 2024) there are many definitions of the Hybrid power plant which are listed in**IEA Wind TCP task 50 WP1**. For this study, a Grid-Connected utility scale Hybrid power plant is considered which can be defined as follows

"An HPP that is connected to the electricity transmission network through an single interconnection point, complies with the grid code rules set out by the transmission system operator and has a combined nameplate capacity of greater than 5 megawatts" (IEA Wind TCP 50 WP1, 2024)

IEA Wind TCP task 50 work package 1 research team has put on efforts to develop consistent terms on HPP terminology across research and industrial fields.They have developed a decision tree which includes a multiple definitions of a HPPs. According to the decision tree in Figure 2.2 a Power plant can satisfy multiple definitions of HPP.In this study a grid-connected utility scale renewable HPP is analysed.

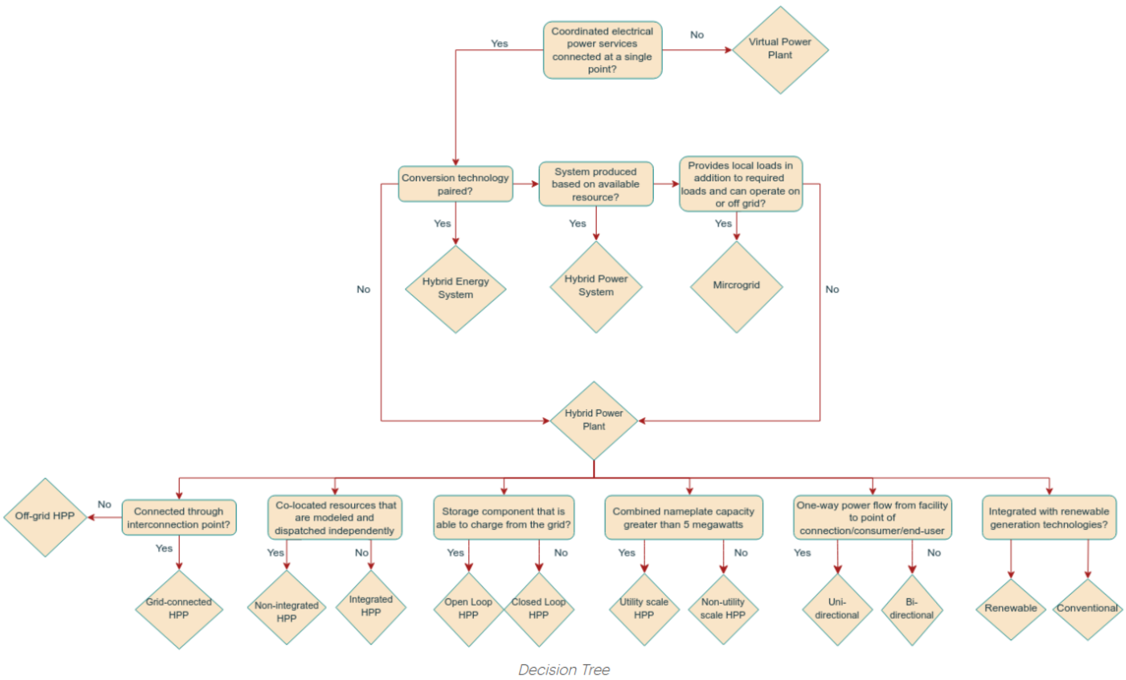


Figure 2.2: HPP Definitions Decision tree (IEA Wind TCP 50 WP1, 2024)

There are many benefits of HPP plants, These benefits can be classified into 2 categories.

- Technical benefits
- Non-technical benefits(economic, others).

2.2.1. Technical benefits

There are many technical benefits of hybrid power plants like

1. **Stable output:** HPPs have overall reduced energy output variability with respect to individual solar and wind plants.
2. **Increased capacity factor:** HPPs have better capacity factors than individual solar and wind plants due to increased energy output throughout the lifetime of the plant.
3. **Improved efficiencies:** HPPs have better electrical efficiencies for electrical equipment than individual RE plants. Due to increased constant loading on equipment like transformers etc.
4. **Remote & Off-grid applications:** HPPs have storage component in them, which adds an extra benefit being used in remote and off-grid applications.
5. **Grid stability:** HPPs give more confidence to grid operators in forecasting the generation.This is possible due to their(HPP's) relatively stable output than Individual RE plants.
6. **Flexibility and ancillary services:** HPPs can have storage components in them, which adds flexibility to the grid for its ancillary services.
7. **Complementarity:** HPPs can have different RE resources like wind and solar, which mostly complement each other in the generation patterns in a single location. This complementarity helps in sizing the plant to achieve a more stable output.
8. **Optimized land use:** The benefit of optimized land usage is mainly possible with HPPs due to the possibility of using the vacant land in between individual generation resources, unlike in Individual RE plants.

9. **Optimized transmission infrastructure:** HPPs always have a single interconnection point for all generation resources in them, unlike individual RE plants. With more HPPs in the grid, the requirement for new transmission lines decreases and the utilisation of existing transmission lines increases with more variable RE injection into the grid.

2.2.2. Non-technical benefits

There are many non-technical benefits of hybrid power plants like

1. **Cost savings:** Due to shared electrical infrastructure, optimized land use, and lower curtailment, the overall capex and opex costs per MW of HPPs are reduced when compared to individual RE plants.
2. **Decreased amount of time of execution in project development:** Due to simultaneous and independent construction activities in HPP development, the project execution time can be less when compared to individual RE plants of the same sizes.
3. **Increased and more reliable revenue:** Several avenues of revenue streams open up with HPPs, which increase overall revenue per plant for RPDs, due to relatively stable energy output the reliability of the revenue also increases.
4. **Energy security:** By Building many HPPs energy security of the country or province can be increased as HPPs have a combination of different renewable technologies. For example, north-west Europe is good in wind resources and has relatively low solar resources when compared to the North Africa region. By building more HPPs in either of these regions the energy security of that region increases due to the availability of at least 1 resource at any time/season of the year and base load can be supplied by storing excess in peak season in long-term storage components of HPPs.
5. **Diversification of revenue streams:** With HPPs Many types of revenue streams can be generated depending upon the use case, location, and plant installation capacities for example direct PPAs in long-term markets, Selling stored excess in the balancing market, As a balancing service provider(BSP) to the grid through ancillary services market. Corporate PPAs with Industrial customers and offering P2X solutions for producing different green molecules, revenue can be generated by storing them for long-term storage or selling them directly. With a Single HPP, these many revenue streams are possible for the owner of the plant,which might be difficult with individual solar or wind plants.
6. **lowering environmental impact:** Due to HPPs there is a lowered environmental impact compared to individual RE plants.HPPs have optimized land use per MW, so they have less habitat disruption than individual RE plants.HPPs have shared infrastructure This translates to less material usage and reduced impact on the environment during construction, such as less insulation usage on cables due to lesser cable lengths or road building. HPPs have storage components within them, so there is less dependence on backup power from the grid or diesel generator sets, etc. In this way, the overall environmental impact of the plant can be reduced using HPPs.

Out of all the listed technical and non-technical benefits of HPPs, this study only focuses on a few of the quantifiable non-technical benefits like revenues, and revenue streams to understand the HPP interaction with Green NH3 production.

2.3. Haber Bosch process

Ammonia(NH3) has been used in many industries like Fertilizers, Refrigeration, textiles and pharmaceuticals chemicals, and explosives for decades. With growing interest in green chemicals in the energy transition landscape, its uses are getting expanded as shown in Figure 2.3. The production process of Ammonia is invented by Fritz Haber & Carl Bosch process in 1906. So, it is named after them and called the **Haber- Bosch process**. Several other ammonia production processes like Electrochemical processes, Thermocyclic process, Plasma-based methods, Photosynthetic bacterial processes, Partial oxidation, etc have developed over the years and are still under research. This study is on the Haber bosch(HB) process which is a proven technology for over 100 years.

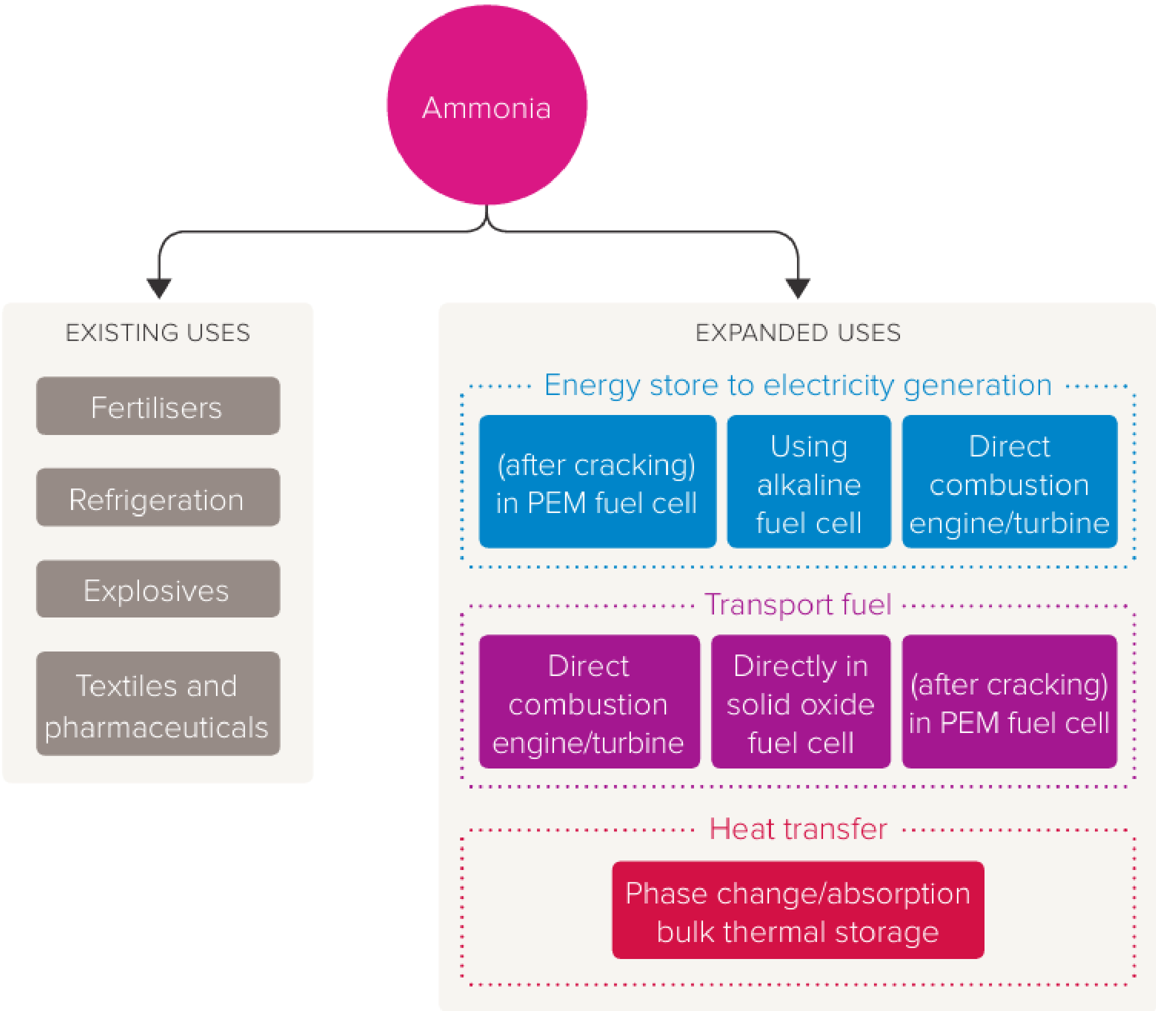


Figure 2.3: Ammonia uses (The Royal Society, 2020)

Conventional Ammonia is produced through Natural gas(Grey) or Coal(Brown/Black), but its production and consumption account for 2% of World CO2 emissions(Bloomberg Carbon Transition Coalition, 2023). Turning different ammonia production processes to green can reduce those emissions. Different colors of ammonia are shown in Figure 2.4 based on the different production processes. Brown, Grey, Turquoise, and blue ammonia are produced from fossil feedstock inputs to the different chemical processes that provide input Hydrogen in the form of syngas (CO+H2) to the Haber-Bosch process. Whereas renewable electricity is input to the electrolysis process which gives green hydrogen as input to the Haber bosch process produces Green ammonia(NH3).

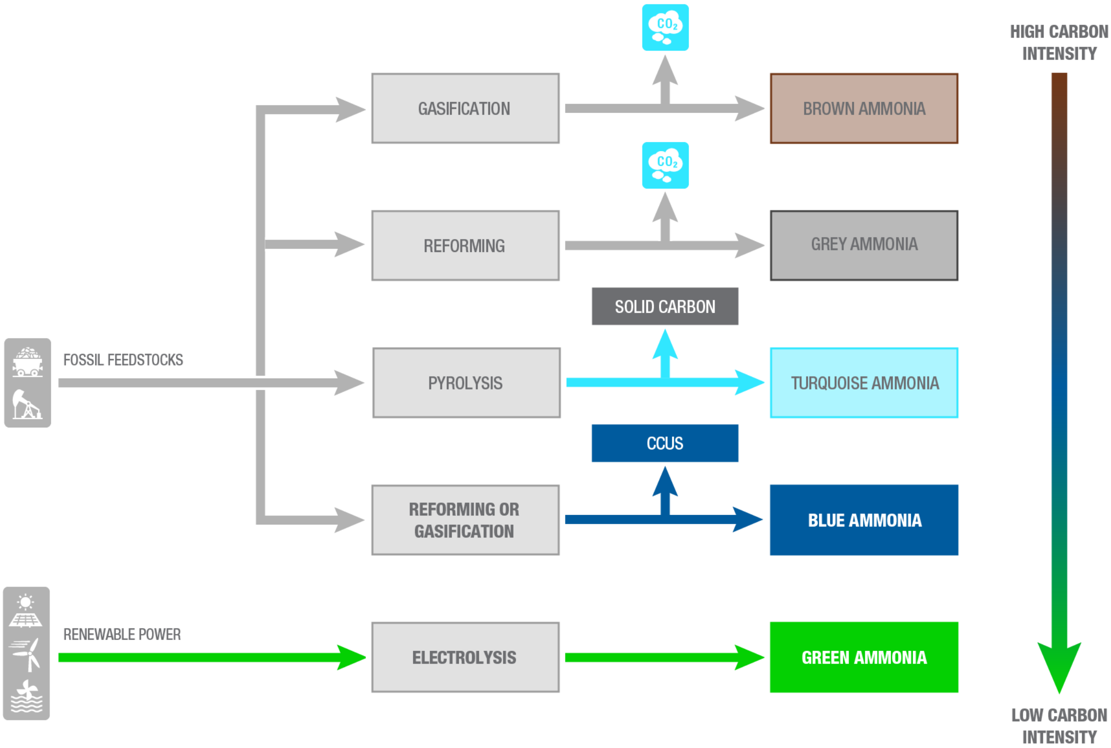


Figure 2.4: Ammonia colors (Ashraf, 2023)

Physical properties	H2	N2	NH3
Molar Mass(g/mol)	2	28	17
Melting point(M.P)	-259.16 °C	-209.86 °C	-77.7 °C
Boiling point(B.P)	-252.879 °C	-195.795 °C	-33.1 °C
HHV(MJ/kg)	141.8	–	22.5
LHV(MJ/kg)	119.96	–	18.646
HHV(kWh/kg)	39.70	–	6.30
LHV(kWh/kg)	33.59	–	5.22
HHV(MJ/L)	12.74	–	17.30
LHV(MJ/L)	10.78	–	12.71
HHV(kWh/L)	3.54	–	4.81
LHV(kWh/L)	3.00	–	3.53
Density(STP- Gaseous state)	0.08988 kg/m3	1.2506 kg/m3	0.769 kg/m3
Density(B.P-Liquid state)	0.07 g/cm3	0.0808 g/cm3	0.6819 g/cm3

Table 2.1: Physical properties of H2,N2 and NH3(Wikipedia contributors, 2024d)

The Haber bosch process is an exothermic equilibrium reaction, which means the reaction releases heat along with the Ammonia when the equilibrium shifts towards the products side.

$$N_2(g) + 3H_2(g) \rightleftharpoons 2\,NH_3(g) \qquad \Delta H^\circ = -92.28 \text{ kJ} \qquad \Delta H_{298K}{}^\circ = -46.14 \text{ kJ/mol} \tag{2.1}$$

Le Chateliers principle: Le Chatelier's principle states that if a dynamic equilibrium is disturbed by changing the conditions, the position of equilibrium shifts to counteract the change to reestablish equilibrium. If a chemical reaction is at equilibrium and experiences a change in pressure, temperature, or concentration of products or reactants, the equilibrium shifts in the opposite direction to offset the change(LibreTexts, 2023).

Temperature range: $400°$C to $650°$C (The Editors of Encyclopaedia Britannica, 2024).
The forward reaction is exothermic. according to Lechatliers principle, the forward reaction is favored if the operating temperature is lowered. The system will respond in a counteracting way by moving the position of equilibrium to the right side. The lower the temperature the better ammonia yield will be.However, Lower temperature slows down the rate of reaction, which means the speed at which reaction proceeds. This means a tradeoff must be made between the rate of reaction and the ammonia yield. A compromised temperature of around $450°$C is used in industries.

Pressure range: 130 atm to 350 atm (Rueda et al., 2024).
There are 4 molecules on the reactant side of the reaction, but only 2 on the product side. If the operating pressure of the reactor increases the reaction will respond by producing fewer molecules, as a counteraction pressure will fall again. So, to get as much ammonia in the equilibrium mixture, reaction needs as high pressure as possible. Around 200 atm pressure is generally used as the operating pressure in industrial-scale reactions.

Catalysts: Iron based catalysts are Fe_3O_4,Fe_3O_4withCO and $Fe_{1\text{-}x}O$. Ruthenium-based catalysts Ru−Ba−K/AC, Ruthenium, alkali earth metals with activated carbon (Rueda et al., 2024).

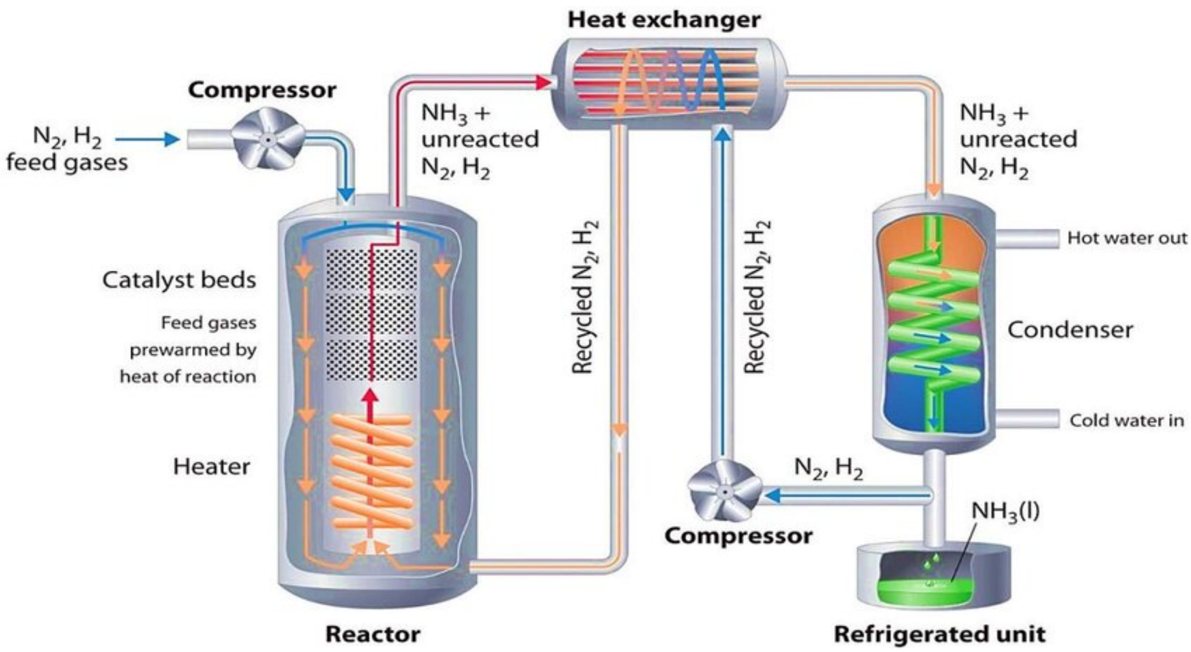


Figure 2.5: Haber Bosch process (Ikpe et al., 2024)

Haber bosch process occurs in five stages:

Stage-1:

H2 is obtained from chemical processes and the selection of these processes varies based on the required nomenclature of ammonia. N2 is obtained from the atmosphere using various N2 separation technologies. H2, N2 as input to the reactor in a gaseous state are called the feed gases to the HB process.

Stage-2:

Feed gases are pumped into the Multi-stage feed compressor to achieve the required pressure. Inside the compressor, the gases are compressed to around 200 atm.

Stage-3:

The pressurized gases are pumped into a tank containing layers of an iron[Magnetite (Fe_3O_4) or wustite (FeO)] or ruthenium[Ru-Ba-K/AC]-based catalyst at a temperature of 450 °C. The Feed Gases H2 and N2 are prewarmed by heat of the reaction in the reactor and are made to flow from bottom to top as shown in Figure 2.5.

Stage-4:

Unreacted H2 and N2 and the ammonia product pass into a cooling tank. The ammonia is liquefied and removed to pressurized storage vessels.Ammonia separation is a crucial step in the HB process. Along with the existing separation process of Condensation, different separation processes like Absorption(Metal Halides) and Adsorption(Zeolites) are being under research.Finally Liquid ammonia is separated and transported or stored in tanks.

Stage-5:

The unreacted H2 and N2 gases are recycled back into the system using recycle compressors to start over again as detailed in Figure 2.6. The Unreacted H2 and N2 will be at lower temperature than the inlet temperatures,so these are made to flow through a heat exchanger to make use of this heat from the outlet of the reactor as shown in Figure 2.5.

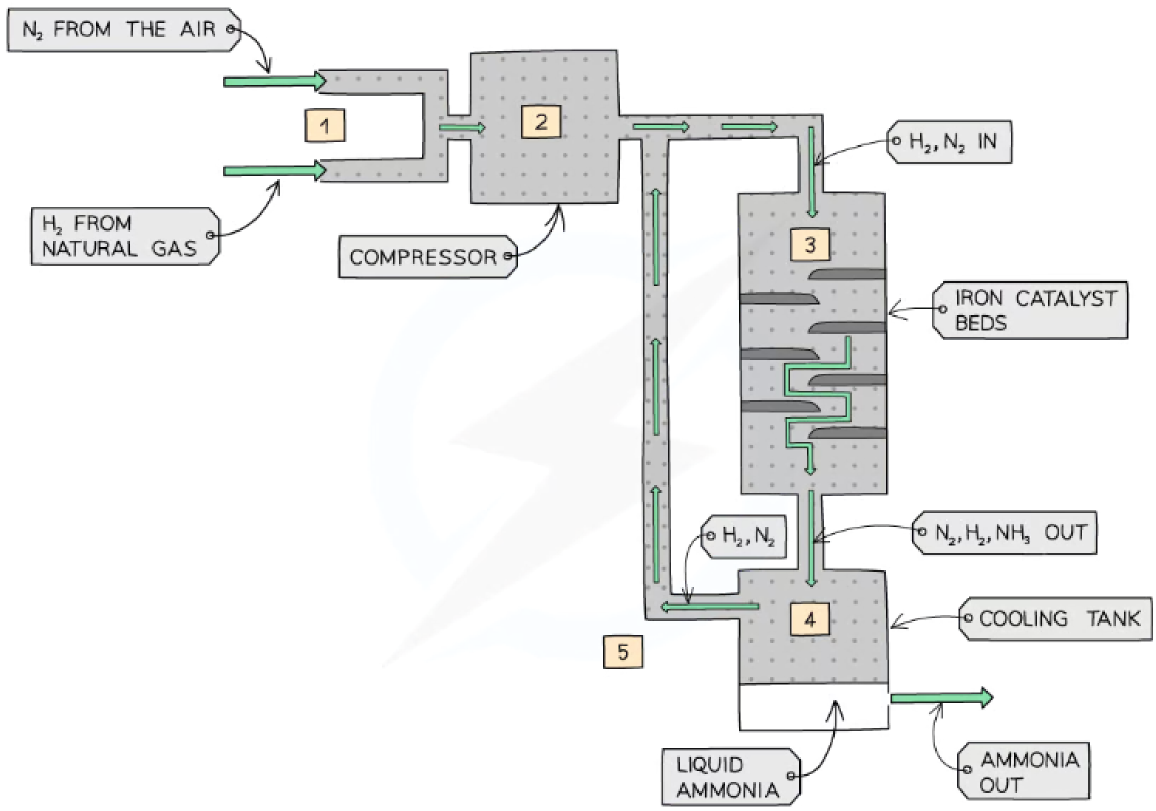


Figure 2.6: HB mass flow diagram (Brennan & Hird, 2024)

2.4. Nitrogen production

3 different nitrogen separation technologies are shown in the Table 2.2.Air separation units(ASU) use a cryogenic distillation process, Pressure swing adsorption(PSA) and membrane-based selective permeation process.All ASU process technology benefits even more from economies of scale than the HB process.Unlike ASU, PSA and Membrane technologies are not scaled up yet to higher N2 production capacities. ASU has the highest N2 purity and lowest energy consumption but has limited process flexibility than PSA.PSA units are compact and inherently modular well suited for smaller production capacities have the best dynamic flexibility but have high energy consumption. The membrane-based process offers benefits like modular configuration with low capital cost but has the lowest purity due to impurities like argon. For both PSA and membrane-based processes, an additional oxygen removal unit(deoxo) unit is required to remove oxygen in N2 gas(Flis & Wakim, 2023). The Capacity range refers to the range of flow rates that the technology can handle.Clearly, ASU has more range than the other 2. The load range (%) in the table refers to the range of operating loads that each technology can handle without significant performance degradation. Here PSA dominates ASU with a higher load range i.e. dynamic flexibility.

