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LIFE CYCLE ASSESSMENT OF AMMONIA PRODUCTION FROM RENEWABLE ENERGY

Master's thesis
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ABSTRACT

Linh Nguyen: LCA of ammonia production from renewable energy
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Mitigating climate change is one of the primary goals of many countries all over the world. A lot of efforts have been made to reduce anthropogenic greenhouse gas emissions, especially from manufacturing industries. Ammonia is an important synthesis chemical due to its essential use in producing fertilizer, which is extremely important to secure the global food supply. In addition, ammonia also has many applications in chemical industries. Currently, ammonia is mainly produced from natural gas. The production process is very energy-intensive and releases high CO_2 emissions. Therefore, more sustainable production pathways are needed to decarbonize the ammonia industry.

Firstly, the thesis aimed to explore the legislative frameworks that incentivize the development of green ammonia in Europe and Estonia, where the case study is located. Secondly, a life cycle assessment (LCA) study was conducted for the green ammonia plant in Estonia to understand the environmental impacts of green ammonia production. The LCA results were used to analyze the environmental impacts of green ammonia production, as well as identify the most relevant impact categories linked with green ammonia production and the largest contributors to the total environmental impacts in the level of life cycle stages and single processes. The results of the thesis were compared with other studies on green ammonia production and conventional ammonia production via steam methane reforming to understand the relative magnitudes of the environmental impacts of the case study.

The main legislative frameworks affecting ammonia production in Europe are the Renewable Energy Directive and the two delegate acts supporting the Directive. The objectives and strategies set in the European Hydrogen Backbone initiative and 'Estonia 2035' are the motivations for developing a hydrogen supply chain in Estonia. Also, the Estonia Hydrogen Roadmap was created to guide the hydrogen development activities, which aimed to create an abundant and carbon-free hydrogen industry in Estonia by 2050. As hydrogen is an input for ammonia production, the development of green hydrogen supply chain is very necessary to promote green ammonia development.

The environmental impacts of green ammonia production in Estonia were evaluated using the LCA method. It was shown that the green ammonia production system has the highest impacts on resource use (minerals and metals), resource use (fossils), climate change, human toxicity (cancer), human toxicity (non-cancer), and freshwater eutrophication. Throughout the life span of the plant, the electricity consumption for hydrogen production is the major source of environmental impacts. Solar electricity was found to have less environmental impacts than wind electricity in the electricity profile consisting of 25% solar and 75% wind power. In terms of the impacts on climate change, the production of 1 kg of ammonia was estimated to produce 0.925 kg CO_2-eq to the environment. 80% of the emissions came from hydrogen production and 20% came from nitrogen production. Through the comparison with other studies on green ammonia in the literature, the environmental impacts of the case study on climate change and freshwater eutrophication are generally higher than other green ammonia systems. The reasons could be due to a more detailed inventory of the water electrolysis and the inclusion of a solar farm in the system boundary of the thesis. However, further analysis is needed to identify the actual causes of these high environmental impacts compared to other studies. Through comparison with other SMR-based systems, ammonia production from renewable energy is found to have a lower impact on climate change and a higher impact on freshwater eutrophication compared to ammonia production via SMR. These findings are aligned with some of the studies in the literature. In the future, the LCA model for the case study can be improved by using actual data from the plant and expanding the system boundary.

Keywords: life cycle assessment, LCA, ammonia production, green ammonia production, renewable energy, wind, solar, Estonia.

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PREFACE

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Thank you!