	ASU (Cryogenic)	PSA	Membrane
Temperature ($^{\circ}C$)	-195 to -170	20-35	40-60
Pressure (bar)	1-10	6-10	6-25
Purity ($wt\%$)	99.999	99.8	99.5
Energy consumption ($kWh/kgN2$)	0.1	0.2-0.3	0.2-0.6
Energy consumption (GJ/t_NH3)	0.3	0.7-1.0	0.7-2.0
Capacity range ($Nm3/h$)	250-50000	25-3000	3-3000
Load range (%)	50-100	30-100	–
Technology readiness level (TRL)	9	9	8-9

Table 2.2: Comparison of Nitrogen Production Technologies(Rouwenhorst et al., 2021)

2.5. Hydrogen production

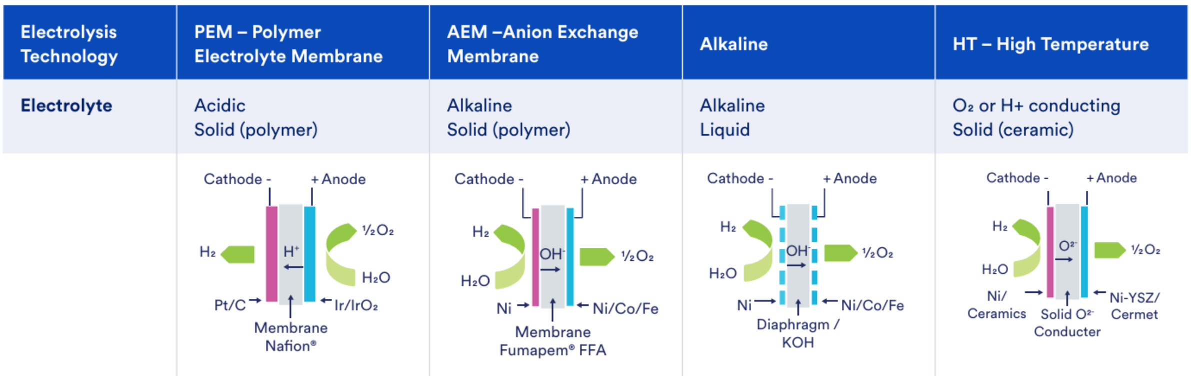


Figure 2.7: Working principle of electrolysis technologies (Flis & Wakim, 2023)

Green Hydrogen is produced by giving input of green electricity to the electrolyzer. Alkaline electrolysis technology is the oldest among all current electrolysis technologies with more than a century of existence. In Norway, the company Norsk Hydro (today´s NEL Hydrogen) was founded around 1905, aiming to use available hydropower in Norway to produce ammonium nitrate via the electrolysis process, to be used as fertilizers. In 1928, the first large-scale electrolysis plant as a source for hydrogen in ammonia production went in operational in Rjukan (Norway)(Ayers et al., 2022). Other recent technologies are Proton exchange membrane(PEM), also called as polymer exchange membrane, Anion exchange membrane(AEC) and Solid oxide electrolysis(SOEC), also called High-temperature electrolysis. The working principle behind these technologies is clearly shown in Figure 2.7.Each of these technologies has different electrolytes and ions are transferred from cathode to anode or vice versa.

Comparision of different hydrogen production technologies are given in Table 2.3. Operating temperatures of Alkaline, PEM and AEM are below 100°C, whereas the SOEC has 500°C-900°C of operating temperature, which make SOEC more compatible with HB process. The exothermic heat output of the HB process can be used to provide sufficient operating temperature to SOEC, making the system more efficient and even sometimes crossing 100% efficiency. The operating pressure of all the technologies are far below the operating pressure requirement of the HB process.Compression requirements for these electrolysis technologies are much lower than that of HB process.Out of all electrolysis technologies, SOEC has the lowest system energy consumption, which makes it more efficient,even without integrating with the HB process. Both Hot rampup and cold rampup times for Alkaline, PEM, AEM technologies are in few minutes to 1hour, whereas SOEC has a cold ramp uptime of almost 10 hours, which is similar to the HB process. The minimum load percentage is the lowest power level at which the electrolyzer can operate stably.With intermittency in renewables, PEM is getting popular due to its lower minimum load % and also its lesser ramp-up times.The TRL of SOEC is between 5-6, which is a technology demonstration stage, so it takes a considerable amount of time to understand the characteristics of SOEC. This study excludes the SOEC and HB process integration.

	Alkaline	PEM	AEM	SOEC
Operating temperature ($°C$)	60-95	50-80	40-80	500-900
Operating pressure (bar)	Conventional tech: atmospheric pressure. Modern tech: up to 30 bar (50 among startups)	Up to 80 (350 among startups)	Up to 35 with potential for much higher in the future	0-2
Hydrogen purity(vol.%)	>99.5	99.99	–	99.99
System energy consumption (kWh/kgH_2)	50-78	50-83	57-69	38 (with steam import) 48 (without steam import)
Stack lifetime (full load hours)	60,000-100,000	50,000-90,000	5,000-40,000	20,000-50,000
Degradation rate ($\%/1000$ hours)	0.13	0.25	0.4	0.55-1%
Ramp up time hot idle to nominal power	60s	10s	30 minutes	10 minutes
Cold ramp up time	30-60 minutes	5 minutes	20 minutes	>600 minutes
Minimum load	10-40%	5-10%	10-20%	>3%
Technology readiness level (TRL)	9	8-9	–	5-6

Table 2.3: Comparison of Hydrogen Production Technologies (Flis & Wakim, 2023),(Rouwenhorst et al., 2021)

3

Modelling and System Description

Modelling of green ammonia production in this study is done in HyDesign.**HyDesign** is an Opensource tool and this project repository can be accessed in GitHub. It is written in the programming language Python using the OpenMDAO framework to connect different functional components.OpenMDAO is an open-source framework for efficient multidisciplinary analysis and optimization, developed by the National Aeronautics and Space Administration(NASA). Detailed architecture of the HyDesign is shown in Figure 3.1.

3.1. HyDesign Architecture

In general, a numerical model can be very complex, multidisciplinary and heterogeneous.It can be decomposed into a series of smaller computations that are chained together by passing variables from one to another. In OpenMDAO all these numerical calculations are made inside a component that represents the smallest unit of computational work the framework understands(OpenMDAO Development Team, 2024). Different types of components exist in OpenMDAO, but only explicit components are used in HyDesign to keep a clear distinction between the inputs and outputs of the components.

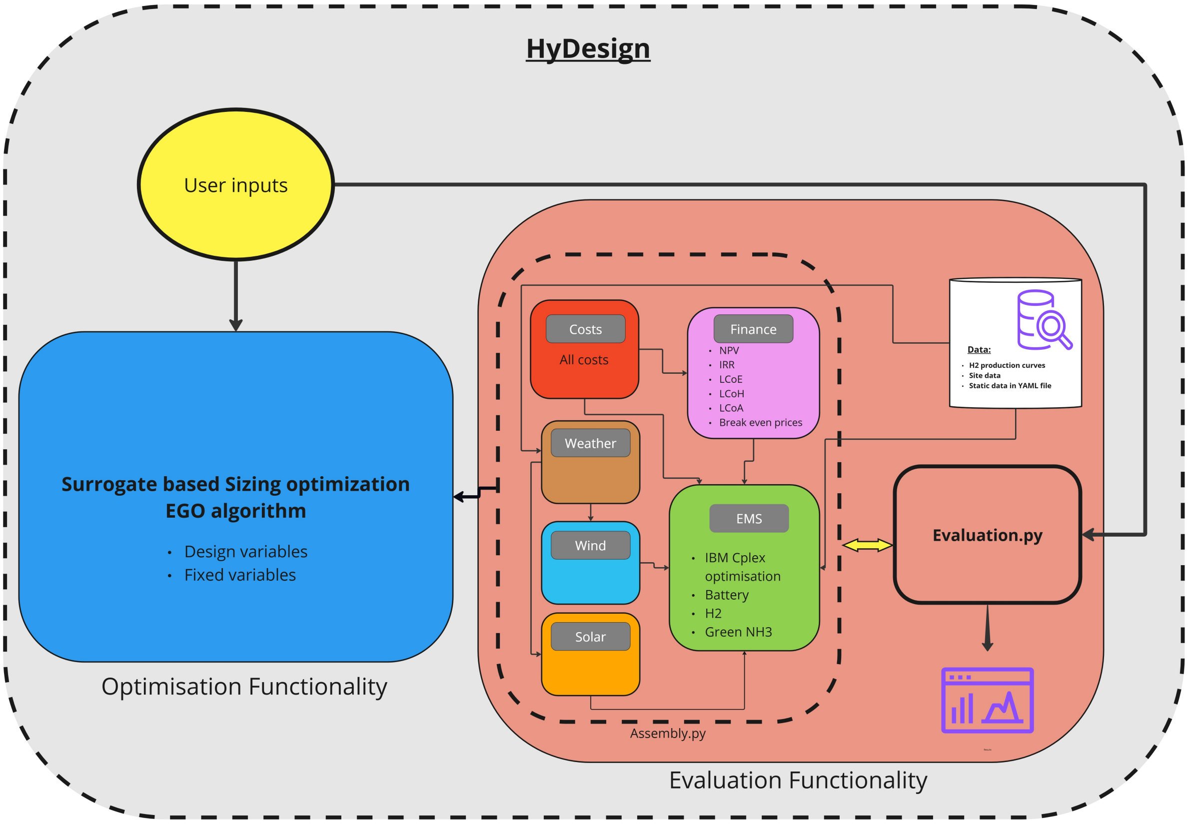


Figure 3.1: HyDesign Architecture

Different components currently exist in the HyDesign. A few of such components are wind component, solar component, weather component, cost component,finance component, and EMS component.HyDesign currently serves 2 functionalities. First is the evaluation of a design given as input by the user and second, optimizing the size of the design given as the input. The evaluation functionality is discussed further in the section 3.2. Sizing optimization functionality is described in section 3.4. Detailed information about all the components and equations of existing generating sources, batteries, and electrolyzers are shared in the HyDesign detailed paper(Murcia Leon et al., 2024). Since HyDesign is made using Python and OpenMDAO, both are open-source projects, it is very hassle-free to scale and enhance the functionality of this tool.For example, other renewable generation resources can be added to the current system through additional explicit components for each new generation source. Once these additional components are made necessary information on weather, cost, and EMS functionality for these extra components can be added to existing components. But, other non-generation parts of the HPP system like battery, H2 production, etc are only modeled inside the EMS, cost, and finance components of the HyDesign. Similarly, GNH3 production will be modelled inside the EMS of HyDesign. Architecture is shown in section 3.1.

3.2. EMS Modelling

"An energy management system (EMS) is a system of computer-aided tools used by operators of electric utility grids to monitor, control, and optimize the performance of the generation or transmission system. Also, it can be used in small-scale systems like microgrids" (Wikipedia contributors, 2024b).

EMS functionality mainly includes monitoring, controlling, and optimization of the energy system.EMS currently formulated in HyDesign can only optimize the revenue of the RPD based on the given inputs of renewable energy source generation time series, and offtake prices of the energy vectors and molecules to be produced. As mentioned in the section 1.1, profits of RPDs are shrinking in the rapid energy transition landscape. RPDs must diversify their revenue streams by producing different energy vectors and molecules. So, This existing EMS functionality will evaluate the given inputs and only suggest the RPD with the optimized production plan for a year by making scheduling choices between the production and storage in each timestamp (1 hour in this study) of different energy vectors like electrical energy(EE), green Hydrogen(GH2), and green ammonia(GNH3).

EMS in HyDesign is modelled as an explicit component of OpenMDAO.EMS is formulated as a linear optimization problem and coded using the IBM Cplex optimization environment.The IBM Cplex optimization environment has restrictions on the number of variables and constraints to be used in the free community version. For this reason, the code is structured in a way that the batch size of the optimization can be changed in the EMS component. The Batch size takes integer values of the number of days. Here Batch size means the time for which a single optimization iteration will be run in IBM Cplex.

The existing linear optimization problem in the HyDesign EMS is shown below:

Objective function-1: Existing objective function in EMS optimization problem of **HyDesign(V1.4.1)** is denoted by EE+GH2.This means EMS only has choice between 2 types of energy vectors either electrical energy(EE) or green Hydrogen(GH2).

$$\textbf{\textit{EE+GH2}} : \max_t \sum_t \{P_{hpp}(t) \cdot price_{elec}(t) + m_{H2}(t) \cdot price_{H2}(t)\} - I_b \tag{3.1}$$

Constraints:

$$
\begin{aligned}
0 \leq P_{hpp}(t) &\leq G_{MW} && (3.2)\\
P_{hpp}(t) &= P_w(t) + P_s(t) + P_{batt}(t) - P_{ptg}(t) - P_{curt}(t) && (3.3)\\
P_{curt}(t) &\geq 0 && (3.4)\\
I_b &\geq 0 && (3.5)\\
-P_{battMW} \leq P_{batt}(t) &\leq P_{battMW} && (3.6)\\
E_{battMWh}(1 - Batt_{DOD}) \leq E_{SOC}(t) &\leq E_{battMWh} && (3.7)\\
E_{SOC}(t+1) &= \begin{cases} E_{SOC}(t) - P_{batt}(t)\Delta t \eta_{ch} & \text{if } P_{batt} < 0 \\ E_{SOC}(t) - P_{batt}(t)\Delta t/\eta_{disch} & \text{if } P_{batt} > 0 \end{cases} && (3.8)\\
0 \leq P_{ptg}(t) &\leq P_{ptgMW} && (3.9)\\
m_{H2}(t) &= HPC(P_{ptg}(t)) && (3.10)\\
HPC(P_{ptg}(t)) &= \eta(P_{ptg}(t)) \cdot P_{ptg}(t) \cdot 1000/HHV && (3.11)
\end{aligned}
$$

Variables:

Power to electrolyzer in MW $(P_{ptg}(t))$

Power curtailment in MW $(P_{curt}(t))$

HPP power generation sent to grid in MW $(P_{hpp}(t))$

Grid capacity in MW(G_{MW})

Power generation from Wind in MW $(P_w(t))$

Power generation from Solar in MW$(P_s(t))$

Battery Power capacity in MW$(P_{batt}(t))$

Battery Energy capacity in MWh$(E_{battMWh})$

Electricity price in €/MWh$(price_{elec}(t))$

Hydrogen selling price in €/MWh$(price_{H2}(t))$

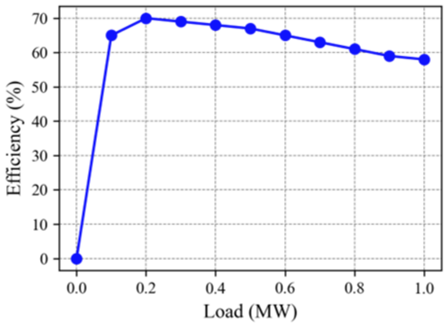
Instantaneous time (t)

Efficiency (η)

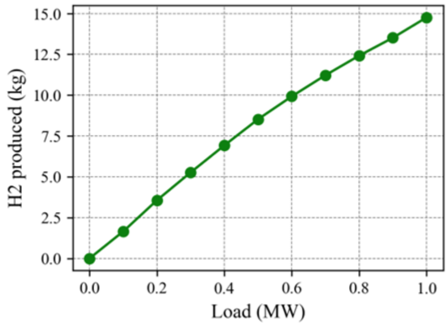
Mass of hydrogen produced in kgs/hr$(m_{H2}(t))$

Battery Depth of Discharge$(Batt_{DOD})$

Numerical limit of Battery Power capacity given as a external input by user of HyDesign(P_{battMW})



(a) Efficiency curve for PEM electrolyzer(Gupta et al., 2024).



(b) Hydrogen production curve for PEM electrolyzer(Gupta et al., 2024).

Figure 3.2: Efficiency and hydrogen production curve for PEM electrolyzer(Gupta et al., 2024).

Numerical limit of electrolyzer power capacity given as a external input by user of HyDesign(P_{ptgMW})

Optimization keep track of battery level$(E_{SOC}(t))$

Battery ramping penalty(l_b)-is the penalty to control the amount of battery degradation.

HPC denotes the non-linear hydrogen production curve which is a function of the electrolyzer's non-linear efficiency curve $\eta(P_{ptg}(t))$, and load $(P_{ptg}(t))$. HPC is modeled using piecewise linear approximation and thus,EMS optimization is solved using linear programming(Gupta et al., 2024).The efficiency and hydrogen production curve for 1MW of PEM is shown in Figure 3.2.

3.2.1. HPP+GNH3 system architecture

Since EMS is formulated as a linear optimization problem, the Haber bosch process is modelled as a simple black box that has few inputs and produces outputs.This can be seen in Figure 3.3. This way of black-box modelling will help in linearising the non linear chemical processes.

Different internal stages of the HB process as described in section 2.3 are not explicitly modelled, because only inputs and outputs matter for the linear EMS modelling.

Inputs to the black-box HB model are the feed gases like H2, N2 and green electricity to the Haber Bosch process. Outputs of the Haber Bosch process are the GNH3 and exothermic heat output. The system architecture for HPP+GNH3 is shown in the Figure 3.3

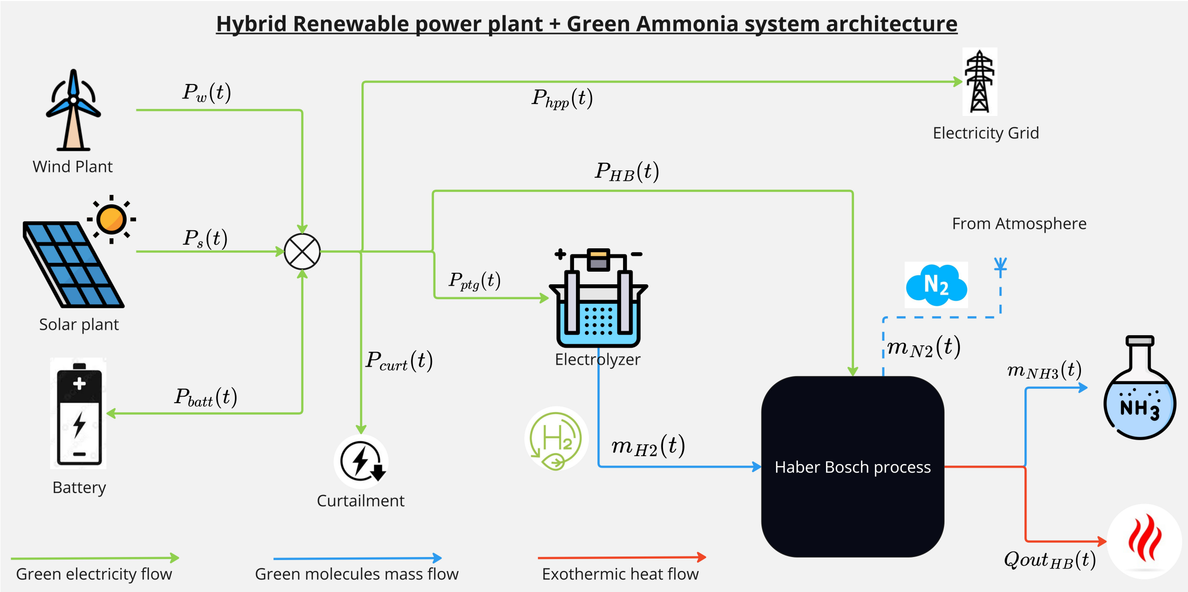


Figure 3.3: HPP+GNH3 system architecture.

In HyDesign, the Annual generation patterns are kept the same for all 25 years of the lifetime.HyDesign replicates this annual generation pattern for 25 years with degradation. So, this study only analyses yearly data for the HPP+GNH3 system.1 hour is considered the minimum timestamp of this study. There are different types of states available for electrolyzers, like Off, On and Standby modes similarly HB process also has off and on modes but standby mode is still in the research phase. The ramp rate of most of the electrolyzers is in the range of minutes, as mentioned inTable 2.3. In contrast, the ramp rate of both conventional and green HB processes is in the range of a couple of hours. The clear differences between the conventional HB process and green HB process are shown inTable 3.1. Since this study excludes the dynamic behaviour of the HB processes, no special considerations will be taken for startup and shutdown time delays and related system dependencies.

	Conventional (Grey) Haber Bosch process	**Green Haber Bosch process**
Startup Heating	Process heat from steam for SMR process.	Electric startup heaters.[4]
Land footprint	Large chemical plants near thermal power plants with significant land usage.	Evolving designs and R&D made it possible to have fit whole equipment in **4-5 modular containers**.[3]
Exothermic heat output	Is completely recovered for recycling.[4]	Currently not fully recovered. Can be stored as thermal heat for future use. Can generate additional revenue to RPDs.[4]
Startup & Shutdown times	Cold startup/shutdown - **24 to 72** hrs, Hot startup - **5 to 12** hrs[4].	R&D is carried on, few technology licensors claim ramp up time of few minutes[4] .
Capacity of the plants	Standard sizes are in the range of metric ton per day-**1500MTPD**.[4]	**300-600TPD** range and even much smaller containerized solutions have **4-5TPD**.[3]
Economic feasibility	Due to economies of scale, it is cheaper and feasible.	Costlier due to the high cost of its associated infrastructure and GH2.
Carbon footprint	$1.673 \quad t_{CO2}/t_{NH3}$[1]	$0.38 - 0.53 \quad t_{CO2}/t_{NH3}$[1]
Flexibility	Not flexible, Only continuous operation(on) or shutdown(off) no standby mode.[4]	R&D is carried on to improve the flexibility and standby mode of the green HB process.
Lifetime of the plant	Long lifetime around **50 years**.[2]	Yet to be known, pilots are commissioned 2-3 years ago.

Table 3.1: Few key differences of Conventional and Electrified HB processes[1](Smith et al., 2020),[2](IEA, 2021),[3](AmmPower Corp, 2024).

3.2.2. Mass Modelling

Mass modelling is one of the most important aspects of HB process modelling. After thorough literature research, 3 different options are chosen for the mass modelling. Each of the 3 options have their own advantages and drawbacks.

1. Mass balance
2. Equilibrium Lookup table
3. Equilibrium constants.

Mass balance

The law of conservation of mass implies that mass can neither be created nor destroyed, although it may be rearranged in space, or the entities associated with it may be changed in form(Wikipedia contributors, 2024a).

So, as per the chemical reaction shown in Equation 2.1,the mass of GNH3 produced $(m_{\text{NH3}}(t))$ must be equal to the mass of green hydrogen and nitrogen taken from the atmosphere.Consequently Equation 3.15 and Equation 3.16 are additional constraints in the EMS optimization.From Equation 3.17 till Equation 3.19 additional time-independent equations are calculated before the execution of the optimization loop. Equation 3.17 is the maximum GH2 that can be produced in a given HPP+GNH3 system.It is formulated using the HPC of a given P_{ptgMW}.

[4]Information collected from various interviews, and conference discussions with industrial professionals, site engineers, refer Figure 2.1

$$0 \leq m_{H2}(t) \leq H2_{max} \tag{3.12}$$
$$0 \leq m_{N2}(t) \leq N2_{max} \tag{3.13}$$
$$0 \leq m_{NH3}(t) \leq Am_{size} \tag{3.14}$$
$$m_{N2}(t) = m_{H2}(t)/Feedratio \tag{3.15}$$
$$m_{NH3}(t) = m_{H2}(t) + m_{N2}(t) \tag{3.16}$$
$$H2_{max} = HPC(P_{ptgMW}) \tag{3.17}$$
$$N2_{max} = (H2_{max}/Feedratio) \tag{3.18}$$
$$Am_{size} = (1 + 1/Feedratio) * H2_{max} \tag{3.19}$$

$H2_{max}$ – Maximum GH2 production in HPP+GNH3 system in kgs

$N2_{max}$ – Maximum N2 production in HPP+GNH3 system in kgs

Am_{size} – Maximum GNH3 production in HPP+GNH3 system in kgs

Mass of Nitrogen ($m_{N2}(t)$) is input to the HB black box model.Usually, nitrogen is extracted from the atmosphere using different separation technologies as described in section 2.4. The required capacity of nitrogen is not independently modelled as a separate constraint,since nitrogen is only used in the HB process of this system and is abundant in the atmosphere. There is no need for storage of N2 which further concludes that nitrogen can only be extracted from the atmosphere whenever wanted. These reasons paved to path to model N2 production depending on GH2 production to produce N2 whenever there is a requirement for NH3 production in the system.

	H2	N2	NH3
Moles	1.5	0.5	1
Mass(Kgs)	0.17647	0.82353	1
Molar mass(g/mol)	2	28	17

Table 3.2: Moles and Masses of HB process

1 Mole of GNH3 requires 0.5 mole of N2 and 1.5 moles of H2.Feed ratio is the ratio of the Mass of H2 over the mass of N2 for 1 kg production of GNH3, as listed in Table 3.2, for 1 kg NH3 production we need 0.17647 kgs of H2 and 0.82353 kgs of N2. The feed ratio is an important parameter in the equilibrium dynamics of the Hb process, but for the simplicity of linear EMS optimization, the feed ratio is kept constant throughout the lifetime of the simulation.

$$Feedratio = 0.17647/0.82353 = 0.214285 \tag{3.20}$$

Although mass balance is the simplest and easiest form of representation of the chemical process, it has some drawbacks like not considering the operational conditions of the HB process. Another drawback is that mass balance always provides more mass of ammonia than the actual extractable mass of ammonia from the reactor due to the equilibrium reaction of the HB process.

Equilibrium Lookup table

As clearly explained in section 2.3 due to le chateliers principle the equilibrium of HB process shifts towards reactants or products based on the operating conditions of the reaction. This means it is important to look at the percentage of ammonia produced in the reactor at different operating conditions of the reaction process. Such percentage ammonia values are given in then the Figure 3.4

t (°C)	T (degr. abs.)	$\frac{p_{NH_3}}{p_{N_2}^{1/2} p_{H_2}^{3/2}}$	$-\log \frac{p_{NH_3}}{p_{N_2}^{1/2} p_{H_2}^{3/2}}$	Percentage of NH_3 at equilibrium			
				at 1 atm	at 30 atm	at 100 atm	at 200 atm
200	473	0.1807	0.660	15.3	67.6	80.6	85.8
300	573	1.1543	0.070	2.18	31.8	52.1	62.8
400	673	1.8608	0.0138	0.44	10.7	25.1	36.3
500	773	2.3983	0.0040	0.129	3.62	10.4	17.6
600	873	2.8211	0.00151	0.049	1.43	4.47	8.25
700	973	3.1621	0.00069	0.0223	0.66	2.14	4.11
800	1,073	3.4417	0.00036	0.0117	0.35	1.15	2.24
900	1,173	3.6736	0.000212	0.0069	0.21	0.68	1.34
1,000	1,273	3.8679	0.000136	0.0044	0.13	0.44	0.87

Fritz Haber presented his original ammonia synthesis results in his Nobel lecture in 1920.
Reprinted with permission from The Nobel Foundation. ®©[2]

Figure 3.4: HB Equilibrium Lookup table (Klemola, 2021).

At $200°$C temperature and 200 atm pressure the percentage production of ammonia is highest among all other operating conditions. This means Higher pressures and lower temperatures will favour the HB equilibrium to move towards the reactant side, but lowering temperature will slow down the reaction kinetics so there should be a tradeoff in operational temperature and reaction output. Based on the discussions with professionals during market research about GNH3 plants it was understood that Feedratio also changes with changes in operational conditions of the reaction.

Implementation of this look-up table in the optimization loop is not straightforward and is more complicated than the mass balance. Additional variables like Temperature and pressure will also be added to the optimization problem. Also, linear interpolation and extrapolation techniques must be used to interpolate or extrapolate the value of the percentage NH3 produced if the operational conditions required for the reaction are in between or outside the range of temperature and pressure values shown in Figure 3.4. This method of mass modelling is simple yet more accurate than mass balance.

Equilibrium constants

"The equilibrium constant of a chemical reaction is the value of its reaction quotient at chemical equilibrium, a state approached by a dynamic chemical system after sufficient time has elapsed at which its composition has no measurable tendency towards further change. For a given set of reaction operational conditions, the equilibrium constant is independent of the initial analytical concentrations of the reactant and product species in the mixture. Thus, given the initial composition of a system, known equilibrium constant values can be used to determine the composition of the system at equilibrium. However, reaction parameters like temperature, solvent, and ionic strength may all influence the value of the equilibrium constant"(Wikipedia contributors, 2024c).

The most accurate form of mass modelling is by calculating the equilibrium constants from the given operational conditions using the equations shown below.

$$\log_{10}(K_p) = \frac{2250.322}{T} - 0.85430 - 1.51049 \log_{10} T - 2.58987 \times 10^{-4} T + 1.48961 \cdot 10^{-7} T^2 \quad (3.21)$$

$$K_p = \frac{P_{NH_3}}{P_{N_2}^{0.5} \cdot P_{H_2}^{1.5}} = \frac{\frac{n_{NH_3}}{n_T} P_T}{\left(\frac{n_{N_2}}{n_T} P_T\right)^{0.5} \left(\frac{n_{H_2}}{n_T} P_T\right)^{1.5}} = \frac{n_T}{P_T} \cdot \frac{n_{NH_3}}{n_{N_2}^{0.5} \cdot n_{H_2}^{1.5}} \quad (3.22)$$

$$P_{NH_3} = \frac{n_{NH_3}}{n_T} P_T; \; P_{N_2} = \frac{n_{N_2}}{n_T} P_T; \; P_{H_2} = \frac{n_{H_2}}{n_T} P_T \quad (3.23)$$

n_{H_2}	Hydrogen moles (kmol)	P_T	Total pressure (atm)
n_{N_2}	Nitrogen moles (kmol)	P_{NH_3}	Ammonia partial pressure (atm)
n_{NH_3}	Ammonia moles (kmol)	P_{H_2}	Hydrogen partial pressure (atm)
n_T	Total moles (kmol)	P_{N_2}	Nitrogen partial pressure (atm)

Equation 3.21,Equation 3.22,Equation 3.23 are referred from a scientific paper(Sánchez & Martín, 2018). For a given reaction's operational conditions like temperature T and Pressure P_T equilibrium constant K_p can be calculated using Equation 3.21.Once the K_p is obtained then subsituting K_p value in Equation 3.22 will give a relation between n_{NH_3},n_{H2} and n_{N2}.Using the mass balance relation in Equation 3.16 and this number of moles relation we can find the number of moles of H2, N2 and NH3 that exist in the equilibrium reaction.

This way of mass modelling is relatively more accurate than the other 2 options described previously. Although this method is accurate but adds more non-linearity to the linear optimisation problem in the EMS, because of this reason this method is not considered in further steps of this study .Out of the other 2 options for mass modelling mass balance is adopted for the further steps of this study since mass balance produces higher values of ammonia than the equilibrium look table. The highest percentage of ammonia in the look table is 85% whereas in the mass balance equation, it is 100% conversion. this enables us to analyse the extreme case of highest value addition in HPPs+GNH3 plants.

3.2.3. Power Modelling

Over the years energy consumption of various electrolysis-based HB processes has had a downward trend and still tends to improve with advancements in research and increasing competition between the equipment manufacturers. Figure 3.5 shows the exponential decreasing trend of energy consumption for green(electrified) HB process with increased ammonia production capacity. The legend in the Figure 3.5 lists different manufacturers of electrified HB process. Following this trend it can be expected that with an increase in the production size of the green HB plant, the specific energy consumption(kwh/kg of NH3) might decrease.

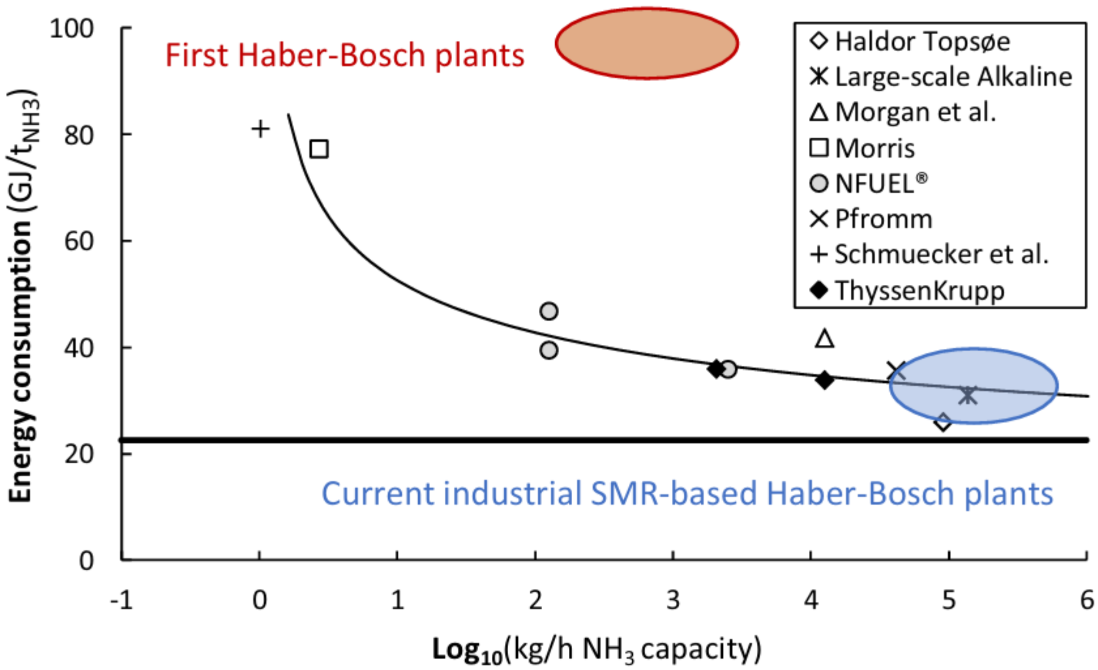


Figure 3.5: Electrified HB Energy consumption trend (Rouwenhorst et al., 2021).

Since each timestamp of this study is **1 hour**. Power and Energy terms can be interchanged because Power = Energy per unit time. The energy requirement per Kg of GNH3 production is in the range of 10.3-12.3 kWh/Kg of NH3.This number includes all the processes that consume electrical energy like compression, N2 separation from the atmosphere and Hydrogen production. Out of all these processes hydrogen production has the largest share in energy consumption. Break down is shown in Figure 3.6 . Air separation unit and Auxiliary power consumption like compression, and condensation uses very little power in comparison to H2 production for 1 kg of GNH3 production.

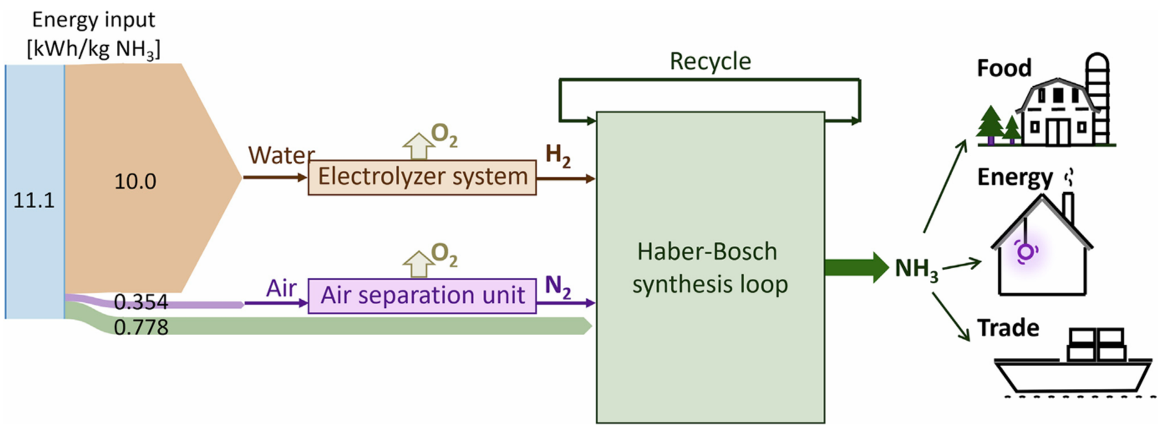


Figure 3.6: Energy consumption breakdown of HB process (Jain et al., 2022).

Specifications of Green(Electrified) HB process systems made by different companies are referred to get quantitative data for HB energy consumption.AMMpower is a Canadian clean energy company focused on the production of green ammonia. AMMpower's IAMM- Complete solution is taken as one of the industrial reference(AmmPower Corp, 2024) for the Electrified HB process. KAPSOM is a Chinese chemical solution provider for power to X solutions. It also supplied the world's first green ammonia plant in 2021.KAPSOM's GA-2000 plant is taken as another industrial reference(KAPSOM, 2024). This plant has a rated output capacity of 2000 Metric Ton per annum(TPA). Along with industrial references a published scientific paper used in Figure 3.6 is also compared(Jain et al., 2022).

Detailed energy consumption breakdown of electrified HB process using various references is shown in Table 3.3. As per the Table 3.2 1 kg of NH3 requires 0.17647kg of H2. Here the energy required for 0.17647 kg of H2 is calculated using an energy requirement of 50.10 kWh/kg value from HPC. This value is more than the HHV value of H2 as listed in this Table 2.1. This is due to the fact that some additional system losses will be there in the conversion from electrons to molecules and vice versa. Since HPC already includes the energy consumption for the H2 production, the respective kWh/0.17647kg of H2 value must be subtracted from different reference's HB energy consumption values, and then the energy consumption of only the HB process is obtained. This onlyHB(kWh/Kg of NH3) row includes processes like air separation units, startup heaters, pre & post-compression,s and condensations. With a pessimistic ideology amongst the 3 values in Table 3.3 the highest consumption value is modelled as an additional constraint in the EMS optimization.

$$P_{HB}(t) = 3.46 * m_{NH3}(t)/1000 \tag{3.24}$$

$P_{HB}(t)$ – HB power consumption in MW

The % of energy consumption for H2 over NH3 is in the range of 71%-86% according to the Table 3.3. Even from the discussions with industrial professionals, it is also confirmed that almost 90% of the energy consumption of electrified HB process is for the GH2 production.

	IAMM	**Scientific paper**	**KAPSOM**
Total HB (kWh/kg of $NH3$)	10.3^{1}	11.1^{2}	12.3^{3}
H2 ($kWh/0.17647kg$ of $H2$)	8.84	8.84	8.84
Only HB (kWh/kg of $NH3$)	1.46	2.26	3.46
$H2/NH3$ energy consumption(%)	85.85%	79.66%	71.89%

Table 3.3: Energy consumption breakdown of HB process using various references. [1](AmmPower Corp, 2024),[2](Jain et al., 2022),[3](KAPSOM, 2024).

3.2.4. Heat Modelling

HB process has an Exothermic heat output ΔH° of 46.14kJ/mol and mass output. After unit conversion, the final equation of heat output in MWh is written as

$$0 \leq Qout_{HB}(t) \leq Therm_{cap} \tag{3.25}$$
$$Qout_{HB}(t) = m_{NH3}(t) * 46.14 * 2.77778 * 10^{-7}/0.017 \tag{3.26}$$
$$Therm_{cap} = Am_{size} * 46.14 * 2.77778 * 10^{-7}/0.017 \tag{3.27}$$

$Qout_{HB}(t)$ – Exothermic Heat output in MWh
$Therm_{cap}$ – Maximum Exothermic Heat output in HPP+GNH3 system in MWh

This Equation 3.26 Equation 3.26 are considered as additional constraints in the EMS optimization.

Electric startup heaters

After various discussions with industry professionals, it was understood that the operational temperature of the electrified HB process is supplied through electric startup heaters. Whereas in conventional grey ammonia plants, these operational temperatures are obtained through process heat that comes from the steam methane reforming process which also supplies input feed gases to the HB process. The Exothermic heat in grey ammonia production is recovered and used in steam generation, preheating feed gases, and other parts of the front-end(before HB process) process of the reforming. some quantity of heat is inevitably lost to the environment.

Meanwhile, the exothermic heat of the electrified HB process can be stored as thermal energy for further use. it can be used in district heating systems etc and can make additional revenue for the developer. It can also be used to provide operational temperature for electrolyzers but since the operational temperature requirements of electrolyzers are much less than the HB process, this reflects that whole heat is not fully utilized in recovery. Currently, most of the heat output of the electrified HB process is not fully recovered in the front-end process of the plant, so this exothermic heat can create additional revenue for the GNH3 developer if the HPP+GNH3 system is properly designed.

Electric startup heaters are the proprietary technology of technology licensors of the HB process.Thermon is a Canadian company known for their expertise in industrial process heating. During an interview, they have presented that their products circulation heaters and immersion heaters are compatible and can be used as a electric startup heater for GNH3 plants. Thermon's immersion heaters can deliver temperatures of $650°$C(Thermon, 2024) which is more than the requirement of HB operational temperature. These Thermon heaters have power consumption up to **5MW**(Thermon, 2024).

Standby mode of HB process

As shown in Table 3.1 conventional HB plants do not have any concept of standby mode since the plant load factor(PLF) is almost 100%[1] for the conventional plants for maximizing production for profit of the plant owner. This is possible due to the constant electricity supply from the NG/Coal thermal power plants in the front end. The plant load factor is very similar to the capacity factor(CUF or CF).In GNH3 plants to achieve a constant output flow of GNH3 for maximum profit to the developer, constant electricity and GH2 inputs are required. However, constant flows of both EE and GH2 are difficult due to fluctuations in renewable energies. Any interruption in this constant flow of EE and GH2 will cause the electrified HB plant to trip and go into shutdown mode. As discussed in thesubsection 3.2.1, the startup and shutdown times of the HB process are in the range of a couple of hours. This implies that switching to an electrified HB process is a hassle process yet inevitable due to fluctuations in renewable energies. This creates a necessity for standby mode for the electrified HB process. For example, electrolyzers have stand mode which helps them avoid time delays from switching from off to on or vice versa. Instead, the quick jump can be made from standby mode to on or vice versa.

To keep the electrified HB process in standby mode it is necessary to provide operational temperature to the system all the time, which is not possible with electric startup heaters alone. **Professor Dr.Fokko Mulder** from Delft University of Technology saw this as a research challenge and filed a patent named "Periodic Ammonia production" which is a methodology of operating the electrified HB process by taking an exothermic heat loop. This methodology enables the electrified HB process to be always in on or standby mode. Schematic of the patented methodology is shown in

[1] Information from interviews with HB site supervisors and engineers.

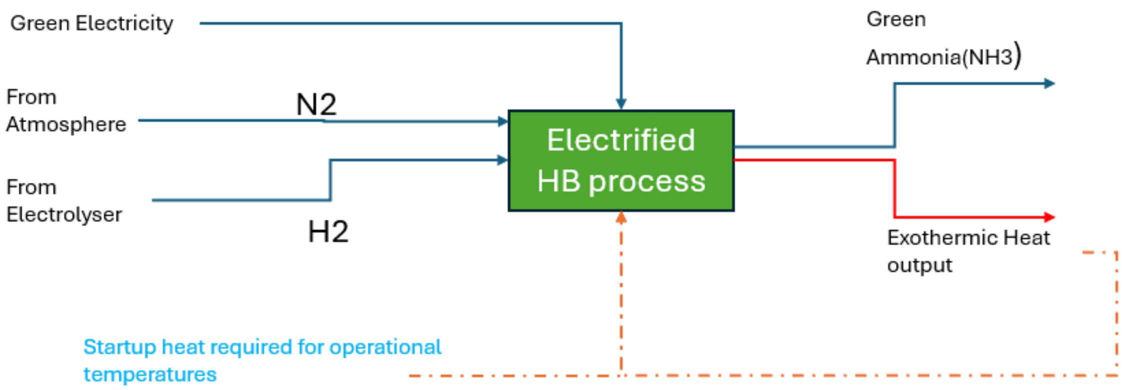


Figure 3.7: Schematic of a patented methodology of HB standby mode (Mulder, 2023).

Along with this research study, validation of the above-patented methodology is conducted in an entrepreneurial way through the TUdelft Impact studio. Multiple interactions with different industrial stakeholders are done in different ways like interviews, emails, and conference discussions. All such interactions helped this study to get the latest market information and key qualitative data for this study. The research process flow diagram is already shown in Figure 2.1. This research study excludes the standby mode of the green HB process in the modelling, analysing, and optimization parts of the study.

3.2.5. Different Objective functions of EMS

The EMS optimization problem formulated in the section 3.2 describes the EMS with an objective function making choices with 2 types of energy forms EE and GH2.In this study 3rd form of energy vector GNH3 is also added, so it is necessary to make multiple combinations of objective functions to have different combinations of multiple revenue streams to the RPDs.All possible combinations of energy vectors for the objective function of EMS are listed in Table 3.4.

1 Energy vector	2 Energy vectors	3 Energy vectors
EE	EE+GH2	EE+GH2+GNH3
GH2	**EE+GNH3**	
GNH3	GH2+GNH3	

Table 3.4: Combinations of energy vectors for objective function in EMS

Objective function-2: Choice between either electrical energy(EE) or Green Ammonia(GNH3).This objective function is the main focus of this research study. The actual value addition of GNH3 to HPPs is analyzed through the optimum value of this objective function.

$$\textbf{\textit{EE+GNH3}} : \max_t \sum_t \{P_{hpp}(t) \cdot price_{elec}(t) + (m_{NH3}(t) \cdot price_{NH3}(t))/1000\} - I_b \tag{3.28}$$

$price_{NH3}(t)$ – Green Ammonia selling price in €/Tonne

Objective function-3: Choice between 3 types of energy vectors electrical energy(EE), Green Ammonia(GNH3) or Green Hydrogen(GH2).This type of 3 revenue streams in GNH3 plants are yet to be explored by RPDs.Based on interviews with industrial professionals it came to know that this is something more complex and hard to realize in this current market scenario having difficulties in finding off-takers for green molecules. Analysis and optimization of results obtained with this objective function were excluded in this study.

$$\textbf{\textit{EE+GH2+GNH3}} : \max_t \sum_t \{P_{hpp}(t) \cdot price_{elec}(t) + m_{H2}(t) \cdot price_{H2}(t) + (m_{NH3}(t) \cdot price_{NH3}(t))/1000\}\} - I_b \tag{3.29}$$

Objective function-3: Only electrical energy(EE) in the objective function means that revenue is solely dependent on EE production.

$$\textbf{\textit{EE}} : \max_t \sum_t \{P_{hpp}(t) \cdot price_{elec}(t)\}\} - I_b \tag{3.30}$$

All Constraints of EMS

All constraints are listed below along with the additional constraints made for GNH3 plants.

Existing constraints:

$$\begin{aligned}
0 \leq P_{hpp}(t) &\leq G_{MW} \\
P_{hpp}(t) &= P_w(t) + P_s(t) + P_{batt}(t) - P_{ptg}(t) - P_{curt}(t) \\
P_{curt}(t) &\geq 0 \\
I_b &\geq 0 \\
-P_{battMW} &\leq P_{batt}(t) \leq P_{battMW} \\
E_{battMWh}(1 - Batt_{DOD}) &\leq E_{SOC}(t) \leq E_{battMWh} \\
E_{SOC}(t+1) &= \begin{cases} E_{SOC}(t) - P_{batt}(t)\Delta t \eta_{ch} & \text{if } P_{batt} < 0 \\ E_{SOC}(t) - P_{batt}(t)\Delta t/\eta_{disch} & \text{if } P_{batt} > 0 \end{cases} \\
0 \leq P_{ptg}(t) &\leq P_{ptgMW} \\
m_{H2}(t) &= HPC(P_{ptg}(t)) \\
HPC(P_{ptg}(t)) &= \eta(P_{ptg}(t)) \cdot P_{ptg}(t) \cdot 1000/HHV
\end{aligned}$$

Additional GNH3 constraints:

$$\begin{aligned}
0 \leq m_{H2}(t) &\leq H2_{max} \\
0 \leq m_{N2}(t) &\leq N2_{max} \\
0 \leq m_{NH3}(t) &\leq Am_{size} \\
0 \leq Qout_{HB}(t) &\leq Therm_{cap} \\
m_{N2}(t) &= m_{H2}(t)/Feedratio \\
m_{NH3}(t) &= m_{H2}(t) + m_{N2}(t) \\
P_{HB}(t) &= 3.46 * m_{NH3}(t)/1000 \\
Qout_{HB}(t) &= m_{NH3}(t) * 46.14 * 2.77778 * 10^{-7}/0.017
\end{aligned}$$

Additional equations: These are time-independent equations. All below equations result in upper limits of the variables in the additional constraints added to the EMS due to GNH3 addition in the system.

$$
\begin{aligned}
Feedratio &= 0.17647/0.82353 = 0.214285 \\
H2_{max} &= HPC(P_{ptgMW}) \\
N2_{max} &= (H2_{max}/Feedratio) \\
Am_{size} &= (1 + 1/Feedratio) * H2_{max} \\
Therm_{cap} &= Am_{size} * 46.14 * 2.77778 * 10^{-7}/0.017
\end{aligned}
$$

Since the optimization solver mainly focuses on the objective function and related variables in it. For every objective function-1,2,3, all the constraints(existing and additional GNH3) are enabled in the code while generating results.

3.3. Financial Modelling

Financial modelling in HyDesign is made using 2 explicit components of OpenMDAO framework. All the costs of the generating sources, batteries, electrolyzers and HB process are coded in the Cost component. All the financial metrics like Levelised cost of energy(LCOE), Net present value(NPV) etc. are coded in the Finance component. This section only illustrates the costs and financial metrics for green ammonia production in HyDesign.Detailed information about all the costs components and equations of existing generating sources, batteries, and electrolyzers are shared in the HyDesign detailed paper(Murcia Leon et al., 2024).

3.3.1. Cost Modelling

As shown in the Table 3.1, the electrified HB processes are costlier than the conventional HB processes. This is due to the very high costs of the associated infrastructure and GH2 costs since, not many green HB process plants are up and running in the world. With the current market situation, it is difficult to find an off-taker for green molecules, and it might take significant time to achieve economies of scale, but will definitely happen[1].

After an extensive search for costs in the latest academic papers, consultant reports, and available pre-feasibility reports of the announced GNH3 projects. Recent Deloitte's comprehensive report on green ammonia market assessment to government of India(Deloitte India , 2023) is taken as the reference of costs for this study. HB process is a large-scale chemical plant with many internal processes and related equipment.it is possible to make a detailed breakdown of costs for conventional HB plants but for the green HB process, the latest information on detailed cost breakdown of all internal equipment is still hard to get. Conventional plants will have fixed equipment costs and variable fuel and other costs.As shown in **??** the whole HB process is modelled as a black box in process, the total capital expenditure(Capex) and Operational expenditure(Opex) are collected for the whole HB process which includes costs of the all internal processes like compression, N2 separation, condensation, startup heating, etc. Since NH3 storage and transportation are excluded in this study, respective costs are omitted from the total Capex and Opex values.

Since the last few decades, only a few technology licensors of HB process exist in the world. This trend is changing now due to more and more technology licensors emerging in the GNH3 market. All the renowned existing players like **TOPSOE**, **CASALE**,**ThyssenKrupp(Uhde)** have similar cost ranges[2]. Whereas their Chinese counterparts have almost **1/3rd** of costs[2]. Different units of costs are also explored Like Capex costs per size of the ammonia plant for example a typical ammonia plant of 1MMTPA has 600 Million$ which scales with an exponent of 0.6[2].

[1] Different opinions were captured during interviews with different stakeholders of the green ammonia industry.
[2] Interviews and email exchanges with GNH3 Developers and consultants.

	$Capex_{HB}$	$Opex_{HB}$	Remarks
Haber bosch process	2660(€/tonne)	53.2(€/tonne)	Opex=2% Capex

Table 3.5: Capital and Operational expenditure of Green HB process(Deloitte India , 2023).

According to the Deloitte report the impact of renewable energy capacity factor on HB process capex is negligible. Hence the cost figures are taken independent of capacity factors. The penalty price for not meeting the green ammonia demand committed in an hour is called a penalty factor of GNH3. it is taken as 0 and excluded in the further analysis of this study. This is because most of the green ammonia plants will have long-term offtake agreements, and the penalty terms and conditions vary according to the negotiations between suppliers and off-takers. Unlike power-purchase agreements(PPA) and hydrogen purchase agreements(HPA), ammonia purchase agreements are not coined in the industry. There are many memoranda of understanding (MOUs) signed between suppliers and off-takers, but a number of final investment decisions(FIDs) are still less as shown in Figure 1.4. Green Ammonia Sale Agreement(GASA) was coined by the government of India through a recent green ammonia tender in 2024 which subsides the RPDs and makes 10-year green ammonia purchase agreements. Germany also launched a green ammonia tender in 2023 through the H2Global Foundation. Subsidies for green ammonia production are also excluded from this study.

$$Capex_{P2A} = Am_{size} * Capex_{HB} * 365 * 24/1000 \tag{3.31}$$
$$Opex_{P2A} = Am_{size} * Opex_{HB} * 365 * 24/1000 \tag{3.32}$$

$Capex_{P2A}$ – Total Capex of HB process in HPP+GNH3 system in €
$Opex_{P2A}$ – Total Opex of HB process in HPP+GNH3 system in €

Since EMS in Hydesign optimizes the revenue for an RPD, so there might be times when green ammonia is not fully produced in an hour. But costs for the production of such minimal ammonia production must still be considered. For example few hours in a year produce full ammonia capacity, whereas other few hours produce less than full capacity but still, costs are considered equal for all the hours so that the total costs are independent of time and production capacity. Because of these reasons, the known $Capex_{HB}$ and $Opex_{HB}$ values in €/tonne are multiplied by the known maximum ammonia production of the plant Am_{size} and the total number of hours in a year. The final Capex and Opex formulations for HB process in HPP+GNH3 systems can be shown in Equation 3.31 and Equation 3.32.

XDSM

3.3.2. Financial metrics Modelling

All relevant financial metrics are computed in the Finance component of the Hydesign of HyDesign.Along with LCOE and NPV, LCOH, LCOA and NPV/Capex are also computed. All cost values are in €s including capex and opex values of all energy vectors.

$$C_T = C_W + C_S + C_{batt} + C_{H2} + C_{el} + Capex_{P2A} \tag{3.33}$$
$$O_T = O_W + O_S + O_{batt} + O_{H2} + O_{el} + Opex_{P2A} \tag{3.34}$$
(3.35)

C_T – Total Capex of HPP+GNH3 system, C_W – Capex of Wind plant,
C_S – Capex of Solar plant, C_{batt} – Capex of batteries,

C_{H2} – Capex of Electrolyser system, C_{el} – Capex of electrical infrastructure and land,
O_T – Total Opex of HPP+GNH3 system, O_W – Opex of Wind plant,
O_S – Opex of Solar plant, O_{batt} – Opex of batteries,
O_{H2} – Opex of Electrolyser system including water, O_{el} – Opex of electrical infrastructure and land.