Tampere, 30 May 2025

Linh

CONTENTS

LIST OF SYMBOLS AND ABBREVIATIONS

AEL	Water electrolyzer
CMS	Carbon molecular sieves
GHG	Greenhouse gas
GWP	Global warming potential
LCA	Life cycle assessment
LCI	Life cycle inventory
PEM	Polymer electrolyte membrane
PSA	Pressure swing adsorption
PPA	Power Purchase Agreement
RED	Renewable Energy Directive
RFNBO	Renewable fuel of non-biological origin
SMR	Steam methane reforming
TEN-T	Trans-European Transport Network

Al_2O_3	Aluminium oxide
CH_3OH	Methanol
CO	Carbon monoxide
Fe	Iron
H_2	Hydrogen
KOH	Potassium hydroxide
NH_3	Ammonia
OH^-	Hydroxide ion

1. INTRODUCTION

To mitigate climate change, countries around the world have made large efforts to decarbonize industries. In Europe, through a long-term development strategy established by the European Green Deal, Europe aims to become a climate-neutral continent and detach its economic growth from resource use (European Commission, 2021). These long-term goals have become the underlying principles for the development of proposals and policies by the European Commission. The European Green Deal contains ambitious objectives of European countries to (i) reduce 55% of the net greenhouse gas emissions (GHG) by 2030, and (ii) reach net-zero GHG emissions by 2050 (European Commission, 2021). To help achieve these objectives, industrial decarbonization needs to work on solutions to reduce their environmental impacts, especially those that are energy-intensive and produce high emissions.

Ammonia (NH_3) is an important synthesis chemical. It is used extensively in various industrial applications such as polyimides, nitric acid, pharmaceuticals, refrigerants, cleaning solutions and other chemicals (Ghavam et al., 2021). Ammonia is especially essential in producing synthetic fertilizers for food production globally, thus contributing to food security for a growing population. In addition, ammonia can also be considered as a potential energy carrier for energy storage and transportation (Ghavam et al., 2021). Ammonia has an energy density of 4.32 kWh/liter, which is equal to the energy density of methanol (CH_3OH) and two times higher than the energy density of liquid hydrogen (H_2). Compared to hydrogen as an energy carrier, ammonia is easier to liquefy since it liquefies at -33.4°C and at atmospheric pressure, while hydrogen liquefies at -253°C. Ammonia also has other advantages to be used as a potential energy carrier such as non-explosive characteristics, easy storage (33°C at 1 atm), great stability with minimal energy loss, and the possibility for long-term storage (Tilman et al., 2011).

Ammonia is produced via Haber-Bosch by synthesizing from hydrogen and nitrogen. Hydrogen used for ammonia production can be produced through different pathways, using various feedstocks such as coal, natural gas, heavy fuel oil, and coke through different production methods such as reforming, pyrolysis, and gasification. The feedstock used to produce hydrogen affects the amount of GHG emissions of the Haber-Bosch process. Currently, 96% of ammonia is produced from fossil fuel-based hydrogen, which produces high GHG emissions (Ojelade et al., 2023). The remaining 4% is generated from water electrolysis powered by electricity, which also consumes fossil fuels such as coal or natural gas passively to generate electricity (Ghavam et al., 2021). The ammonia production from natural gas produces the highest GHG emissions (up to 2.5 tCO_2-eq / tNH_3) among all production pathways, but it is also the most common way to produce ammonia at the moment (Ghavam et al., 2021).

To make ammonia production become more sustainable, one solution is to produce hydrogen from water electrolysis powered by renewable energy, or produce hydrogen from lower-carbon feedstocks such as biomass, bioethanol, bio-glycerol or biogas (Chisalita et al., 2020). The ammonia production pathway using renewable energy hydrogen via electrolysis is called green ammonia and it has been shown to be one of the most environmentally-friendly pathways to produce ammonia. Ammonia produced from green H_2 is shown to reduce up to 70% GHG emissions compared with the traditional production method from natural gas (Bicer et al., 2016).

Although green ammonia produces less direct GHG emissions than conventional ammonia production from fossil fuels, it is necessary to understand the full environmental impacts of green ammonia production compared to the traditional method. This thesis aims to explore the environmental impacts of green ammonia production from a life cycle perspective using life cycle assessment (LCA). Although there have been many LCA studies on green ammonia production, there is a lack of LCA studies for ammonia production in Estonia. The location of the plant defines the sources of material and energy flows to the system, which creates differences in the total environmental impacts. The case study also uses mixed electricity comprising wind power and solar power in a ratio of 3:1, whose impacts are also different from the systems using 100% wind power or 100% solar power.