Weighted average cost of capital after tax($WACC_{tx}$) here is the weighting sum of the $WACC$s for wind, solar, battery, electrolyzer, HB process and electrical by their corresponding Capex, taking the mean WACC for the electrical costs shared across all technologies.

$$WACC_m = (WACC_W + WACC_S + WACC_{batt} + WACC_{H2} + WACC_{P2A})/5 \quad (3.36)$$

$$WACC_{tx} = (C_W * WACC_W + C_S * WACC_S + C_{batt} * WACC_{batt} + C_{el} * WACC_m + WACC_{H2} * C_{H2} + WACC_{P2A} * Capex_{P2A})/C_T \quad (3.37)$$

The financial model then estimates the yearly incomes (I_y) and cashflow (F_y) as a function of the average revenue over the year(R_y), the tax rate ($r_t ax$) and $WACC_t x$. Net present value (NPV) and levelized costs of energy (LCoE) can then be calculated using the $WACC_t x$ as the discount rate, as well as the internal rate of return (IRR).

$$\text{Revenue } R_y = \text{ is the solution of objective functions } [EE] \text{ or } [EE + GNH3] \text{ or } [EE + GNH3 + GH2] \text{ .} \quad (3.38)$$

$$\text{Net income} = \text{Revenue} - O_T \quad (3.39)$$

$$\text{Annual cashflow}(i_y) = \text{Net income}(1 - r_{tax})(1 - WACC_{tx}) \quad (3.40)$$

$$\text{Cashflow } F_y = \begin{cases} -C_T, & y = 0 \\ i_y, & y > 0 \end{cases} \quad (3.41)$$

$$\text{Net present value } NPV = \sum F_y(1 + WACC_{tx})^{-y} - C_T \quad (3.42)$$

$$0 = \sum i_y(1 + IRR)^{-y} - C_T \quad (3.43)$$

$$\text{Annual EE production } AEP_y = \left\langle \sum P_{hpp}(t)(t) \right\rangle_y \quad (3.44)$$

$$\text{Annual H2 production } AHP_y = \left\langle \sum m_{H2}(t)(t) \right\rangle_y \quad (3.45)$$

$$\text{Annual NH3 production } AAP_y = \left\langle \sum m_{NH3}(t)(t) \right\rangle_y \quad (3.46)$$

$$\text{Grid utilisation factor } GUF = \sum P_{hpp}(t) / \sum G_{MW} \quad (3.47)$$

Levelised Cost of Electricity (LCoE):

LCoE is the ratio of Total costs for electricity production over the total electricity production. The net electricity production NEP_y includes the electricity production for the electrolyzer and HB process. C_T is the total cost for all units of electricity production.

$$NEP_y = AEP_y + \left\langle \sum P_{ptg}(t)(t) + \sum P_{HB}(t)(t) \right\rangle_y \tag{3.48}$$

$$\text{Total Costs for all units of electricity } C_L = \sum_y (O_T(1 + WACC_{tx})^{-y}) + C_T \tag{3.49}$$

$$\text{Total EE production } NEP_L = \sum_y (NEP_y(1 + WACC_{tx})^{-y}) \tag{3.50}$$

$$LCoE = \frac{C_L}{NEP_L} \tag{3.51}$$

Levelised Cost of Hydrogen (LCoH):

LCoH is the ratio of total costs for hydrogen production over the total hydrogen production. The Total hydrogen production NHP_L will taken Annual hydrogen production AHP_y over lifetime with $WACC_{H2}$ as the discount ratio. Total costs for hydrogen production C_{H2L} will also include the costs of electricity for hydrogen production along with the costs of hydrogen production alone. The costs of electricity for hydrogen production are computed using LCoE as shown in Equation 3.52.

$$\text{Opex EE Costs for H2 production } O_{PTG} = LCoE * \sum_y P_{ptg}(t) \tag{3.52}$$

$$\text{Total Costs for H2 production } C_{H2L} = \sum_y (O_{H2}(1 + WACC_{H2})^{-y}) + C_{H2} + O_{PTG} \tag{3.53}$$

$$\text{Total H2 production } NHP_L = \sum_y (AHP_y(1 + WACC_{H2})^{-y}) \tag{3.54}$$

$$LCoH = \frac{C_{H2L}}{NHP_L} \tag{3.55}$$

Levelised Cost of Ammonia (LCoA):

LCoA is the ratio of total costs for NH3 production over the total NH3 production. The Total NH3 production NAP_L will take annual NH3 production AHP_y over a lifetime with $WACC_{P2A}$ as the discount ratio. Total costs for NH3 production C_{H2L} will also include the costs of electricity for NH3 production along with the costs of NH3 production alone. The costs of electricity for NH3 production are computed using LCoE as shown in Equation 3.56.

$$\text{Opex EE Costs for NH3 production } O_{P2A} = LCoE * \langle \sum_y P_{ptg}(t) + \sum_y P_{HB}(t) \rangle \tag{3.56}$$

$$\text{Total Costs for NH3 production } C_{NH3L} = \sum_y (Opex_{P2A}(1 + WACC_{P2A})^{-y}) + Capex_{P2A} + O_{P2A} \tag{3.57}$$

$$\text{Total NH3 production } NAP_L = \sum_y (AAP_y(1 + WACC_{P2A})^{-y}) \tag{3.58}$$

$$LCoA = \frac{C_{NH3L}}{NAP_L} \tag{3.59}$$

Break-Even prices:

The break-even prices are calculated by running an optimisation to minimize the NPV^2 value. NPV can be positive or negative, but while running an optimization to get a minimum price to make the project profitable, we need another non-negative metric.So,NPV^2 is considered the objective function for the internal optimization to compute breakeven prices.

4 types of breakeven prices are calculated in the Finance component of Hydesign which are:

1. **Break-even PPA price for H2** :- The minimum required PPA electricity price $price_{elec}(t)$ for given $price_{H2}(t)$ to break even that means NPV^2 is 0.
2. **Break-even PPA price for NH3**:- The minimum required PPA electricity price $price_{elec}(t)$ for given $price_{NH3}(t)$ to break even that means NPV^2 is 0.
3. **Break-even H2 price**:- The minimum required $price_{H2}(t)$ to break even that means NPV^2 is 0.
4. **Break-even NH3 price**:-The minimum required $price_{NH3}(t)$ to break even that means NPV^2 is 0.

3.4. Sizing optimization

HyDesign has 2 main functionalities **Evaluation** and **Sizing Optimisation** of the given design.EMS of HyDesign takes care of the evaluation function. The Sizing Optimisation functionality is made using the surrogate-based optimization concept. This surrogate-based optimization is used as the outer sizing optimisation to reduce the full model evaluations during a gradient-based optimization (Murcia Leon et al., 2024).This is sizing optimization is forced to only take integer values of the design variables.

$$\text{min } y(x) \tag{3.60}$$

$$y(x) = \begin{cases} -[NPV/C_T](x) \\ -NPV(x) \\ LCoE(x) \\ LCoA(x) \end{cases} \tag{3.61}$$

$$x = [h_c, sp, p_{rated}, \rho_W, \theta_{tilt}, \theta_{azim}, r_{DCAC}, B_{Eh}, Feedratio, N_{wt}, S_{MW}, B_P, PTG_{MW}, G_{MW}, price_{NH3}] \tag{3.62}$$

$$\text{s.t.} \quad D = 2\sqrt{P_{rated}/(\pi sp)} \tag{3.63}$$

$$hh = h_c + D/2 \tag{3.64}$$

$$W_{MW} = N_{wt} p_{rated} \tag{3.65}$$

$$A_w = W_{MW}/\rho W \tag{3.66}$$

$$B_E = B_{Eh} * B_P \tag{3.67}$$

h_c – Turbine rotor clearance w.r.t ground
sp – Specific power of turbine in (W/m2)
p_{rated} – rated power of turbine
ρ_W – Installation density of wind farm in (MW/km2)
θ_{tilt} – Surface title in solar plant
θ_{azim} – Azimuth of the solar plant
r_{DCAC} – DC-AC ratio of solar plant.
B_{Eh} – No of Hours of Battery discharge

N_{wt} – Number of wind turbines in wind plant
S_{MW} – Solar plant rated AC capacity
B_P – Battery power user input
PTG_{MW} – Power to electrolyzer user input

Here the $-[NPV/C_T](x)$ is preferred more as the objective function instead of NPV. This is because NPV is a measure of the absolute profit of the project since it's a summation of the initial investment and the present value of the future revenues. Since it's not normalized, it is often used to compare the returns of different projects with a similar initial investment. For a design problem where the investment varies with a change in the design variables, the use of NPV can be problematic(Mehta et al., 2024).

The variables in orange color are fixed variables in this optimization whereas the variables in violet text are the design variables. Fixed variables are fixed throughout the optimization search space, design variables change within the defined limits.

4

Site Selection and Modelling Checks

To generalise and justify the value addition(if any) of the GNH3 system to the HPP system, different types of resource data must be analysed through the developed model. Different locations across the world will have different renewable resource characteristics. Evaluating the value addition in at least a few of the selected locations will provide some confidence in the results to achieve the research goal. what are the few theoretical and practical aspects that must be chosen for the site selection hypothesis for research validations will be discussed in further sections of this chapter. Along with the site selection method, different modelling checks are also explained.

4.1. Site Selection

In this vast world renewable resource distribution is not very uniform. Regions which have rich wind potential have average or below-average solar potential, whereas regions which have good solar potential have very minimal wind potential. For example, Northwest Europe has good wind potential but average solar potential, whereas Saudi Arabia has good solar potential and average wind potential. One of the benefits of the HPPs is the relatively stable output due to the complementarity of the renewable resources as listed in subsection 2.2.1. Since, the study is about HPPs with GNH3 system, to achieve a stable output from HPP, it is logical to have a generation source with complimentary resource distribution. The Focus of the study is HPP+GNH3 plant with wind and solar as a renewable resource. So, the site selection hypothesis will only be focused on the wind and solar potentials of the site.

Based on the complementarity requirement of HPPs, 4 extreme combinations of wind and solar potentials are listed.

1. Good wind + Bad solar
2. Good wind + Good solar
3. Bad wind + Bad solar
4. Bad wind + Good solar

Here Good and Bad terms are relative to each of the renewable resources. Free opensource resources like Global wind atlas and Global Solar atlas are referred to search for the regions which match listed 4 combinations of extremity of potentials. Along with complementarity, individual resource characteristics and their location at a global scale also play a major role in site selection for this study.

Starting with solar resources, different seasons are caused by the earth's rotation around the sun. The

Tropic of Cancer[23°27'N], also known as the Northern Tropic, is the Earth's northernmost circle of latitude where the Sun can be seen directly overhead. This occurs on the June solstice when the Northern Hemisphere is tilted toward the Sun to its maximum extent(Wikipedia contributors, 2024f). It also reaches 90 degrees below the horizon at solar midnight on the December Solstice. The **Tropic of Capricorn[23°27'S]** (or the Southern Tropic) is the circle of latitude that contains the subsolar point at the December (or southern) solstice. It is thus the southernmost latitude where the Sun can be seen directly overhead. It also reaches 90 degrees below the horizon at solar midnight on the June Solstice. Its northern equivalent is the Tropic of Cancer (Wikipedia contributors, 2024g).

A solstice is one of the two times of the year when the positioning and tilt of Earth relative to the sun results in the most amount of daylight time(June solstice) or the least amount of daylight time in a single day(December solstice). Equinox is one of the two times of the year when the amount of daylight and nighttime hours are equal in length. The vernal equinox(March) marks the start of spring, and the autumnal equinox(September) marks the start of fall(Dictionary.com, 2024).

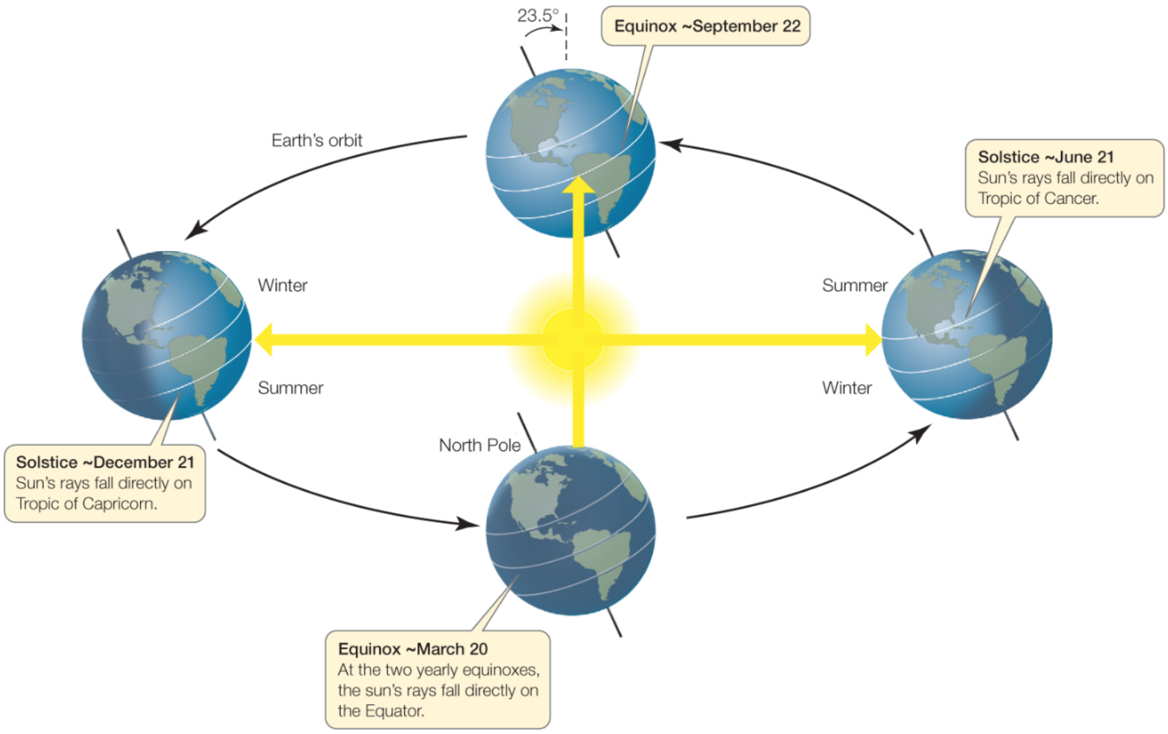
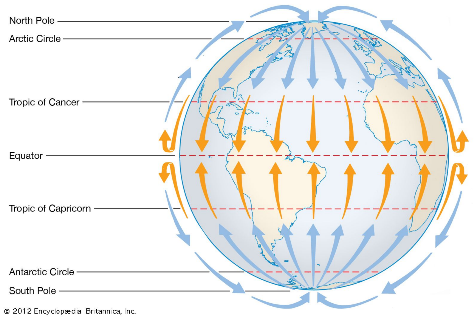


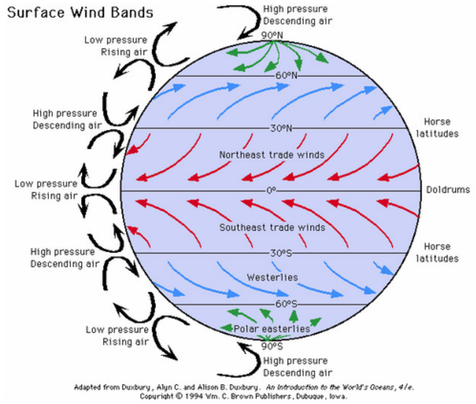
Figure 4.1: The Tilt of Earth's Axis of Rotation (Macmillan Learning, 2024).

As shown in Figure 4.1. The possibility of the overhead sun at any location on Earth at any time of the year is only between the tropic of Cancer and the tropic of Capricorn. For solar panels to produce maximum energy direct normal(perpendicular) irradiation is required. Hence we can deduce that most of the solar-rich regions are in between the tropics of Cancer and Capricorn. The same observation can be seen in the PV power potential map of the global solar atlas.

The heat of the Sun causes winds around the world. It heats the tropical zone more than the polar regions because its rays are more direct at the equator. The hot and light air in the tropics rises seen in Figure 4.2a and flows toward the two poles. Meanwhile, the cold and heavy air from the poles moves toward the equator(Britannica Kids, 2024). Due to the Earth's self-rotation on its axis causes the Coriolis effect which helps determine the direction of planetary, or global, winds by causing them to curve, or deflect, as the Earth rotates. In the Northern Hemisphere, winds curve to the right in the direction of motion. Air moving toward the equator curves to the west, while air moving away from the equator curves to the east can be clearly shown in Figure 4.2b. This pattern is reversed in the



(a) Wind generation(Britannica Kids, 2024)



(b) Planetary(global) winds (James, 2024).

Figure 4.2: Global wind patterns.

Southern Hemisphere, where winds curve to the left in the direction of motion winds moving toward the equator curve to the west, and winds moving away from the equator curve to the east. The difference in temperature between land and sea also influences global winds. Offshore sites across different coastal areas of the world are rich in wind potential due to lower surface roughness and uniform topography in comparison to land causing lesser obstruction to wind flows.

These planetary winds are generated in altitudes much higher(>40k Km) than the wind power plants which are in atmospheric boundary layer level(1km height). Still, the planetary wind patterns are important since they are the cause of the generation of different wind zones across the global. From Figure 4.2 the high pressure descending air flows after latitudes near to tropics and poles. Low-pressure ascending air is near the equator. This is the reason why the wind power potential seen in the global wind atlas is less between the tropics [30°N -30°S] and more above the tropics.

From Figure 4.1 and Figure 4.2 it is evident that the global wind and solar patterns change significantly around the tropics [23°27'N -23°27'S] and have complimentary patterns. Keeping these global patterns in site selection and also with the 4 combinations of extremity mentioned earlier Few regions are shortlisted with the help of global solar and wind atlas power potential maps as shown in the table.

Good Wind + Good Solar	**Good Wind + Bad solar**	**Bad Wind +Bad Solar**	**Bad wind + Good solar**
Namibia Chile Perth, Australia	New Zealand St,johns, Canada Bella core Canada Japan islands	Democratic republic of congo Chengdu china	Saudi Arabia Sudan

Table 4.1: Few selected regions for HPP model verification.

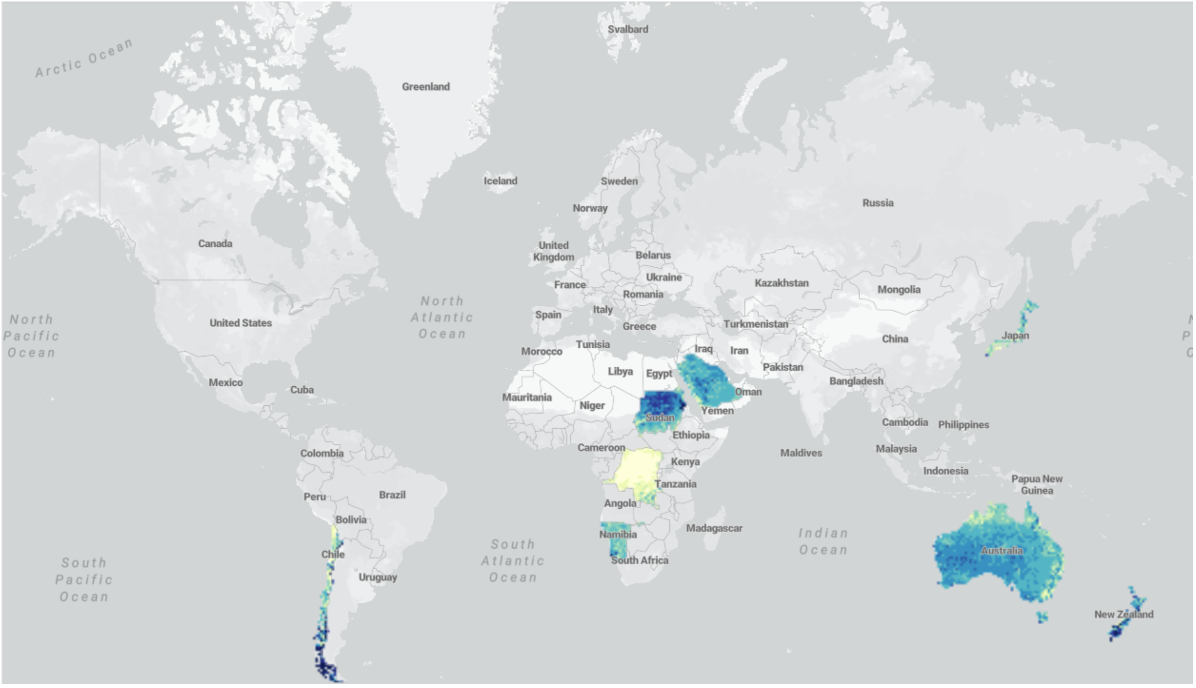


Figure 4.3: Few selected countries' wind potential (National Renewable Energy Laboratory, 2024)

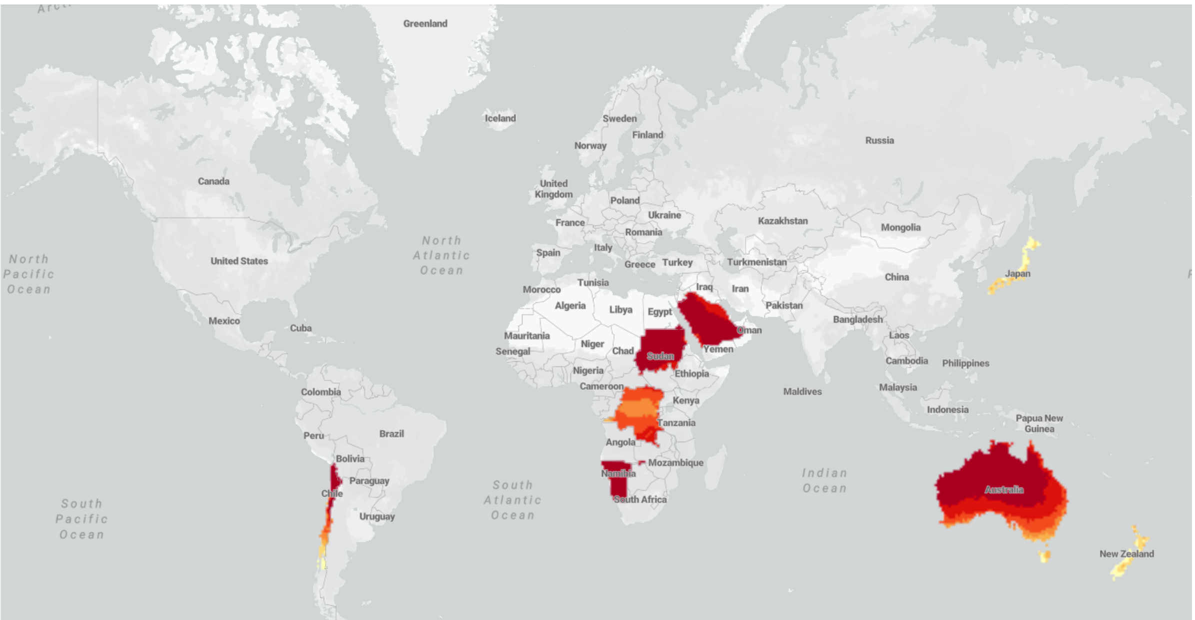


Figure 4.4: Few selected countries' solar potential (National Renewable Energy Laboratory, 2024)

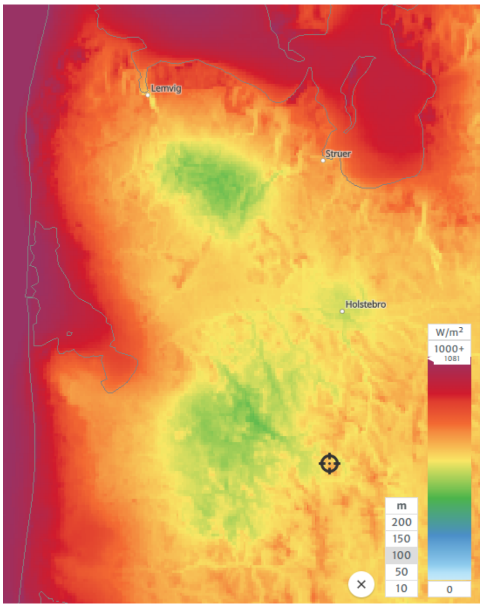
The selected countries are either inside the tropical region or near the verge of the tropical region. In a few of the selected countries in Figure 4.3 and Figure 4.4 it is clearly visible that few regions with dark red solar potential have lighter blue wind potential and vice versa. Based on a brief theoretical explanation of global resource patterns a hypothesis can be made that these locations can be well fitted for model verifications of HPPs because of their complimentary resource potentials. A Detailed resource analysis on annual and diurnal patterns is well suggested for justification of the hypothesis, but it is excluded from this study.

Along with resource potential, there are also other important aspects in site selection like suitable land area, Distance to Grid substation and port facilities. Topology is important for wind resources due to changes in surface roughness and turbulence characteristics. similarly, topology is also important for the solar resource, a level-graded land is preferred to avoid inter-panel and inter-array shadows on panels. To avoid huge power transmission losses and leakage losses due to the transportation of green molecules, it is strongly recommended to search a site near the grid substation and port facilities.

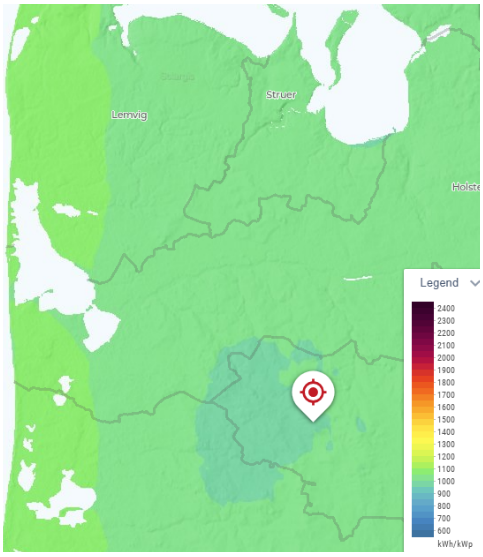
This explained site selection hypothesis is the first step for making a site selection criteria. Site selection criteria are important to select appropriate sites which cover all extreme cases of resource characteristics, this helps in observing the HPP generation behaviours through developed mathematical models and extensions to such models. Due to the limited availability of data, this study is confined to a single location for analysis of GNH3 model results.

4.2. Base case study

Due to the latest hourly resource data availability issues and weather-correlated electricity price availability issues at all sites. An existing site in the Hydesign database is considered as the base case for the rest of this study. The site is in **Denmark** and electricity prices for the year **2012** are taken for this study.



(a) Basecase wind power potential(Global Wind Atlas, 2024).



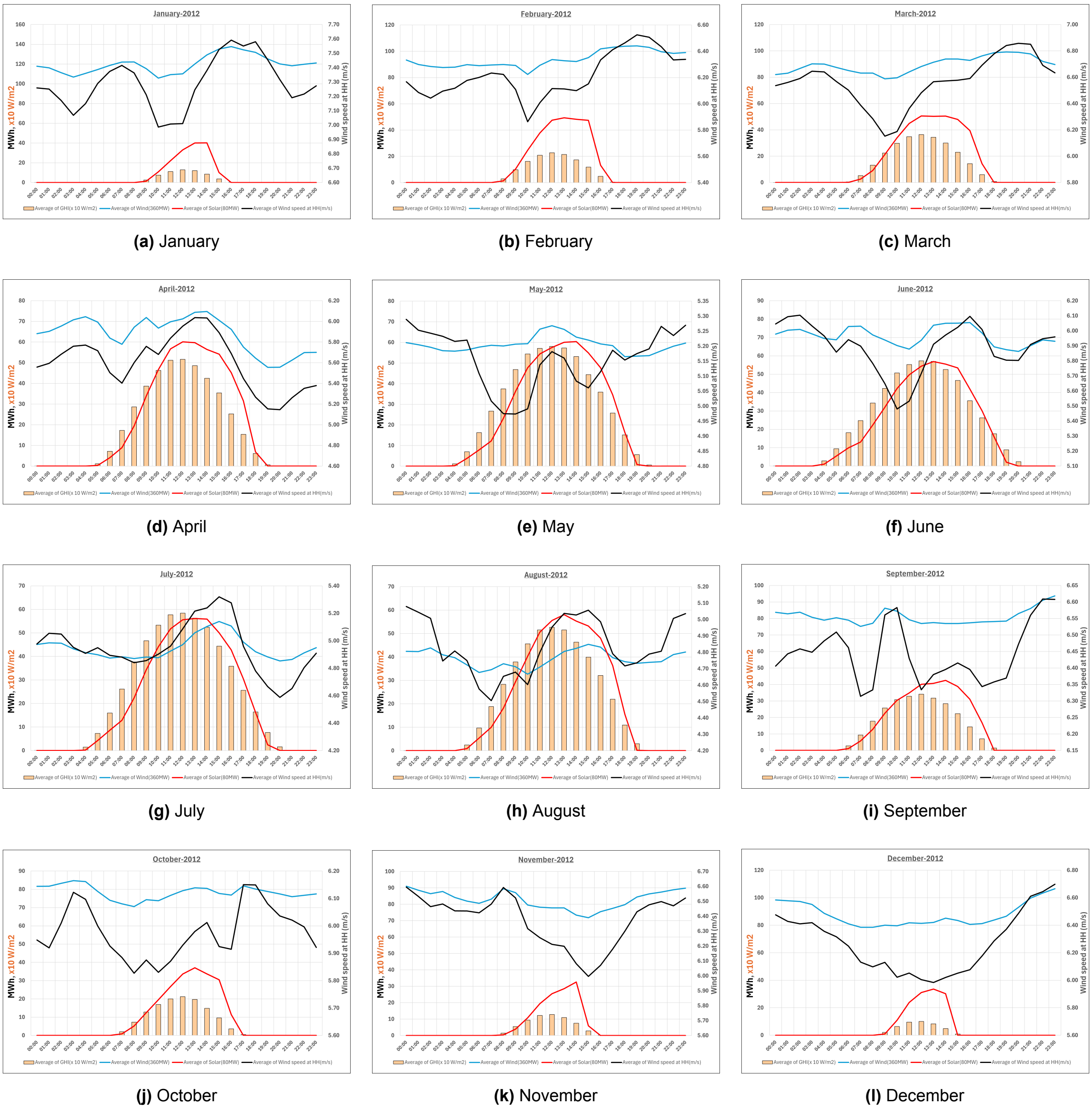
(b) Basecase solar power potential(Global Solar Atlas, 2024).

Figure 4.5: Basecase renewable resource power potentials at
Latitude: $56^{\circ}.227322^{'}$N, Longitude :$8^{\circ}.594398^{'}$E, Altitude:85m

4.2.1. Base case resource details

For a base-case site, the average diurnal resource and generation profiles for all months in 2012 are shown in Figure 4.6. The wind speed is calculated from the weather component of the Hydesign, whereas the Global horizontal irradiance(GHI) and solar generation are calculated from the solar component.The Wind generation is calculated from the wind component. From the overview of the 12 monthly resource profiles in Figure 4.6 it is clear that GHI is increasing trend from March till September, out of these months, the April to August months were good GHI hence good solar generation.During April to August, the mean wind speed values show a decreasing trend, consequently lower wind generation.But from September to March Wind speed has an increasing trend resulting in higher wind generation.During these months of good wind generation, the solar generation is worse.

Summer months April to August solar generation is good and wind generation is relatively worst.In contrast in the winter months September to March wind generation is good and solar generation is relatively worst.The annual wind plant generation, solar plant generation and their sum named as total generation is shown in Figure 4.7c.



(a) January **(b)** February **(c)** March

(d) April **(e)** May **(f)** June

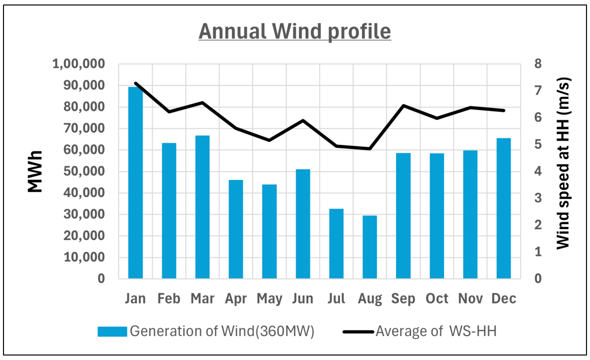
(g) July **(h)** August **(i)** September

(j) October **(k)** November **(l)** December

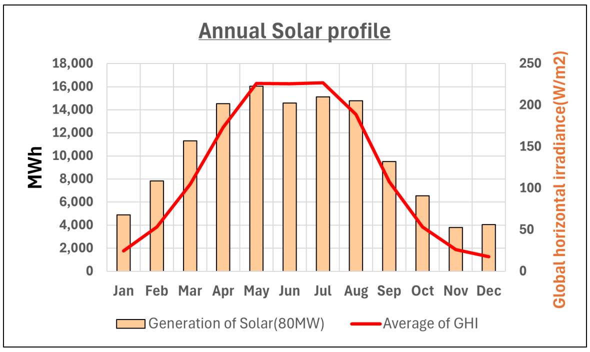
Figure 4.6: Average diurnal resource profiles and generation profiles for all months in 2012.

In Figure 4.7a the wind generation follows the mean wind speed profile. For a 360MW-rated wind plant capacity has a total annual generation of 662.59 Giga watt hours(GWh). This can also be written as 662.59 million units(kWh) of electricity.This wind plant has a capacity factor(CF) of 21%.Out of all months July and August have least wind generation. January, March and December have highest wind generation.The percentage change of generation from month to month is more in transition from june to july and august to September.

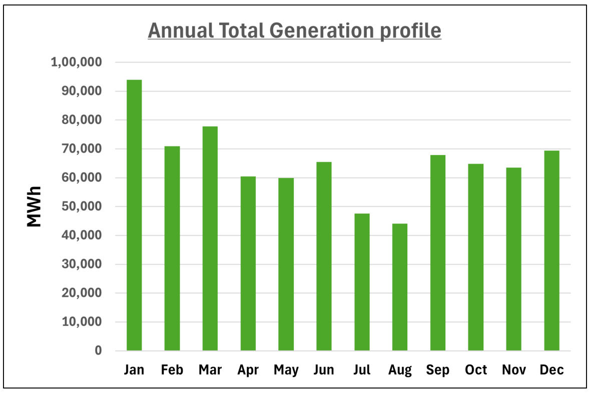
In Figure 4.7b the solar generation follows the average GHI profile. For a 80MW-rated solar plant capacity has a total annual generation of 123GWh and CF of 17.55%.Out of all months January, November and December have least solar generation. May to August months have the highest solar generation. The percentage change of generation from month to month is more in transition from jan to Feb and august to september.



(a) Annual Wind resource and generation profile.



(b) Annual Solar resource and generation profile.

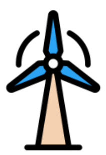


(c) Annual Total generation profile.

Figure 4.7: Annual resource and generation profiles.

In Figure 4.7c the sum of wind and solar plant generations are shown. This sum is termed as a total generation. The total annual generation of 785.61GWh.Out of all months July and August have the least total generation. January to march and December have the highest total generation.The percentage change of generation from month to month is more in transition from june to july and august to September.From all the 3 profiles in Figure 4.7 it is clearly evident that Total generation exactly follows the annual wind profile. This is mainly due to higher rated wind plant capacity than solar plant.

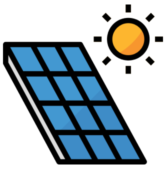
4.2.2. Base case technical details



Wind-rated power capacity: **360MW**

- Number of turbines (N_{wt}): **90 Turbines**
- Wind turbine rated power (p_{rated}): **4MW**

- Wind turbine rotor diameter (d): $\sim$ **119 m**
- Hub Height (hh) : $\sim$ **70 m**
- Specific power of turbine in(sp): **360 W/m2**
- Turbine rotor clearance w.r.t ground(h_c): **10 m**
- Installation density of wind farm (ρW): **5 MW/km2**
- land area use of wind farm (A_{wpp}): **72 km2**



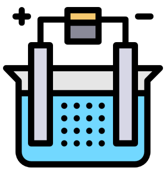
Solar-rated power AC capacity (S_{MW}): **80 MW**

- Solar DC/AC ratio (r_{DCAC}): **1.5**
- Surface title in solar plant (θ_{tilt}): **50°**
- Azimuth of the solar plant (θ_{azim}): **210°**
- Solar farm land use per MW : **1 km2/MW**
- land area use of solar farm (A_{pvp}): **80 km2**

Battery power capacity (B_P): **20 MW**

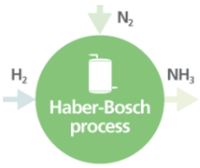
- Battery discharge hours (B_{Eh}): **4**
- Battery depth of discharge ($Batt_{DOD}$): **90 %**
- Battery charge/discharge efficiency (η): **98.5 %**

Grid capacity (G_{MW}): **300 MW**



Electrolyzer rated power capacity (PTG_{MW}): **150 MW**

- High Heat Value of hydrogen (HHV): **39.3 kWh/kg**
- water consumption: **9.4 l/kg**
- H2 production curve: **PEM Electrolyzer**
- Penalty factor H2 : **0**
- Hydrogen selling price ($price_{\mathrm{H2}}(t)$) : **5 €/kg**



$Feedratio$: **0.214285**

- Penalty factor NH3 : **0**
- Ammonia selling price ($price_{\mathrm{NH3}}(t)$) : **950 €/Tonne**

4.3. Modelling checks

In the section 3.2 different equations are introduced in the Hydesign EMS model. Before analyzing the results of this model, it is necessary to perform some modelling checks to ensure the reliability of the results and this exercise also gives confidence in the functioning of the model, since there is no benchmark power to ammonia(P2A) model to refer to as earlier mentioned in **??**.

It is recommended to check the model in different sites using different input resource data. But as earlier mentioned, only the base case site is used for modelling checks and generating results in this study. Objective function- 2 (***EE+GNH3***) in Equation 3.28 is used for modelling checks. Hourly Simulations for the evaluation of a user input design are made by running the evaluate.py file in HyDesign. HyDesign Architecture can be referred to in Figure 3.1. The results graphs and CSV files are then analyzed using Microsoft Excel software.HyDesign replicates this annual generation pattern for 25 years with degradation. So, modelling checks are performed only for the annual results, but not the lifetime of 25 years. All the parameters in the results are given as 8760 hourly values in CSV, these are termed as output arrays from here on in this study.

1. **No NAN:** As a first step of check, all arrays of extracted output parameters must have numerical values. Errors such as Not a number(NAN) should not be seen in any cell of any parameter array. For the base case results this check is satisfied by the model.

2. **Not above max values:** All the output parameters like $P_w(t)$, $P_s(t)$, $P_{batt}(t)$, $P_{hpp}(t)$, $P_{curt}(t)$, $P_{ptg}(t)$, $P_{HB}(t)$, $m_{\mathrm{H2}}(t)$, $m_{\mathrm{N2}}(t)$, $m_{\mathrm{NH3}}(t)$, $Qout_{HB}(t)$ must have their maximum of model generated values below the expected rated capacities at any hour(out of 8760) of the year. For the base case results this check is satisfied by the model.

3. **Not below min values:** All the output parameters listed in the last check must have their minimum of model-generated values above the minimum limits shown in section 3.2 at any hour(out of 8760) of the year. For the base case results this check is satisfied by the all parameters of the model except $P_{hpp}(t)$. There are 32 hours in a year where the $P_{hpp}(t)$ value is less than **0**. All 32 values are very small and have non-zero decimal values after 7^{th},15^{th} and 16^{th} decimals. Such minute deviations are neglected. Such deviations can occur while reading the CSV format data in Excel.

4. **Electrical Energy balance:** Electrical energy(EE) must be balanced in the system, this means generation over a period must be equal to consumption plus outflow to the grid over the same period.

$$\sum_{y}(P_w(t) + P_s(t)) - \sum_{y}(P_{hpp}(t) + P_{curt}(t) + P_{ptg}(t) + P_{HB}(t) + P_{batt}(t)) = 0 \tag{4.1}$$

   This EE balance must be checked annually and also hourly for all 8760 hours.

   - **Annual:** For the base case results this annual check is satisfied by the model.

   - **Hourly:** For the base case results this hourly check is satisfied by the model except for 89 hours in a year where EE balance does not exist. But, all these 89 hours have very minimal deviations are very small have and have non-zero decimal values after 13^{th},14^{th} and 15^{th} decimals. Such minute deviations are neglected. Such deviations can occur while reading the CSV format data in Excel.

5. **HPP output less than grid capacity:** At any hour $P_{hpp}(t)$ must always be less than G_{MW}.For the base case results this check is satisfied by the model.

6. **HPP capacity factor:** The capacity factor of HPP plant (CF_{Hpp}) must always less than the capacity factor of wind (CF_{wind}).For the base case results this check is satisfied by the model.

$$CF_{Hpp} <= CF_{wind} \tag{4.2}$$

7. **$P_{ptg}(t)$ and $P_{curt}(t)$ relation:** Always $P_{ptg}(t)$ value must be greater than the $P_{curt}(t)$ since the optimisation solver must assign the EE to energy forms and then if it is excess it must be curtailed but not otherwise. For the base case results this check is satisfied by the model.

8. **$P_{ptg}(t)$ and $P_{HB}(t)$ relation:**
   - **Non zero $P_{HB}(t)$ for zero $P_{ptg}(t)$ values:** It is not practically possible to produce NH3 without H2 production, so it is not possible to have a non -zero $P_{HB}(t)$ for zero $P_{ptg}(t)$.For the base case results this check is satisfied by the model.
   - **$P_{HB}(t)$ values for max($P_{ptg}(t)$):** For max values of $P_{ptg}(t)$ it is only possible to get $P_{HB}(t)$ values $<=$ its max value.For the base case results this check is satisfied by the model. Always $P_{HB}(t)$ has maximum value for max $P_{ptg}(t)$ in the base case.

9. **Mass balance:** Mass must be balanced in the system, this means the mass of generated H2 and N2 over a period must be equal to the mass of produced NH3 in that period.

$$\sum_{y}(m_{\text{H2}}(t) + m_{\text{H2}}(t)) = \sum_{y}(m_{\text{NH3}}(t)) \tag{4.3}$$

   This mass balance must be checked annually and also hourly for all 8760 hours.
   - **Annual:** For the base case results this annual check is satisfied by the model.
   - **Hourly:** For the base case results this hourly check is satisfied by the model.

10. **$P_{HB}(t)$ and $m_{NH3}(t)$ relation:**
    - **Non zero $m_{NH3}(t)$ for zero $P_{HB}(t)$ values:** It is not practically possible to produce NH3 without a power supply to HB process, so it is not possible to have a non-zero $m_{NH3}(t)$ for zero $P_{HB}(t)$. For the base case results this check is satisfied by the model.
    - **$m_{NH3}(t)$ values for max($P_{HB}(t)$):** it is only possible to get max $m_{NH3}(t)$ values for max values of $P_{HB}(t)$.For the base case results this check is satisfied by the model. Always $Qout_{HB}(t)$ has maximum value for max $m_{NH3}(t)$ in the base case.

11. **$Qout_{HB}(t)$ and $m_{NH3}(t)$ relation:**
    - **Non zero $Qout_{HB}(t)$ for zero $m_{NH3}(t)$ values:** HB process produces exothermic heat only when covalent N-H bonds are produced in HB process. so it is not possible to have a non-zero $Qout_{HB}(t)$ for zero $m_{NH3}(t)$.For the base case results this check is satisfied by the model.
    - **$Qout_{HB}(t)$ values for max($m_{NH3}(t)$):** it is only possible to get max $Qout_{HB}(t)$ values for max values of $m_{NH3}(t)$.For the base case results this check is satisfied by the model. Always $Qout_{HB}(t)$ has maximum value for max $m_{NH3}(t)$ in the base case.

12. **$m_{N2}(t)$ and $m_{H2}(t)$ relation:**

    - **Non zero $m_{N2}(t)$ for zero $m_{H2}(t)$ values:** N2 production is modelled in a way that only the required amount of N2 will be produced whenever there is H2 production.No N2 storage or oversizing of N2 production. so it is not possible to have a non-zero $m_{N2}(t)$ for zero $m_{H2}(t)$. For the base case results this check is satisfied by the model.

    - **$m_{N2}(t)$ values for max($m_{H2}(t)$):** it is only possible to get max $m_{N2}(t)$ values for max values of $m_{H2}(t)$.For the base case results this check is satisfied by the model.Always $m_{N2}(t)$ has maximum value for max $m_{H2}(t)$ in the base case.

13. **$m_{NH3}(t)$, $m_{H2}(t)$ and $m_{N2}(t)$ relation:**

    - **Non zero $m_{NH3}(t)$ for zero $m_{H2}(t)$ values:** NH3 production is only possible when H2 and N2 is produced. so it is not possible to have a non-zero $m_{NH3}(t)$ for zero values of either $m_{H2}(t)$ or $m_{N2}(t)$. For the base case results this check is satisfied by the model.

    - **$m_{NH3}(t)$ values for max values of ($m_{H2}(t)$) and ($m_{N2}(t)$) :** it is only possible to get max $m_{NH3}(t)$ values for both max values of $m_{H2}(t)$ and $m_{N2}(t)$ .For the base case results this check is satisfied by the model.Always $m_{NH3}(t)$ has maximum value for max $m_{H2}(t)$ and max $m_{N2}(t)$ in the base case.

Out of all 13 modelling checks listed above, the coloured checks are specifically for the added GNH3 model. All cyan-coloured checks are made only dependent on the HB process, so testing them on one site data will be enough to verify the functioning of related equations. whereas the orange-coloured checks are dependent on the HPP system before HB process, so it is recommended to do these 2 model checks on data from different sites.Since the optimization solver will change its decision based on the site data. All 13 modelling checks are successfully satisfied by adding GNH3 equations in the EMS model with the base case site data.

5

Results and Discussions

For this study, an available site in the HyDesign data repository is choosen and all technical details are listed in subsection 4.2.2. The resource potentials along with annual wind and solar generation values and plots are shown in subsection 4.2.1. The Whole study focuses on the results of this single base case site, but the general logical relations are deduced from these results which can apply to different sites in a similar way.

5.1. Base case results

Complete details of the base case site can be found in section 4.2.After verifying the HPP+GNH3 model through all modelling checks listed in section 4.3 results were generated using the Objective function 1 (*EE*) and 2 (*EE+GNH3*) in EMS optimization out of 7 possible objective functions mentioned in subsection 3.2.5. All the necessary constraints and equations are detailed in section 3.2.There are a certain list of assumptions made during this study all such assumptions are listed in next section:

5.1.1. Assumptions and Exclusions

- Time frame: This study considers 1 hour as the timeframe for all simulations. The electricity spot prices are also only available for each hour of the year in HyDesign. So, all analysis and optimizations are performed over this time frame of 1 hour.

- Grid intake: Always required electrical energy for HB process and GH2 production is supplied through wind and solar generation. There is no additional electrical energy intake from the grid.

- Mass modelling: Out of 3 options described in the section 3.2, mass modelling is implemented in generating the results.Since mass modelling also offers 100% mass conversion to ammonia from GH2 and N2.This 100% conversion assumption helps to look at the extreme(maximum) case of value addition in the HPP+GNH3 system.

- Startup heaters: Electric startup heaters are considered in this study to provide operational temperatures to the HB process. The Starting time of such heaters is in the range of a few minutes, so there will not be any delay in providing operational temperatures to HB process. Since, starting time is only in few minutes but the time frame of simulation is 1Hr the effects of such delays are neglected in this study. The power consumption of the electric startup heaters are assumed to be implicitly considered in Only HB part of HB process power consumption.

- Compressors and Condensor: Similar to electric startup heaters power consumption of condensers and all different compressors like Multi-stage feed compressors, recycle compressors and refrigeration compressors are assumed to be implicitly considered in Only HB part of HB process power consumption.

- Ramp up/down dynamics: The startup and shutdown times of the whole HB process are in the range of hours as stated in Table 3.1 unlike the electrolyser which have only a few minutes Table 2.3. R&D is still carried on to improve the flexibility of the green HB process. Although few licensors of the HB process offer flexible green HB processes, those claims yet be proven on the ground.Renewable dynamic distributed ammonia project(REDDAP) the world's first dynamic power to ammonia project was recently commissioned on 26th August 2024 (State of Green, 2024).This study excludes the operation of standby mode of HB process and does not analyse the flexibility of the green HB process.

Scenarios	Electrolyser mode	H2 Production	HB process mode	NH3 Production
Scenario-1	Off	✖	Off	✖
Scenario-2	Off	✖	Standby[1]	✖
Scenario-3	Off	✖	On	✖
Scenario-4	Standby	✖	Off	✖
Scenario-5	Standby	✖	Standby[1]	✖
Scenario-6	Standby	✖	On	✖
Scenario-7	On	✔	Off	✖
Scenario-8	On	✔	Standby[1]	✖
Base Case Scenario	**On**	✔	**On**	✔

Table 5.1: Possible Operating scenarios of HPP+GNH3 system $\forall[P_w(t), P_s(t)]$.

All possible operating scenarios for all values of wind and solar generations are listed in Table 5.1.This means that only 9 situations are physically possible in HPP+GNH3 $\forall[P_w(t), P_s(t)]$.But,8 out of 9 situations cannot produce ammonia.Whereas in base case scenario both hydrogen and ammonia are produced.This explains why only base case scenario is being used in this study to analyze the HPP interaction with GNH3.

- Constant $Feedratio$: In an interview with Ammonia energy association(AEA) personnel it was known that in real world scenario $Feedratio$ usually changes with fluctuations of $P_{HB}(t)$ in the HB process.But, in this study dynamics are excluded.so,$Feedratio$ is kept constant throughout the simulation.

- Ammonia Transport: Ammonia offtake is considered to be at the same point of production.So, in this study, all types of ammonia transportation are excluded from modelling, so related costs are also excluded.

- Ammonia storage: This study excludes all types of storage of produced ammonia. This means seasonal storage of electricity in the form of ammonia is not included. All units of produced ammonia can be delivered for offtake without any storage.Since ammonia storage is not there conversion of ammonia back to hydrogen and then to electricity is excluded in this study. Related costs of ammonia storage are also excluded.

- Hydrogen Offtake: This study excludes the possibility of separate hydrogen offtake. Either EE or GNH3 can only be delivered as an output from the HPP+GNH3 system.

[1]Information collected from various interviews, and conference discussions with industrial professionals, site engineers, refer Figure 2.1

- Hydrogen Storage: No separate hydrogen storage is used in the simulations of this study.This means seasonal storage of electricity in the form of hydrogen is not included.Since hydrogen storage is not there, the conversion of hydrogen back to electricity is excluded in this study All units of produced hydrogen are only used to produce ammonia.Related costs of hydrogen storage are also excluded.

- Nitrogen Storage: Nitrogen as feedinput to GNH3 HB process is modelled as a complete dependant of $m_{H2}(t)$ and $Feedratio$.Since nitrogen is not used anywhere else in the system, the production of nitrogen is only necessary when there is hydrogen production for GNH3 this eliminates the requirement for Nitrogen storage. So, this study excludes nitrogen storage and related costs. Nitrogen production in the model of this study is independent of the type of production technologies stated in Table 2.2.

- Heat Storage and transport: There is no separate heat storage included in the model. The heat produced is quantified in terms of MWh. All produced heat is wasted in this base case study and no revenue is being generated from it.Since, there is no usage or revenue from generated heat, transportation of heat in any form is also excluded from this study. Neither the heat storage is modelled nor it is included in the revenue calculation. All revenue streams and costs related to heat storage, usage and transportation are excluded.

- HB process lifetime: Unlike conventional HB plants which have a long life time like 50 years as mentioned in Table 3.1 the new green HB plants' lifetime is still uncertain.Only few pilots in the world are up and running since last 2-3 years certainly this period is not enough to judge the lifetime of the green HB process.In an interview with one of the vice presidents of the renowned ammonia technology licensor TOPSOE it was known that green HB process has a disadvantage of steel fatigue due to vibrations of reactor vessels caused by intermittency of renewables. Such a steel fatigue can bear around 10,000 cycles. Based on this number of fatigue cycles it was estimated green HB process equipment can last for around 20 to 30 years. In this study, the lifetime of the green HB process is assumed as 25 years to match with standard renewable plants' lifetime.

- Repetition over lifetime: As earlier mentioned in the subsection 3.2.1 annual generation patterns are replicated for all 25 years with degradation. This means from year 2 to 25 the annual generation patterns are the same as that of year 1, only addition is degradation. Like annual generation patterns, $price_{elec}(t)$ repeated for years 2 to 25 but without any change. This means for all 25 years in the lifetime of the plant, the electricity prices are the same for any particular hour of the year.

- Fixed hydrogen price: Green Hydrogen price $price_{H2}(t)$ is constant at **5 €/kg** whole throughout the lifetime of the HPP+GNH3 system.Dynamic hydrogen prices are excluded from this study since at present hydrogen supply is only made through offtake agreements with upfront fixed hydrogen prices.

- Fixed Ammonia price: Green Ammonia price $price_{NH3}(t)$ is constant at **950 €/tonne** whole throughout the lifetime of the HPP+GNH3 system.Dynamic hydrogen prices are excluded from this study since at present ammonia supply agreements are only made through offtake agreements with upfront fixed ammonia prices.

After all the above assumptions and exclusions, the simulation was run for the base case scenario using the evaluation file in HyDesign.Technical and Financial results of the base case site for the base case scenario are presented in the next sections.

5.1.2. Technical results

Objective function 1 (*EE*) and 2 (*EE+GNH3*) were run in EMS optimization to evaluate the base case site for the base case scenario. Monthly total renewable generation, HPP output and ammonia output for *EE* and *EE+GNH3* are presented in Figure 5.1.First and foremost observation is that the electrical energy yield from HPP when only *EE* objective was run is much more than the electrical energy yield from HPP when *EE+GNH3* was run. From here on electrcial energy yield is termed as the HPP output in both objective functions and objective function will be termed as obj.The preliminary reason for such decrease in HPP output of *EE+GNH3* is due to additional revenue stream from ammonia.Since HPP +GNH3 system has ammonia as a additional revenue stream,optimization solver will distribute some part of the total generation into hydrogen and ammonia generation.This distribution of total generation into electrical energy or into ammonia is driven by many factors like revenue, price and quantity.Details on these factors will be discussed in further parts of this chapter.In Figure 5.2 we can clearly see that HPP output of *EE* is almost at the same level of total renewable generation histograms since, in *EE* obj HPP output is produced only as electrical energy. The small difference between total generation and HPP output of *EE* is called curtailed energy. Curtailment or curtailed energy is defined as the generated energy which exceeds the grid capacity limit which usually be wasted when not used in further processes of the HPP system.

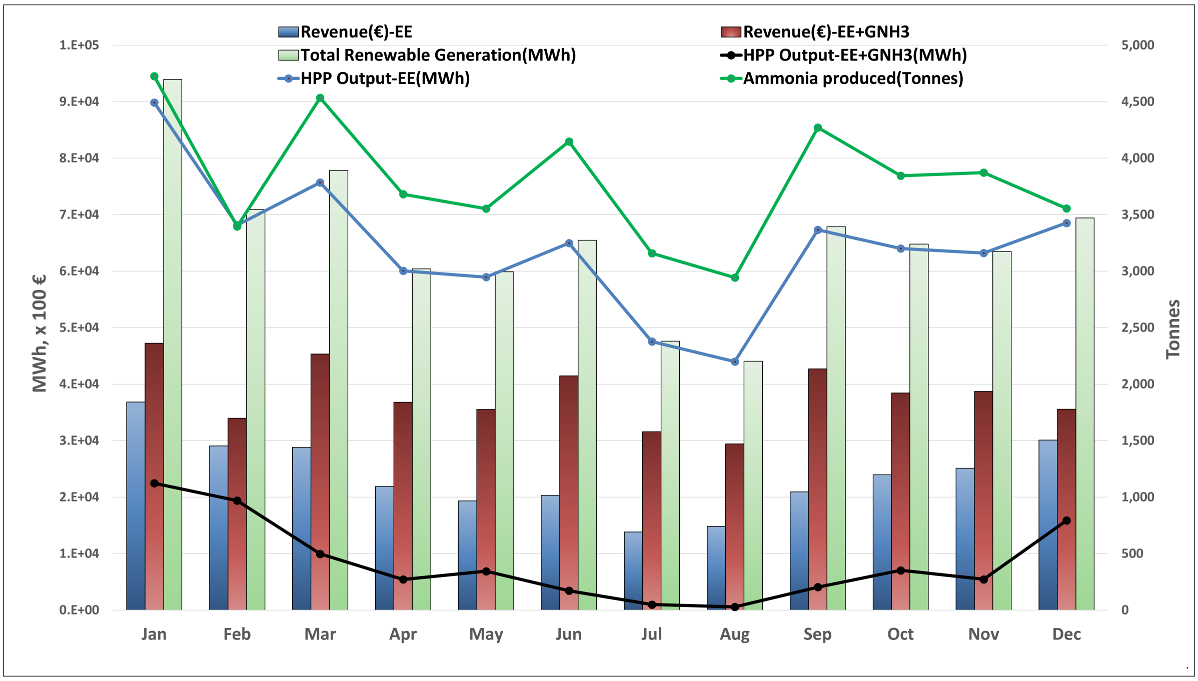


Figure 5.1: Monthly Revenues with HPP+GNH3 system outputs.

Interestingly, along with HPP output of *EE*, ammonia produced in *EE+GNH3* also follows the same profile trend of total renewable generation but HPP output of EE+GNH3 doesnot fully follow this trend.This is because here in HPP+GNH3 system the solver chooses to produce more ammonia than the electrical energy by supplying more generation to electrolyser and HB process, the leftover generation was taken as the HPP output in form of electrical energy.Since, all leftover is taken as HPP output in *EE+GNH3* obj, the curtailment value is always 0 in this case as shown in Figure 5.2.Optimization solver will always try to maximize revenue using the given obj function.Equation 3.38 shows how revenues are calculated in both objective functions.Revenues are multiplication of deliverable quantity of energy vector and price at which the energy vector is sold. Although HPP output of *EE* is more than that of *EE+GNH3*, the revenue of *EE* is less than revenue of *EE+GNH3* due to additional revenue stream of ammonia.

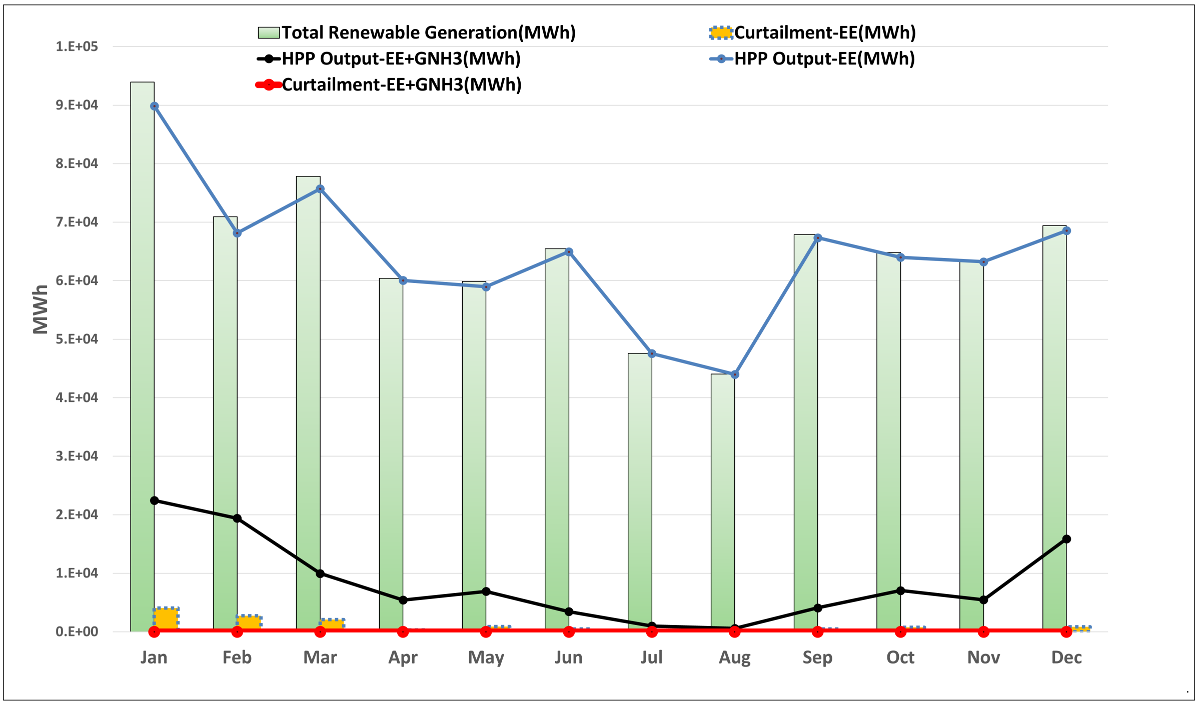


Figure 5.2: Monthly Grid Curtailment values of objective functions *EE*, *EE+GNH3*.

Revenue of *EE+GNH3* also follows the total renewable generation trend because revenue is dependant on 2 factors price and quantity.With a fixed ammonia price,revenue now only dependant on the quantity of ammonia production, ammonia production exactly follows the total renewable generation trend therefore revenue of *EE+GNH3* also follows it.In a similar way trend of revenue of *EE* also be argued on price and quantity, but here the price of electricity is not fixed. In Figure 5.1 Revenue of *EE* does not exactly follow the total generation trend although HPP output of *EE* exactly follows the trend this is because of variable hourly electricity prices.

To know whether if there is any value addition due to ammonia in HPP+GNH3 system, it is important to know the root cause of the revenue difference of *EE*,*EE+GNH3*.To understand the variable electricity price effect on the revenue of *EE* and consequently on the revenue difference of *EE*,*EE+GNH3* the average electricity prices are plotted with difference in revenues in Figure 5.3.

$$\text{Revenue Difference} = \text{Revenue of } EE{+}GNH3 - \text{Revenue of } EE. \tag{5.1}$$

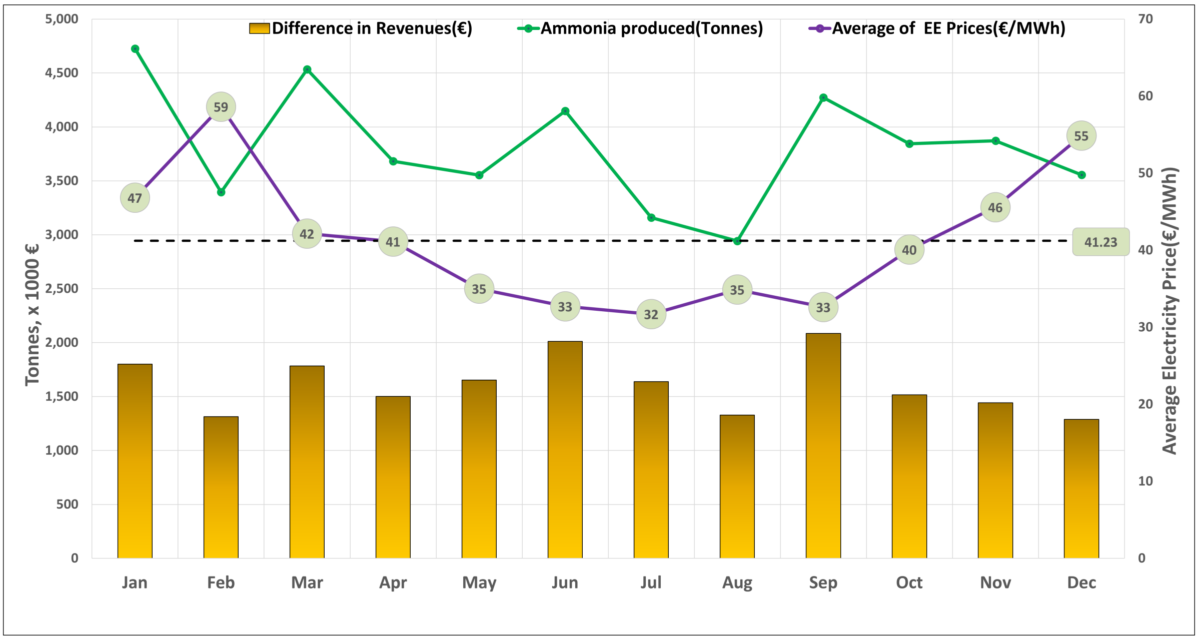


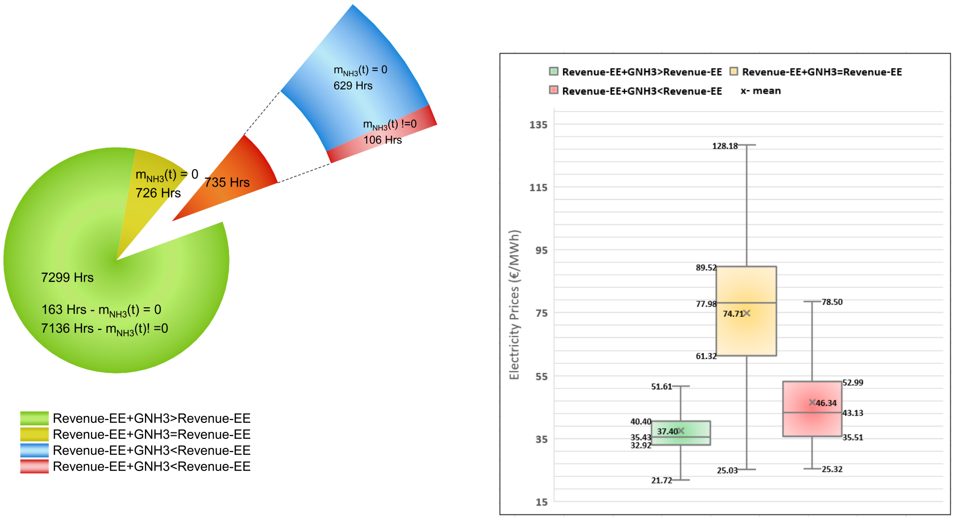
Figure 5.3: Monthly average electricity prices along with the difference in revenues of *EE*,*EE+GNH3* .

Whenever there is a increase electricity price the difference in revenue and ammonia production decreases.In February, August and October-December the average electricity prices are more than their previous months consequently ammonia production and difference in revenue decreases. This is because whenever there is a increase in electricity price the solver tries to maximize the overall revenue by increasing electricity production and consequently ammonia production will decrease.Difference in revenue will also decrease due to increase in revenue of *EE*.

$$\text{Revenue Difference} \propto \text{Ammonia production} \propto 1/\text{Electricity price}. \tag{5.2}$$

Closely observing the Figure 5.1 and Figure 5.3 In February when the HPP output of *EE* is less than that of March yet still revenue of *EE* in February is slightly greater than March this is due to electricity price in February is more than price in march.In same way the revenue of *EE* in August is more than that of July although HPP output of *EE* July is more than August, due to higher electricity price in August.This provides an evidence that amongst the price and quantity for revenue of *EE*, electricity price becomes the boosting factor is increasing the revenue.whereas in revenue of *EE+GNH3* boosting factor is always ammonia production quantity since ammonia price is always fixed in this study.

Now dissecting results further to know the percentage of time in a year where revenue of *EE+GNH3* is more than revenue of *EE* might help to understand many other hidden relations that cause the actual value addition. Out of 8760 hours in a typical calendar year, the revenue of *EE+GNH3* can be more, equal or less than the revenue of *EE*.These are the only 3 possible cases of the revenue difference.The Annual time share of all 3 possible cases of revenue difference with electricity prices are shown in Figure 5.4.



(a) Annual time share of 3 possible cases of revenue difference.

(b) Box chart of electricity prices for 3 possible cases of revenue difference.

Figure 5.4: Annual time share of 3 possible cases of revenue difference with electricity prices

As shown in Figure 5.4a 83.32% of the time the revenue of *EE+GNH3* is greater than the revenue of *EE*. 8.29% of the time both revenues are equal and 8.32% of the time the revenue of *EE+GNH3* is lesser than the revenue of *EE*. In Figure 5.4b the box chart of electricity price ranges are shown for all 3 revenue difference cases. In these boxcharts few outlier prices are excluded, outliers are the values which standout in the data.Outliers are usually plotted above maximum(upper whisker) and below minimum(lower whisker) of box chart.Along with whiskers, boxchart also shows median, mean and 1st and 3rd quartile values of the data. 1st quartile is 25th percentile which indicates the median of the lower half of the data when sorted in increasing order.Similary 3rd quartile is 75th percentile which is the median of the upper half of the data when sorted in increasing order. The area in box chart between 1st quartile and 3rd quartile is called interquartile range(IQR).

Clearly the IQR is smallest for the greater *EE+GNH3* revenue case than other 2 cases.The box chart of equal revenue case has the highest median price and also highest IQR than other 2 cases.Even the 1st quartile of this equal revenue boxchart is greater than the 3rd quartiles of other 2 charts.This shows that equal revenue case has the highest price range. *EE+GNH3* revenue lesser case has a boxchart with IQR, median price greater than greater revenue case but lesser than the revenue equal case.This Figure 5.4b helps in getting an overview of the spread of the electricity price range in all 3 cases.

Cases	Hours	Ammonia Production $m_{NH3}(t)$	Curtailment difference [EE-EE+GNH3]	HPP output difference [EE-EE+GNH3]	Average Electricity price [€/MWh]	Remarks
Revenue-EE+GNH3 > Revenue-EE	7136	Not equal to 0	Always > or = 0	Always > 0	37.01 (Min: 12.91, Max: 70.81)	Ammonia production is key advantage for revenue. Battery discharges more in EE than EE+GNH3. Also, Battery operational cycles are more in EE.
Revenue-EE+GNH3 > Revenue-EE	163	0	Always = 0	Always < or = 0	53.83 (Min: 14.38, Max: 100.47)	Lower generation hours, Battery discharges more in EE+GNH3 than EE. Also, battery operation cycles are more in EE+GNH3.
Revenue-EE+GNH3 = Revenue-EE	726	0	Always = 0	Always = 0	74.71 (Min: 25.03, Max: 128.18)	Higher electricity prices drives same outputs in EE and EE+GNH3.Battery operation is exactly same in both EE,EE+GNH3.
Revenue-EE+GNH3 < Revenue-EE	629	0	Always = 0	Always > or = 0	44.8 (Min: 25.32, Max: 122.70)	Lower generation hours, Battery discharges more in than EE+GNH3. Also, battery operation cycles are more in EE.
Revenue-EE+GNH3 < Revenue-EE	106	Not equal to 0	Always = 0	Always > 0	55.40 (Min: 32.89, Max: 70.76)	Battery always discharges in EE,75% of the time upto full capacity. Also, battery operation cycles are more in EE

Table 5.2: Comparison of Revenue Difference Cases

Table 5.2 comprises a detailed comparison of all 3 revenue difference cases in year of 8760 hours.In all three revenue cases the ammonia selling price $price_{NH3}(t)$ is constant at **950 €/tonne**.Starting with the first case - the revenue of *EE+GNH3* is more than revenue of *EE*. Out of 7299 hours, 7136 hours in this case produced ammonia and had HPP output difference always > 0, this means always the electrical energy output from *EE* is more than *EE+GNH3*. Because of lower electricity prices, quantity must be increased to improve revenue so, battery discharges more in *EE* than in *EE+GNH3*, also battery operation cycles are more in *EE* .Similarly, the curtailment difference is always > or = to 0.All energy in *EE* can only be converted to electrical energy, the remaining energy is curtailed due to grid capacity limit G_{MW}.whereas most of the energy in *EE+GNH3* is sent to ammonia production first and then to delivery of electrical energy to grid,if in case there is anything energy left it will be curtailed.In all 8760 hours of the year the curtailed energy in *EE+GNH3* is always 0 as shown in Figure 5.2.

Out of 7299 hours of first case 163 hours do not produce ammonia yet still the revenue is greater than *EE*.By analyzing in detail, it was understood that these 163 hours are low-generation hours of a year with above-average electricity price.So,the solver tries to optimise the revenue by choosing to generate electricity in *EE+GNH3* over ammonia production or charging battery.So, in these 163 hours always only electricity is produced in both *EE* and *EE+GNH3*.But,the battery discharges more in *EE+GNH3* than *EE* causing HPP output difference always < or = to 0. The curtailment difference is 0 since, these being low generation hours, there is not enough energy remaining to curtail.

In the second case- both revenues are equal,726 hours in a year fall in this case.This case has the highest average electricity price than all other revenue difference cases as shown in Table 5.2.Here, the solver always prioritizes electricity over ammonia production in both *EE+GNH3* and *EE* objectives.Hence, the results of these objectives are same, always the curtailment difference and HPP output difference are exactly equal to 0. Even the battery operation in both objectives of this case is exactly same. The ammonia production in all these hours is always 0. This is evident that when the electricity price is higher both objectives unanimously produce electricity following a similar way of operating the assets like storage systems like batteries in this case.

In third case-the revenue of *EE+GNH3* is less than revenue of *EE*.Out of 735 hours,629 hours does not produce any ammonia.By analyzing in detail, it was understood that these 629 hours are low-generation hours of a year with above-average electricity price and more than the median value in the box chart of this case shown in Figure 5.4b.So,the solver tries to optimise the revenue by choosing to generate electricity in *EE+GNH3* than ammonia.So, in these 629 hours always only electricity is produced in both *EE* and *EE+GNH3*.But,the battery discharges more in *EE* than *EE+GNH3* causing HPP output difference always > or = to 0. The curtailment difference is 0 since, these being low generation hours, there is not enough energy remaining to curtail.

Out of 735 hours of third case 106 hours produce ammonia yet still revenue of *EE+GNH3* is lesser than *EE*.The average electricity price is more than the 3rd quartile in box chart of this case shown in Figure 5.4b. The main reason for the lesser revenue of *EE+GNH3* although ammonia production is non-zero is due to full battery discharge in *EE*.79 hours out of these 106 hours battery discharges up to its full capacity in *EE* providing more electrical energy and improving revenue of *EE*.HPP output difference is always > 0 in this case which means more electrical energy is delivered in *EE* than *EE+GNH3*. Curtailment difference is always equal to 0 in this case since the solver always tries to prioritize the electrical energy delivery over ammonia production or charging the battery.

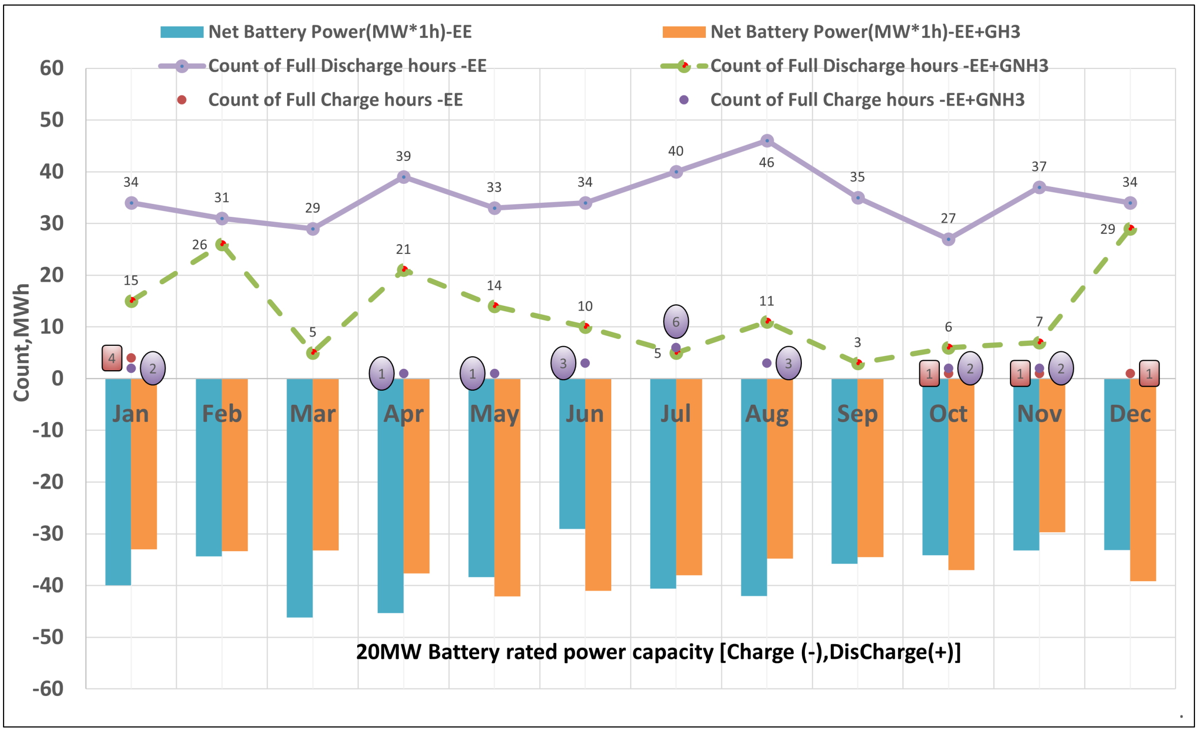


Figure 5.5: Monthly net battery power with a count of full discharge and charge hours of *EE* and *EE+GNH3*.

Last case in Table 5.2 specifically highlights that even with higher electricity prices and non-zero ammonia production, the revenue improvement can only happen through battery discharge operation.This means along with electricity price, battery operation is also important for understanding the value addition caused by GNH3 in HPP+GNH3 system.

Figure 5.5 clearly plots the monthly count of full discharge hours and charge hours of *EE* and *EE+GNH3* along with net battery power of *EE* and *EE+GNH3*.Here, net battery power means the sum of the charged power(- sign) and discharged power(+ sign), the resulting power will have either (+) or (-) sign indicating the net state of battery operation in a period of observation.

It is very clear in Figure 5.5 that in all 12 months of a year the full discharge hours count of the *EE* is more than the *EE+GNH3*. This is because in *EE* revenue can be improved only through delivering more electrical energy with less curtailment, so solver charges batteries in high total renewable generation hours and discharges it in lesser generation hours.Whereas in *EE+GNH3* solver always tries to produce more ammonia by suppling power to electrolyser and HB process to optimise the hourly revenue.Solver chooses to generate more ammonia than storing energy in a battery for discharge in later hours, because of this full discharge hours in *EE+GNH3* are less than the *EE*.Interestingly the profile of full discharge hour count in *EE+GNH3* follows the average monthly price profile in Figure 5.3.Whenever there is a increase in average electricity price there is a increase in full discharge hour count in *EE+GNH3* for example in months of February, April, August, December this relation can be clearly noticed.This is because whenever there is price hike solver tries to produce more electrical energy in *EE+GNH3* through improving battery discharge operation.But *EE* full discharge hour count doesnot depend on the electricity profile,since it depends on the total generation profile this will be explained further in the report.

The number of full charge hours are much lesser in both *EE+GNH3* and *EE* compared to their count of full discharge hours.This is because of the fact that to maximise revenue always delivered energy must be maximised through more battery discharge than charge,so need for discharge is more than the charge.Count of full charge hours is more in *EE+GNH3* in *EE* because it is better to deliver more electrical energy than saving in a battery in *EE*.

The net state of the battery in both *EE* and *EE+GNH3* for each month of a year is always negative as shown in Figure 5.5.This means the -sign(charging) is more than the + sign(discharging), which means that batteries are getting charged more often than they are discharging.Although full charge hours count is less than full discharge hours count in both *EE+GNH3* and *EE*,net power is with always -sign.This is because more number of times batteries are charged with lesser amount of energies. In relative comparison of net state of battery in *EE+GNH3* and *EE* it is understood that most of the times *EE* has more net negative(charging) power than *EE+GNH3*.This is because of more battery operations of *EE* than in *EE+GNH3*.More battery operations means more charging with small amounts of energy and more discharging up to its full discharge capacity, these operations together are named as battery operation cycles are stated in Table 5.2.

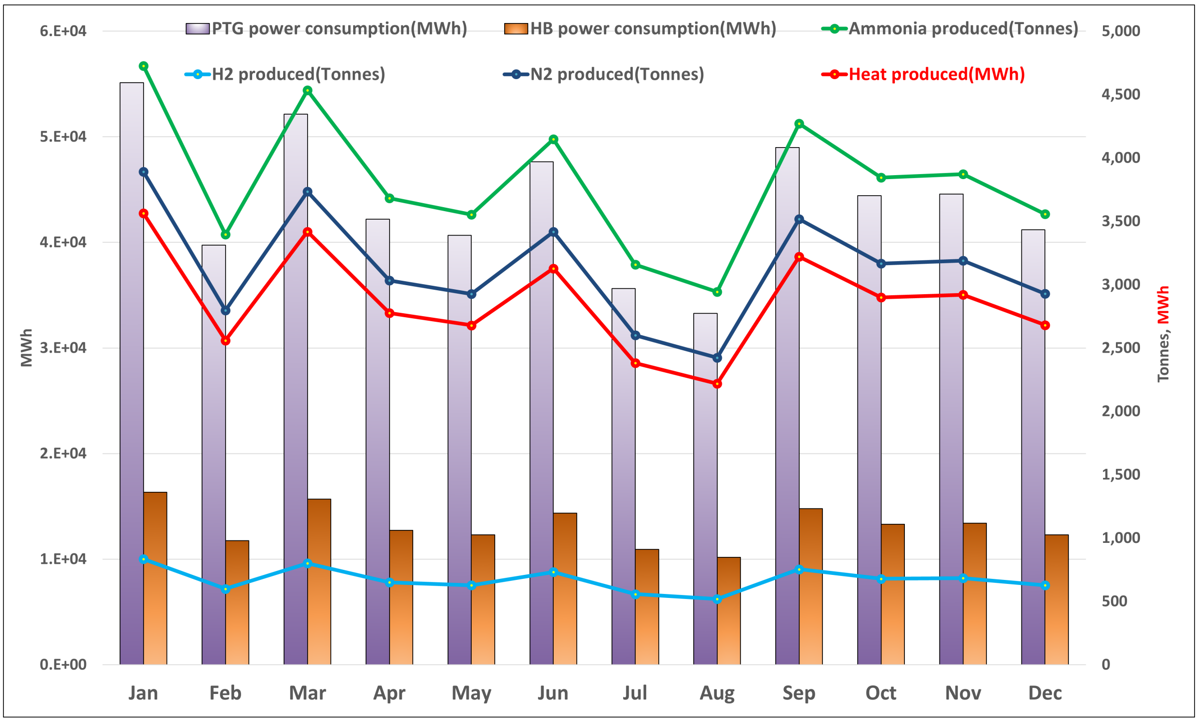
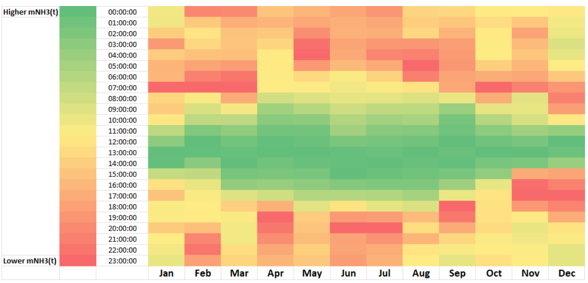


Figure 5.6: Monthly values of HB process inputs and outputs.

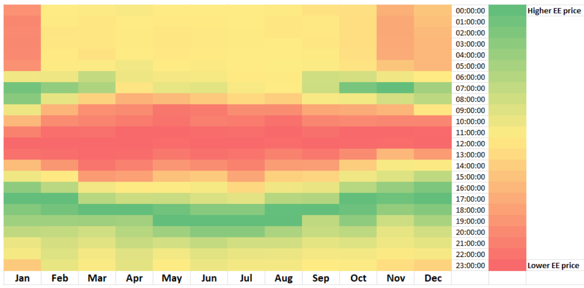
Figure 5.6 shows all the inputs and outputs of HB process in *EE+GNH3* shown in Figure 3.3.The monthly profiles of HB power consumption $(P_{HB}(t))$ and power to electrolyser $(P_{ptg}(t))$ follow the ditto trends.These both follow the same trend of ammonia production which has similar trend of total renewable energy generation.The hydrogen mass produced, nitrogen mass produced and heat energy produced have ditto trends like that of ammonia production since they all are related through linear equations shown in subsection 3.2.5. The heat energy produced is presented in MWh on left y-axis in Figure 5.6.

Till now all results are presented for 12 months of a year.But to understand the dependance of ammonia production and HPP outputs on solar and wind profiles, it is necessary to look at their diurnal profiles for each month of a year.Figure 5.7 shows a multiple figures of monthly diurnal profiles presented as a heatmap with varying color range between maximum and minimum values shown in legends.In all the figures green color indicates the maximum value and red color indicates the minimum value. Color ranking is done on each month independantly for all 24 hours of a day.For example in Figure 5.7a in January,May months the lowest ammonia production are at 7:00am,4:00am. Both these hours show dark red color, but need not necessarily have the same numerical value. The correct way of interpretation this color ranking is only in January 7:00am is least ammonia production hour, whereas only in May 4:00am is least ammonia production hour same way of interpretation applies for maximum values in green color.

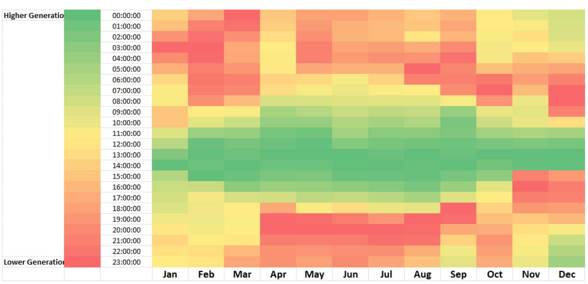
Amongst all the monthly diurnal profiles shown in Figure 5.7 only the electricity prices are presented in averages, rest all figures are presented in sum values.This means the value of a particular hour of a month in a figure is sum of all numerical values of that particular hour in all days of that month.But for electricity price in Figure 5.7b values are averaged.



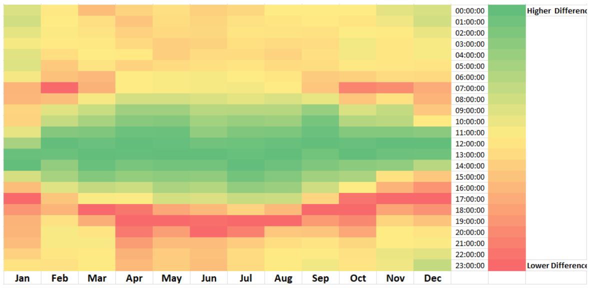
(a) Monthly diurnal profile of ammonia production.



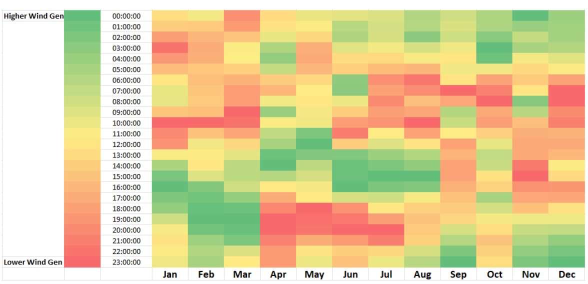
(b) Average monthly diurnal profile of electricity price.



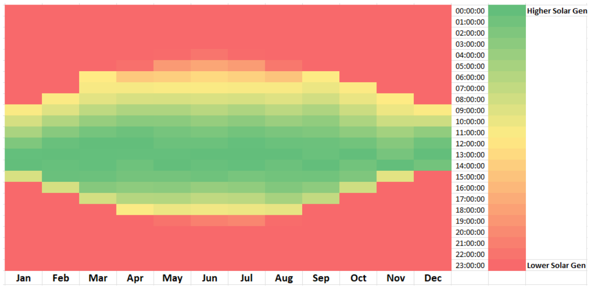
(c) Monthly diurnal profile of total renewable generation.



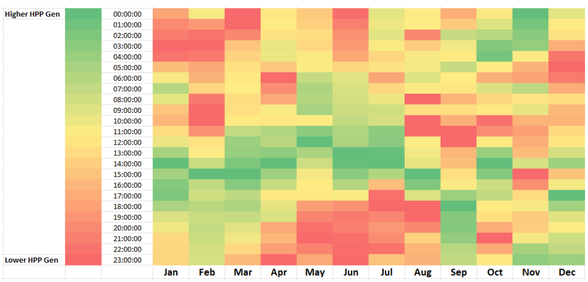
(d) Monthly diurnal profile of revenue difference.



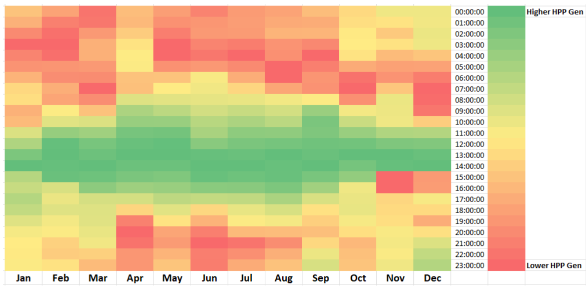
(e) Monthly diurnal profile of wind generation.



(f) Monthly diurnal profile of solar generation.



(g) Monthly diurnal profile of EE+GNH3 electricity generation.



(h) Monthly diurnal profile of EE electricity generation.

Figure 5.7: Monthly diurnal profiles

Monthly diurnal profile of Ammonia production in Figure 5.7a, revenue difference in Figure 5.7d and electricity price in Figure 5.7b follow a relation mentioned in Equation 5.2.The green cloud between 8:00 to 17:00 hours in ammonia production and revenue difference exactly matches the red cloud in average electricity price heatmap. This means ammonia production is maximum whenever the average electricity price is lesser, consequently the revenue difference between *EE+GNH3* and *EE* is maximum follow ammonia production trend. As earlier pointed in Figure 5.1 the ammonia production follow the total renewable energy generation trend, similarly here also the green cloud in ammonia production is mainly because of the green cloud in total renewable energy generation monthly diurnal profile in Figure 5.7c.

The total renewable energy generation monthly diurnal profile is overlapped result of wind and solar monthly diurnal profiles in Figure 5.7e and Figure 5.7f.The solar diurnal profile complements with wind diurnal profile as earlier explained in subsection 4.2.1.Because of this complimentary profiles and The total renewable generation has a green cloud matching with solar green cloud although wind rated power capacity in this base case site is 4 times more than the solar rated power capacity. Hence complementarity of the renewable resources play a major role in total renewable generation which is the key driving factor for ammonia production along with electricity price.

There is no particular green cloud or pattern is visible in monthly diurnal profile of wind generation in Figure 5.7e.Similarly, no clear pattern is visible in *EE+GNH3* electricity generation,but heatmap of *EE+GNH3* electricity generation slightly matches with the wind generation since wind rated power capacity is more than solar power.Interestingly the monthly diurnal profile of *EE* electricity generation in Figure 5.7h does not follow the red cloud in electricity price heatmap.Ideally to maiximise revenue the electricity proudction must be increased in hours with more electricity price but in this case the electricity generation in *EE* is complementing this logic. That means the electricity generation is more in hours with lesser average electricity price, this is due to HPP output of *EE* is dependant on the total renewable energy generation.

5.1.3. Financial results

The value addition in base case scenario is seen as a revenue increase in subsection 5.1.2 without any inclusion of costs.Table 3.1 mentions that the green HB process are more costly than the conventional HB process due to its associated infrastructure and huge GH2 production costs.So to understand the value addition in terms of financial metrics including associated green HB process costs, different financial metrics are computed using the equations listed in subsection 3.3.2.

Table 5.3 shows the comparision of the different financial metrics in HyDesign for both *EE* and *EE+GNH3* in lifetime of 25 years. Light orange color and light green color in the table show the lower value and higher value for a particular financial metric.Although revenue is more for the *EE+GNH3* the NPV/-Capex, NPV anf IRR is more for the *EE*. This is due to higher costs of GNH3 system.But, the LCOE of the *EE* is greater than the *EE+GNH3* due to heavy curtailment of 12.9 GWh in *EE*, whereas the curtailment in *EE+GNH3* is 0.

	EE+GNH3	*EE*
NPV/CAPEX	-0.135	0.305
NPV [MEuro]	-104.0	112.5
IRR	0	0.09
LCOE [Euro/MWh]	44.09	44.82
LCOH [Euro/kg]	8.4	NA
LCOA [Euro/kg]	2.5	NA
Revenue [MEuro]	1196.6	712.6
Total CAPEX [MEuro]	771.5	368.5
Total OPEX [MEuro]	13.9	5.8
penalty lifetime [MEuro]	0	0
Capacity factor wind	21.0%	21.0%
Capacity factor solar	17.6%	17.6%
Capacity factor HPP	2.6%	20.0%
Break-even NH3 price [Euro/kg]	1083.5	NA
Break-even PPA price for NH3 [Euro/MWh]	104.0	29.3
$price_{NH3}(t)$	950	950
Total annual renewable energy	785.6	785.6
Annual Wind energy generation [GWh]	662.6	662.6
Annual Solar energy generation [GWh]	123	123
AEP [GWh]	101.5	772.3
GUF	0.0	0.3
Annual H2 production [tonnes]	8061.8	0
Annual consumption of electrolyser [GWh]	525.6	0
Annual NH3 production [tonnes]	45683.9	0
Annual consumption of HB process [GWh]	158.1	0
Annual heat production of HB process [GWh]	34.4	0
Total annual curtailment [GWh]	0	12.9

Table 5.3: Financial Metrics comparision of *EE* and *EE+GNH3* for lifetime of 25 years.

As earlier mentioned in subsection 3.3.2 different types of break even prices are calculated using the simple optimization using SciPy library in python.The objective of all such optimizations is to minimize NPV^2.The minimum required $price_{NH3}(t)$ to break even that means NPV^2 is 0 is called Break-even NH3 price. Break-even NH3 price is 1083.5 €/kg which is more than the input $price_{NH3}(t)$ of 950 €/kg. Similary minimum required PPA electricity price $price_{elec}(t)$ for given $price_{NH3}(t)$ to break even that means NPV^2 is 0 is called Break-even PPA price for NH3.Break-even PPA price for NH3 is 104 €/kWh which is much more than the average electricity price of 41.23 €/kWh. This Break-even PPA price for NH3 is less in *EE* due to more HPP output in *EE* than in *EE+GNH3*.

5.2. Sensitivity analysis

Until now the results presented in subsection 5.1.2 and subsection 5.1.3 are for base case site for a base case scenario.Using those, it is hard to generalize the relation between various technical parameters and financial metrics.So sensitivity analysis is carried out in this study to understand the general trends between technical parameters and financial metrics.

Out of various sensitivity analysis methods One-factor-at-a-time sensitivity(OFAT) approach is chosen for this study.**”One of the simplest and most common approaches is that of changing one-factor-at-a-time (OFAT), to see what effect this produces on the output”**(Wikipedia contributors, 2024e). This method involves moving one input variable, keeping others at their baseline (nominal) values listed in subsection 4.2.2 and then returning the variable to its nominal value, then repeating for each of the other inputs similarly.

The changes due to change in input variables are calculated using gradient ratio. Gradient ratio formula is shown below in Equation 5.3. For example, if variable X is an input variable and variable Y is output variable then the gradient ratio is the percentage change ratio of Y over the percentage change of X. Gradient ratio is unitless number since it is a ratio.For example if the gradient ratio is 2 which means that for 1% increase in X, Y will increase 2%.

$$\text{Gradient Ratio} = \frac{\text{Percentage Change in } Y}{\text{Percentage Change in } X} \tag{5.3}$$

Average gradient ratio is an average of multiple gradient ratios for different iterations of inputs and corresponding outputs. Let's consider N iterations, where in each iteration: * X_i is the input value. * Y_i is the corresponding output value. Then, the gradient ratio for the i-th iteration is:

$$\text{Gradient Ratio}_i = \frac{\text{Percentage Change in } Y_i}{\text{Percentage Change in } X_i}$$

where:

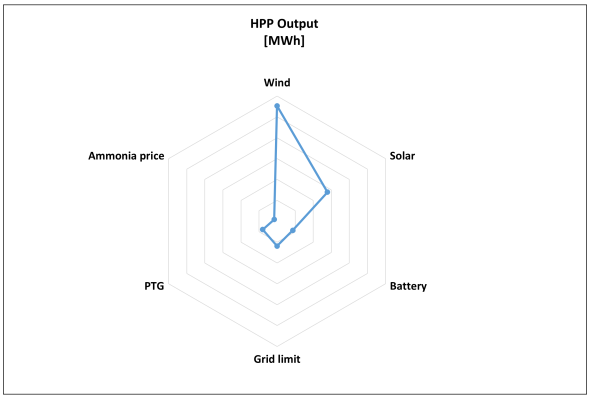
$$\text{Percentage Change in } X_i = \frac{X_{i,final} - X_{i,initial}}{X_{i,initial}} \times 100\%$$
$$\text{Percentage Change in } Y_i = \frac{Y_{i,final} - Y_{i,initial}}{Y_{i,initial}} \times 100\%$$

The average gradient ratio across all N iterations is:

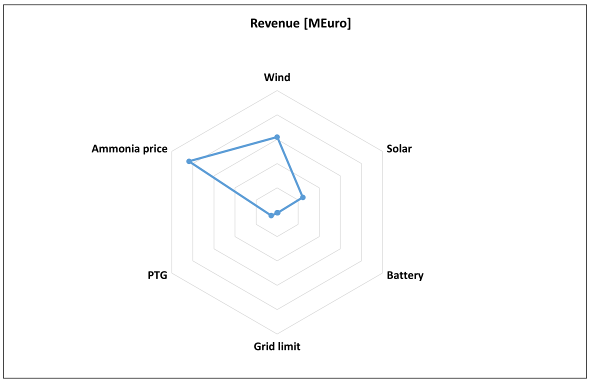
$$\text{Average Gradient Ratio} = \frac{1}{N} \sum_{i=1}^{N} \text{Gradient Ratio}_i$$

This provides a measure of the average sensitivity of the output Y to changes in the input X across multiple iterations.Figure 5.8 shows the gradient ratio radar diagrams of various technical outputs and financial metrics of *EE+GNH3*.Because this sensitivity analysis's aim is to generalize the trends, the absolute values of gradient ratio's are removed from all sub figures of Figure 5.8.The elecicity prices are kept constant in whole sensitivity analysis, since hourly electricity price is not in control of renewable power developer(RPD) they are excluded from this sensitivity study.Only input parameters like wind capacity,solar capacity ,battery capacity, electrolyser capacity, grid limit and ammonia price which can be modified during plant design stage or contract negotiation with offtaker are considered in this sensitivity study.

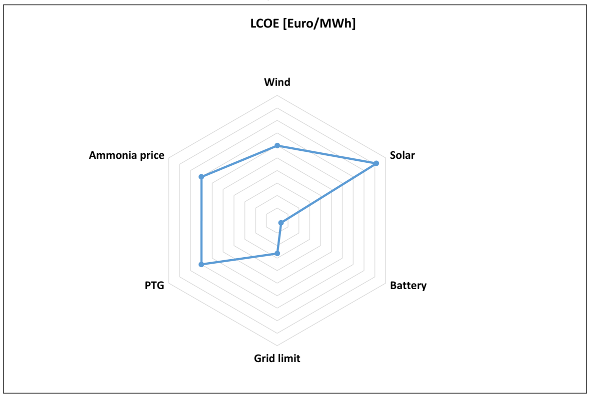
The spokes or radii in the gradient ratio radar diagram represent the various input parameters are changed using OFAT method. The title of the radar diagrams represent the output which changes.In Figure 5.8a HPP output of *EE+GNH3* changes with different spokes.Clearly wind capacity has a higher(outward from center of web) gradient ratio than all others,this means HPP output of *EE+GNH3* increases more with increase in wind capacity than any other spoke in the radar chart.This is mainly due to the dependency of HPP output on continuous profile of wind resource than the solar resource. In Figure 5.8b revenue of *EE+GNH3* changes with different spokes.Clearly ammonia price has a higher(outward from center of web) gradient ratio than all others,this means revenue of *EE+GNH3* increases more with increase in ammonia price than any other spoke in the radar chart. similar relation is also seen in Figure 5.7 and Figure 5.3.



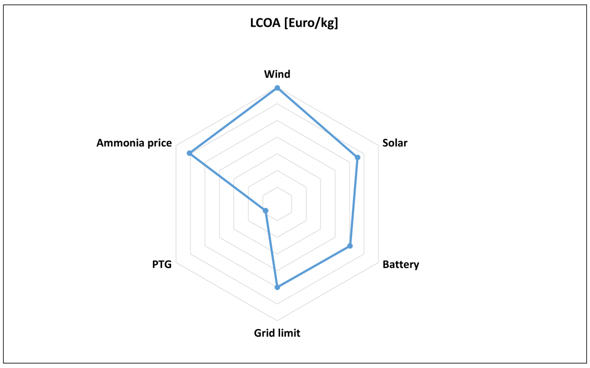
(a) Gradient ratio radar diagram of HPP output of EE+GNH3.



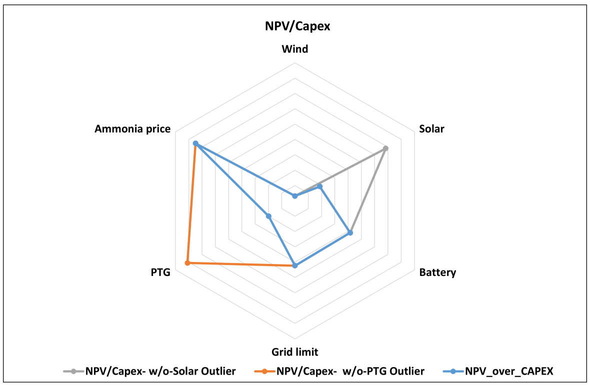
(b) Gradient ratio radar diagram of revenue of EE+GNH3.



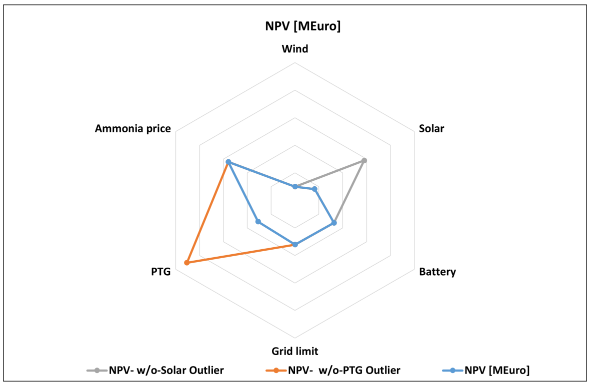
(c) Negated gradient ratio radar diagram of LCOE of EE+GNH3.



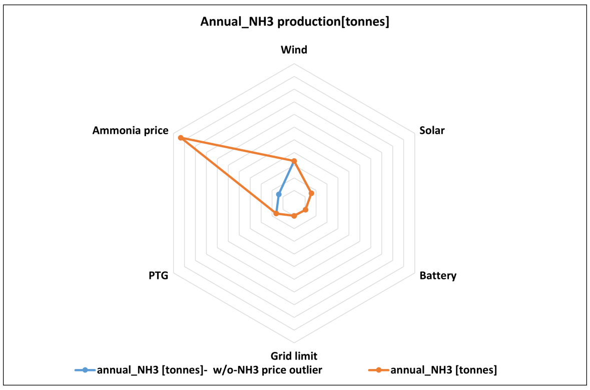
(d) Negated gradient ratio radar diagram of LCOA of EE+GNH3.



(e) Gradient ratio radar diagram of NPV/Capex of EE+GNH3.



(f) Gradient ratio radar diagram of NPV of EE+GNH3.



(g) Gradient ratio radar diagram of ammonia production of EE+GNH3.

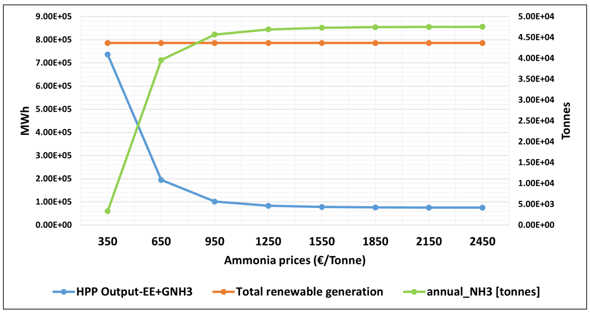
Figure 5.8: Gradient ratio radar diagrams of various outputs and metrics of EE+GNH3.

In Figure 5.8c LCOE of *EE+GNH3* changes with different spokes, but here the gradient ratios are negated.Clearly solar capacity has a higher gradient ratio than all others, this means LCOE of *EE+GNH3* decreases more with an increase in solar capacity than any other spoke in the radar chart.This is because increasing in solar capacity increases the HPP output of *EE+GNH3* more than any other spoke after wind.But wind power is costlier than solar power,so the LCOE decrease is more for solar capacity increase.In Figure 5.8d LCOA of *EE+GNH3* changes with different spokes, but here the gradient ratios are negated.Clearly wind capacity, Ammonia price and solar capacity have higher gradient ratios than all others, this means LCOA of *EE+GNH3* decreases more with an increase in wind capacity than any other spoke in the radar chart.This is because increasing in wind capacity increases total renewable generation in *EE+GNH3* which yields ammonia production for a given grid limit.Similar to wind capacity, solar capacity also yield more ammonia production due to more total renewable energy generation.Whereas ammonia price increase will yields more revenue due to more ammonia production as earlier described in Figure 5.7 and Figure 5.3.

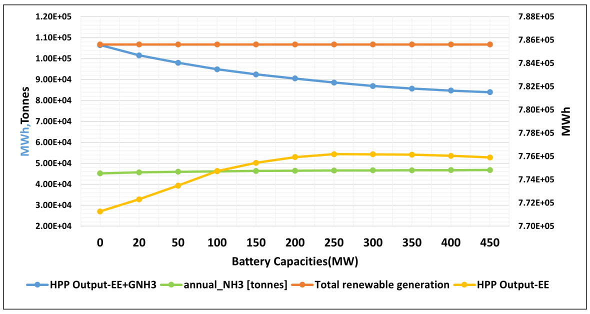
For NPV/capex and NPV in Figure 5.8e and Figure 5.8f three radar charts are overlapped. Each of the three charts shows different spokes for highest gradient ratio.NPV, NPV/Capex will be more when system outputs from *EE+GNH3* with lesser costs,so with increase in ammonia price costs of system does not increase but output ammonia production increases and hence revenue improves results in higher NPV and NPV/Capex.The other 2 charts in grey and orange colour in Figure 5.8e and Figure 5.8f are without outlier samples in the calculation of the average gradient ratio shown in Equation 5.2.

Similary in Figure 5.8g has 2 overlapped radar charts one with ammonia price outlier and other without outlier. Clearly in without outlier radar chart wind capacity has higher gradient ratio than all the others.This is due to increase in wind capacity yields in higher total renewable energy generation which most likely improves the ammonia production for a given grid limit.In chart with outlier, ammonia price has the highest gradient ratio because of solver preference to produce ammonia for higher ammonia price.

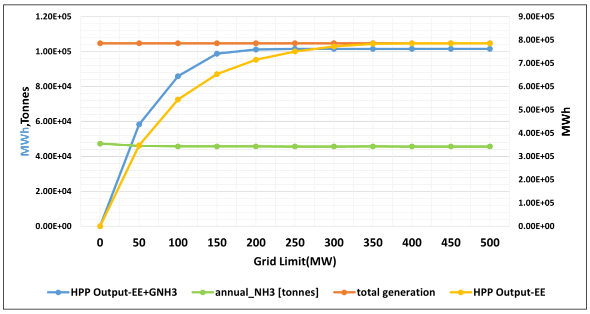
The absolute numerical values of changes in ammonia produced,HPP output of *EE+GNH3* and HPP output of *EE* for changes in various input parameters are shown in Figure 5.9.The 6 subfigures in Figure 5.9 shows changes in 6 different input parameters which are spokes in previously shown gradient radar charts. The range of x-axes in all 6 subfigures in Figure 5.9 are the value range for gradients in Figure 5.8.In few subfigures of Figure 5.9 when the x-axis start with 0 the first gradient ratio is discarded in average gradient ratio calculations of such input parameters.The Change in ammonia prices in Figure 5.9a shows a exactly complementary trend for HPP output of *EE+GNH3* and ammonia production in *EE+GNH3*. The total renewable generation remains constant since there is no change in wind or solar capacity.This complementarity between HPP output and ammonia production is due to solver preference to choose ammonia production over electricity output to improve revenue for a constant total renewable energy generation.The outlier mentioned earlier for Figure 5.8g is also clearly visible in Figure 5.9a.When ammonia price changes from 350 €/kg to 650 €/kg there is a steep increase in ammonia production than the remaining all price increases from 650 €/kg to 950 €/kg and so on.



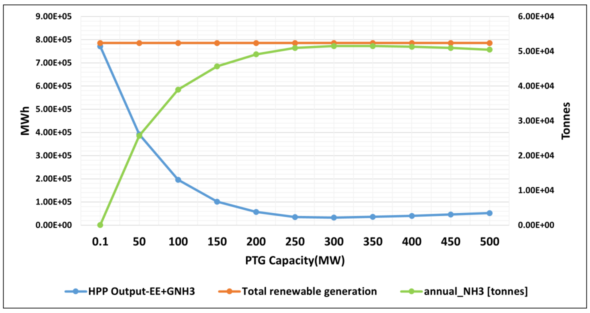
(a) Change in outputs of EE+GNH3 for changes in ammonia prices.



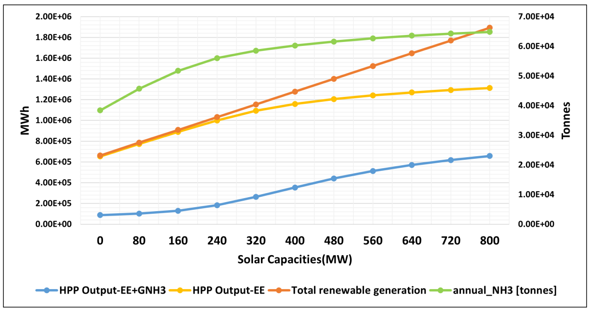
(b) Change in outputs of EE+GNH3 for changes in battery capacities.



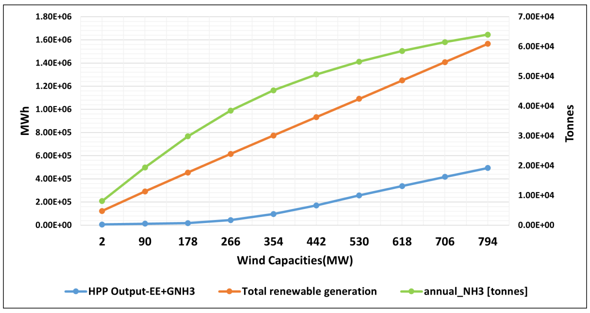
(c) Change in outputs of EE+GNH3 for changes in grid limits.



(d) Change in outputs of EE+GNH3 for changes in electrolyser capacities.



(e) Change in outputs of EE+GNH3 for changes in solar capacities.



(f) Change in outputs of EE+GNH3 for changes in wind capacities.

Figure 5.9: Change in outputs of EE+GNH3 for changes in various input parameters.

With an increase in battery capacity in Figure 5.9b there is a very slight increase in ammonia production and a significant decrease in HPP output of *EE+GNH3*.This is because of increased battery capacity, the solver shifts energy with lesser electricity price to produce more ammonia by storing it in the battery, due to this HPP output decreases for a constant total renewable energy generation and constant grid limit.But in the case of *EE* the HPP output increases with an increase in battery capacity this is mainly due to no ammonia production in *EE* and the solver saves the extra energy in the battery instead of curtailing it.This can also be seen in gradient radar charts in Figure 5.8g battery gradient ratio is very minimal but still positive.Whereas in Figure 5.8a the battery radar chart is very small but negative(inwards to the center in smallest web).

With an increase in grid limit in Figure 5.9b there is very slight decrease in ammonia production capacity and then later ammonia production remains constant. This is due to fact that increasing in grid limit is decreases the curtailment hence the HPP output of *EE+GNH3* increases.When HPP output of *EE+GNH3* increases ammonia production decreases for a constant total renewable energy generation.In case of *EE* the HPP output increases with increase in grid limit up to threshold of total renewable energy generation. The curtailment of *EE* decreases with increasing grid limit reaches 0 when the HPP output reaches the threshold.

With an increase in electrolyser rated capacity in Figure 5.9d the ammonia production increases and

HPP output of *EE+GNH3* decreases.The total renewable energy generation is kept constant.Ammonia production increases because more hydrogen is produced when electrolyser capacity is increased, whereas the HPP output decreases because the solver chooses to improve revenue by producing more ammonia by providing more renewable energy to the electrolyser than delivering it to the grid.

With the increase in solar capacity in Figure 5.9e the ammonia production increases and the HPP output of *EE+GNH3* also increases.Unlike other subfigures in Figure 5.9 the curves are smoother in Figure 5.9e this conveys that gradient ratios for all iterations of solar capacity change have almost similar values. The HPP output of *EE* increases linearly with an increase in solar capacity and then start to saturate after exceeding the grid limit of 300MW. Similarly with the increase in wind capacity in Figure 5.9f the ammonia production increases and the HPP output of *EE+GNH3* also increases.Unlike other subfigures in Figure 5.9 the curves are smoother in Figure 5.9f this conveys that gradient ratios for all iterations of wind capacity change have almost similar values.

In all 6 subfigures of the Figure 5.9 one common trend is observed.Whenever a single input parameter is changed keeping all other inputs at their base(nominal) valuesin OFAT sensitivity approach,always there exists atleast 2 bottlenecks one for ammonia production and one for HPP output of *EE+GNH3* or *EE*.Such bottlenecks are listed below

1. **Ammonia price change**: Electrolyser capacity,grid limit and total renewable generation are the bottlenecks.
2. **Battery change**: Electrolyser capacity,grid limit and total renewable generation are the bottlenecks.
3. **Grid limit change**: Electrolyser capacity and total renewable generation are the bottlenecks.
4. **Electrolyser capacity change**: Grid limit and total renewable generation are the bottlenecks.
5. **Solar capacity change**: Electrolyser capacity, grid limit are the bottlenecks.
6. **Wind capacity change**: Electrolyser capacity, grid limit are the bottlenecks.

These bottlenecks causes the saturation(flatness of curve) of ammonia production and HPP output curves in all 6 subfigures of the Figure 5.9.The main bottleneck for the ammonia production is the electrolyser capacity because all mass productions are directly dependant on this single parameter as shown in Figure 5.10. The additional equations of HB process which are dependant on this electrolyser capacity are listed in subsection 3.2.5.In the radar chart Figure 5.8e without the PTG outlier clearly electrolyser capacity has highest gradient ration for NPV/Capex which is one of important financial metrics for judgements of RPD.The modelling dependency and gradient dependency on electrolyser capacity makes it crucial aspect for the HPP+GNH3 system,In order to improve the value addition through any additional hydrogen based X systems in the P2X setup.

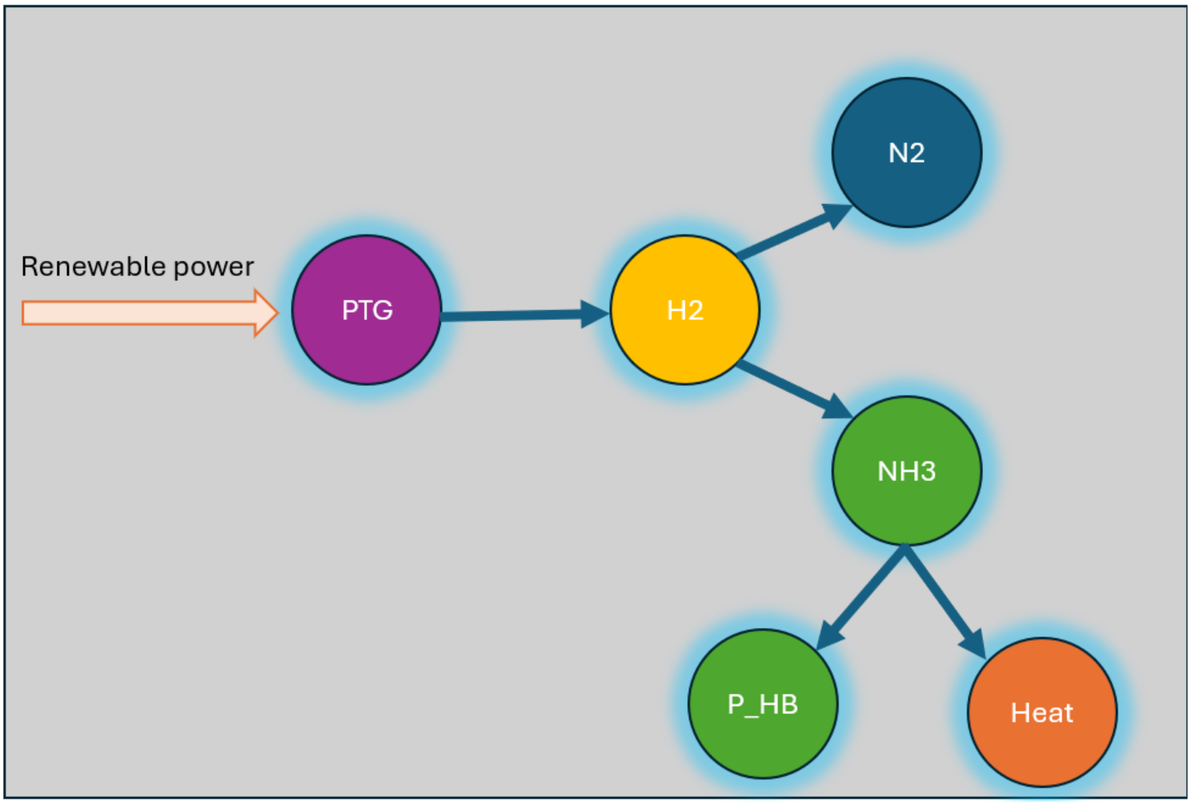


Figure 5.10: Dependancy of HB process parameters on electrolyser capacity.

5.3. Optimization results

Along with evaluation functionality HyDesign also has the sizing optimization functionality which was elaborated in section 3.4. For a given objective of NPV/Capex, LCOA and NPV the sizing optimization was performed using surrogate based optimization to reduce full model evaluations. The results obtained for 3 different financial metrics as objective functions of optimization are shown in Table 5.4.

For maximizing the NPV/Capex the surrogate based sizing optimization yielded 4MW of Wind capacity and 1MW of electrolyser capacity which is unrealistic for a RPD to setup such a plant in a significant space with such low capacities.In Figure 5.8e for a radar chart without solar outlier, the NPV/Capex increases more with increasing solar capacity.The same result can be seen in this surrogate based optimization result also.

	EE+GNH3		
	NPV/Capex	LCOA	NPV
NPV/CAPEX	**0.818**	**0.134**	**0.366**
NPV [MEuro]	**184.167**	**137.469**	**408.773**
IRR	0.12	0.072	0.094
LCOE [Euro/MWh]	31.907	53.163	42.44
LCOH [Euro/kg]	5.932	9.257	7.597
LCOA [Euro/kg]	**0.5**	**0.468**	**0.504**
Revenue [MEuro]	582.545	1758.229	2342.282
CAPEX [MEuro]	225.155	1029.056	1115.378
OPEX [MEuro]	3.251	16.7	18.247
penalty lifetime [MEuro]	0	0	0
Capacity factor wind [-]	0.235	0.208	0.209
Capacity factor solar [-]	0.176	0.176	0.176
Capacity factor HPP [-]	0.155	0.133	0.095
Grid limit [MW]	**300**	**300**	**300**
Wind [MW]	**4**	**788**	**524**
Solar [MW]	**464**	**765**	**800**
Battery Energy [MWh]	**132**	**1132**	**1728**
Battery Power [MW]	**33**	**283**	**432**
PtG [MW]	**1**	**1**	**87**
AEP [GWh]	635.851	1812.968	1104.897
GUF	0.242	0.69	0.42
Annual H2 production [tonnes]	110.018	117.677	9497.967
Annual consumption of electrolyser [GWh]	7.433	7.966	641.011
Annual NH3 production [tonnes]	623.435	666.836	53821.96
Annual consumption of HB process [GWh]	2.157	2.307	186.224
Total annual curtailment [GWh]	1889.04	19451.062	6093.874

Table 5.4: Sizing optimization results for different objective functions of EE+GNH3.

For maximizing the NPV the surrogate based sizing optimization yielded more solar capacity than the wind capacity.In Figure 5.8f for a radar chart without solar outlier, the NPV increases more with increasing solar capacity.The same result can be seen in this surrogate based optimization result also.

For minimizing the LCOA the surrogate based sizing optimization yielded more wind capacity than the solar capacity.The resulted electrolyser capacity is 1MW which is again unrealistic for RPD.In Figure 5.8d the LCOA decreases more with increasing wind capacity.The same result can be seen in this surrogate based optimization result also.

From results of all 3 objective functions it is clear that surrogate based optimization sometimes yields unrealistic sizing results which are not feasible on ground.This can be improved by evaluating more number of models in this optimization shell with more iterations.Currently the presented results of 3 objective functions are evaluated with only 8 models with 2 iterations.This surrogate based optimization also uses gradient approach (Murcia Leon et al., 2024).So,instead of doing full model or partial model evaluations, analytical equations can be formulated using the average gradient ratio approach presented in section 5.2.Formulation of analytical equations for sizing optimization is out of the scope of this study and hence excluded.

6 Conclusion

Although the percentage share of renewable energy in the global energy landscape is increasing rapidly and consistently breaking records for annual installation, there is still a need for tripling up of renewable energy capacity by 2030.The costs and prices of renewable energy declining year by year, this is one of the key reasons for the shrinking of profits for renewable power developers(RPDs). Different strategies can be adopted by the renewable developers to increase revenues like improving financing costs, making multiple revenue streams for individual renewable assets, combining production outputs from different plants in the portfolio to leverage the complementarity of assets, and also entering different energy markets etc.

Along with adding extra capacity of renewable energy in the global energy landscape, it is also important to search for solutions to turn the hard-to-abate sectors to have a net zero or negative carbon footprint. This creates an opportunity for P2X technologies which are becoming popular due to their ability to facilitate the integration of different energy sectors like electricity and hard-to-abate sectors.

The design of a Hybrid power plant(HPP) is a complex problem that combines different assets to maximize the value of the power plant.Although many tools have been developed for either larger hybrid systems, microgrid applications or individual technology plants, there is still a requirement for new tools with capabilities that are specific to utility-scale hybrid power plants.Researchers at the Technical University of Denmark(DTU) are in the process of developing an open-source tool called HyDesign.According to desktop research, it was understood before HyDesign that no other open-source HPP sizing tool in the market could size and optimize the P2X designs.

The purpose of this study is to analyze how can the RPDs improve their economic value by coupling with green ammonia(GNH3) production using HyDesign.In various ways, green ammonia can be produced.But, this study chooses the most prominent and proven technology which existed for more than a century now.Haber bosch(HB) process of ammonia production is modelled in this study.The subresearch questions and main research question are answered below.

6.1. Sub research questions:

How to model and integrate the production of Green Ammonia in HPP design of Hydesign?

HyDesign is built using Python computer programming language and open source framework for efficient multidimensional analysis and optimization called OpenMDAO.OpenMDAO operates with the smallest unit of computational work called components.Amongst different types of components, explicit components were chosen to keep a clear distinction between the inputs and outputs.Each renewable resource and related weather computations of the HPP+GNH3 system are modelled in explicit components.Costs, and financial metrics are also modelled as separate explicit components. HyDesign also has another important explicit component called Energy Management System(EMS).EMS currently formulated in HyDesign can only optimize the revenue of the RPD based on the given inputs of renewable energy source generation time series, and offtake prices of the energy vectors and molecules to be produced. In this EMS component, non-energy-producing parts of the HPP+GNH3 system are modelled.EMS contains a linear optimization problem in which the objective function is modified in this study to cater for the needs of P2X designs, especially P2Ammonia design.With modification in the objective function of EMS different combinations of objectives are now possible to choose based on the requirements of the RPDs.Along with objective functions, a few existing constraints are modified and many new constraints are added to the optimization problem to include the GNH3 in the existing HPP+P2X design.

For the GNH3 system 3 important aspects are there for designing the production of the whole GNH3 plant.The first aspect is mass modelling which can be done in 3 different ways simple mass balance, lookup tables and equilibrium constant calculations.Each of the three methods has its own advantages and drawbacks.Although mass balance has 100% conversion of reactants(H2,N2) to ammonia(NH3),it does not show HB process dependency on operational conditions like temperature and pressure. Lookup tables provide ammonia equilibrium percentages for different operational conditions but for only a few values of temperature and pressure.So, Interpolation and extrapolation must be made for values outside the range of the operational conditions given in the lookup tables. Interpolation and extrapolation within a linear optimization problem create more complexity.Computation of ammonia mass using equilibrium constants is the most accurate among 3 mass modelling methods,but it adds non-linearity to the linear optimization problem.In this study for mass modelling simple mass balance is selected because of its 100% conversion which creates the possibility to analyze the extreme case in GNH3 value addition to the HPP system.Hydrogen production mass is already modelled in HyDesign using a piecewise linear function to linearize the non-linear load curves of the electrolysers.Using this hydrogen mass and assumption of constant H2/N2 mole ratio, nitrogen mass is modelled with a dependency on the mass of hydrogen and feed ratio(ratio of masses of H2/N2 for 1 mole of NH3 production).The size of N2 production is neglected since N2 is abundant in the atmosphere and is available at any point in the lifetime of the plant.Corresponding mass balance equations are modelled as constraints in the EMS optimization problem.

The second aspect is power modelling, after thorough literature and market research, it was understood that the percentage energy requirement in the form of electricity for ammonia production is much less.With advancing latest green ammonia technologies plant sizes are decreasing and hence the energy requirement for green ammonia production is also improving.3 different numerical values are deduced from 2 industrial datasheets and 1 scientific paper.Out of these 3 values the highest number is chosen in a conservatory view. The last aspect of the green ammonia plant is the heat modelling of the plant.Haber bosch process is an exothermic process that releases heat due to N-H bond formation.So,every 1 mole of ammonia produced produces 46.14 kJ of heat always.Hence this linear relationship is modelled as a single linear equation dependent on the mass of the ammonia production.In this way, all 3 important aspects of the green ammonia plant are modelled as additional constraints in the linear optimization problem of the EMS explicit component of HyDesign.

How does the value(economic benefits) of a utility-scale hybrid renewable power plant change with this HPP+GNH3 system design?

The Definition of utility-scale hybrid renewable power plants is referred from the **IEA Wind TCP task 50 WP1**.In this study, only a grid-connected utility-scale renewable HPP is analysed.Results of 2 objective functions of EMS are compared and analyzed to understand the value addition due to GNH3 in the HPP+GNH3 system.1st objective function with only HPP is denoted by *EE* and the second objective with HPP+GNH3 is denoted by *EE+GNH3*.The ammonia offtake price is kept constant throughout the lifetime and The hourly electricity price data of 2012 is available in the HyDesign repository is the same time-series of prices is used for all 25 years of lifetime.In an absolute numerical value comparison of annual results of both *EE* and *EE+GNH3* shows that the overall revenue of *EE+GNH3* is more than *EE*.The revenue always depends on the price and quantity.The actual revenue difference between these objective functions originates from ammonia production and high electricity delivery only possible due to more battery operation driven by high electricity price hours.

$$\text{Revenue Difference} \propto \text{Ammonia production} \propto 1/\text{Electricity price}$$

In those optimizations.Out of 8760 hours in a year more than 80% the time revenue difference is caused by ammonia production driven mostly by the electrolyser capacity and total renewable energy generation which depends upon the renewable sources capacities.Out of the rest 18.5% the year the revenue difference is caused by electricity production which changes due to battery operations driven solely by electricity price.Increasing total renewable energy generation through adding more renewable energy sources or increasing the current rated capacities of renewable sources improves the quantity of ammonia production and consequently revenue of the HPP+GNH3 system.While increasing the total renewable energy generation accordingly electrolyser capacity must also be increased to see a steep increase of ammonia production.Alternatively battery-rated capacity can also be increased to improve the revenue of HPP+GNH3 system.Since,electricity price is not in the control of the RPDs, only resource-rated capacities, electrolyser capacity and battery capacity can be changed.

Along with revenues, other financial metrics like LCOE,LCOA, NPV/Capex, and NPV are also checked for objective functions.The results of these 4 metrics depict that due to higher costs of green hydrogen and green ammonia production and associated infrastructure,the NPV,NPV/Capex is more for the HPP system. whereas increasing resource-rated capacities, electrolyser capacity and battery capacity improve all 4 financial metrics.But, improving all the capacities at a time will not help due to the rise of costs, increasing the solar will improve LCOE, NPV/Capex,NPV and increasing wind capacity will improve LCOA.Increasing electrolyser capacity will also improve the NPV/Capex.Increasing the battery capacity will also improve these additional 4 financial metrics but not to the extent of increasing solar, wind or electrolyser.

What can be the possible Modelling checks(MC) to verify the model and what sensitivity framework be made on a model for this HPP+GNH3 system design?

Before analyzing the results of the simulation run through the added HPP+GNH3 model in HyDesign it is necessary to verify the proper functioning of the model using appropriate modelling checks.Performing these modelling checks will ensure the reliability of the results and this exercise also gives confidence in the functioning of the model, since there is no benchmark power to ammonia(P2A) model to refer to. It is recommended to check the model in different sites using different input resource data.But,only the base case site is used for modelling checks and generating results in this study.13 modelling checks are listed in this report and all 13 modelling checks are performed on the model for the base case site.Out of 13 modelling checks, 7 modelling checks are for an existing model of HPP in HyDesign and the rest 6 modelling checks are specifically for the new GNH3 model. Out of these 6 modelling checks, 2 checks are dependent on both the existing model and the newly added GNH3 model, so testing them on one site data will be enough to verify the functioning of related equations.

In this study one-factor-at-a-time(OFAT) sensitivity approach is used to perform a sensitivity analysis on base case results.The change of output parameters to each input parameter is tracked through gradient ratios.Gradient ratio is the ratio of the percentage change of the output parameter to the percentage change of the input parameter.To increase reliability and decrease the dependence on absolute numerical values, multiple gradient ratios are calculated through multiple iterations of changes in input parameters and resulting output parameters.Finally average gradient ratios are calculated using gradient ratios of all multiple iterations.Results of this sensitivity study give 6 radar charts of different financial metrics and HPP+GNH3 system outputs.These radar charts help to analyze and understand where the value addition happens in the HPP+GNH3 system. The gradient ratio radar charts are also checked with the results of the surrogate-based efficient global optimization(EGO) algorithm existing in HyDesign.For a specific financial metric as an objective function in the EGO algorithm, both sensitivity analysis results and the existing EGO algorithm does the same actions.Hence OFAT sensitivity approach with gradient ratios method is verified and useful for this HPP+GNH3 model.

6.2. Main research question:

How can the value(economic benefits) of utility-scale HPP be optimized by coupling with production of energy carrier Green NH3?

The value in this study is defined as the economic benefit measured by a few financial metrics like revenue, LCOE, LCOA, NPV/Capex, and NPV.The real value addition in a grid-connected utility-scale hybrid renewable power plant lies in the electricity and ammonia prices and associated output quantities. Since the hourly electricity price is not in the control of the RPDs, only the ammonia price and associated output quantities can be improved.In this study, ammonia price is kept constant, since currently ammonia offtake contracts are made with fixed predetermined ammonia price.RPDS have control to negotiate the ammonia offtake price,with this current market situation where GNH3 plants are relatively less and technology is new, RPDs can expect and demand a price premium for such plants.Now, with this only immediate controllable value left is through improving output quantities like ammonia production and electricity delivery.For a single base case site performed in this study with assumptions, it is clear that most of the time in a year ammonia production will yield more revenue to RPD than electricity production.But looking at other financial metrics NPV/Capex, and NPV which also include the associated costs of GNH3 plants,currently with the present market situation with lesser economies of scale of GNH3 plants it is not profitable for RPD to build own operate(BOO) an HPP+GNH3 system in comparison with HPP plant.

Although revenues are higher for an HPP+GNH3 system than an HPP plant other key financial metrics are better for the HPP plant.Using a sophisticated open-source tool like HyDesign, the sizing of HPP+GNH3 plants can be evaluated and optimized to improve key financial metrics like LCOE, LCOA, NPV/Capex, and NPV.In this study, HPP+GNH3 model is added to HyDesign EMS.Out various 3 of mass modelling mass balance approach is chosen to observe the extreme case of value(economic) addition when 100% reactants(H2,N2) to product(NH3) conversion.Since no open-source tool has an HPP+GNH3 model based on the desktop research.To ensure reliability of results and to get confidence in the functioning of the model,13 modelling checks are listed in this study.All 13 checks are successfully satisfied by the HPP+GNH3 model in Hydesign.

For a single base case site with a base case scenario sensitivity analysis is performed using the OFAT method.The sensitivity analysis yielded that for different financial metrics, different components of HPP+GNH3 must be improved to optimize the value(economic) of financial metrics.Increasing solar capacity will improve metrics like LCOE, NPV/Capex, and NPV.Increasing wind improves the LCOA and ammonia production.Increasing electrolyzer capacity will also improve NPV/Capex and ammonia production since all mass productions in the HPP+GNH3 system are dependent on the electrolyser capacity.Increasing battery will also improve a few of these 4 metrics but not to the extent of increasing solar,wind and electrolyser capacity. These results of the OFAT sensitivity analysis is also checked with the HyDesign's existing surrogate based EGO algorithm.For a specific financial metric as an objective function in the EGO algorithm, both OFAT sensitivity analysis results and the existing EGO algorithm does the same actions.Increasing solar, wind, electrolyser capacity and battery all together are expected to improve these metrics but also raise costs significantly, this ignites a thought for a detailed sensitivity analysis to understand to what extent this value(economic) can be optimized using the increase of multiple capacities.The study finds that building a large-scale HPP+GNH3 system is beneficial for RPDs and to society which yields better financial benefits and more green ammonia production which can be used in many hard-to-abate sectors.

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A

Appendix-A

Table A.1: Cost Parameters Overview

Component	Cost	Unit
Wind		
Turbine	640,000	EUR/MW
Civil Works	260,000	EUR/MW
Fixed O&M	12,600	EUR/MW/year
Variable O&M	1.35	EUR/MWh
Solar PV		
PV System	110,000	EUR/MW DC
Hardware Installation	100,000	EUR/MW DC
Inverter	20,000	EUR/MW
Fixed O&M	4,500	EUR/MW/year
Battery Storage		
Energy Cost	62,000	EUR/MWh
Power Conversion System	16,000	EUR/MW
BOP Installation	80,000	EUR/MW
Control System	2,250	EUR/MW
Hydrogen System		
Electrolyzer CAPEX	800,000	EUR/MW
Electrolyzer OPEX	16,000	EUR/MW
Water Cost	4	EUR/m^3
Water Treatment	2	EUR/m^3
Ammonia System		
Haber-Bosch CAPEX	2,576	EUR/tonne
Haber-Bosch OPEX	51.52	EUR/tonne
Storage CAPEX	644	EUR/tonne
Storage OPEX	12.88	EUR/tonne
Shared Infrastructure		
BOS & Soft Costs	119,940	EUR/MW
Grid Connection	50,000	EUR/MW
Land Cost	300,000	EUR/km^2