The research questions of this thesis are:

1. What are the strategies and policies that encourage the development of green ammonia production in Estonia?
2.
    a. What are the environmental impacts of the green ammonia production system?
    b. What are the most relevant impact categories associated with green ammonia production?

c. What are the most environmentally impactful elements in the green ammonia system at the life-cycle stage level and at the single process level?

The structure of the thesis includes 6 chapters. Chapter 2 is a literature review of legislative policies related to green ammonia production, and ammonia production technologies and their environmental impacts. It also introduces LCA methodologies and reviews other LCA studies on ammonia production. Chapter 3 describes the case study in Estonia and explains the LCA model used in the thesis. Chapters 4 and 5 present, interpret, analyze, and discuss the LCA data to answer the research questions. Chapter 6 is a summary of the thesis and highlights the main findings.

2. LITERATURE REVIEW

2.1 Strategies and policies for green ammonia production

This section introduces strategies and policies driving the ammonia economy as well as the hydrogen economy in Europe and Estonia. In Europe, the development of green ammonia is encouraged by the Renewable Energy Directive (RED), which is part of the 'Fit for 55 package'. It sets requirements on the renewable electricity that is used to produce hydrogen and hydrogen derivatives, known as 'renewable liquid and gaseous transport fuels of non-biological origin' (RFNBO). In Estonia's context, the motivation for green ammonia development comes from the European Hydrogen Backbone initiative, as well as long-term strategies from 'Estonia 2035'. The development of a green hydrogen economy in Estonia is facilitated by the Estonia Hydrogen Roadmap, which aims to increase the hydrogen production capacity in the country and reduce the emissions from the production.

2.1.1 European Union's strategies and policies

A policy framework that supports the development of green ammonia is the 'Fit for 55 package', which was a legislative proposal by the European Commission in 2021 ("Fit for 55," 2021). It includes rules and regulations related to all sectors of the economy to help Europe achieve a 55% GHG reduction by 2030 and become net zero by 2050. The adoption of the EU Renewable Energy Directive (RED) is part of the 'Fit for 55' package. EU Directives are legal frameworks that are proposed by the European Commission, then amended and adopted by the European Parliament and the European Council. EU Directives are not directly applicable, but must be transposed into national legislation by all Member States within 18 months after the date entering into force. The first RED version (RED I) was first adopted in 2009. It was replaced by the second version (RED II) in 2018, and the newest version (RED III) in 2023, which is currently in force.

Overall, RED III sets a target of 42.5% renewables share of the EU's overall energy consumption by 2030. Furthermore, RED III encourages European countries to achieve an additional 2.5% indicative increase in renewables share, which increases the total share of renewable energy of the EU up to 45%. In the ammonia production context, RED III strongly emphasizes increasing the consumption of RFNBOs in transport and industry. RFNBO is defined as fuels produced from hydrogen, which derives from renewable energy except biomass sources in the form of heat or electricity, such as synthetic hydrocarbons-, alcohols-, and ammonia-based fuels (JRC, 2023). The ammonia produced via water electrolysis using renewable electricity is also classified as an RFNBO. According to RED III, RFNBOs should account for a minimum of 1% of the total energy usage in transportation, and a minimum of 42% of total hydrogen consumed in industry by 2030. By 2035, the proportion of RFNBOs used in industry shall account for at least 60% of the total hydrogen used in industry. (Directive (EU) 2023/2413, 2023)

Compared to the previous version of RED (RED II), the current version expands the regulations on RFNBOs, not only limited to RFNBOs used as transport fuels but also to those used in industrial sectors. In addition to the REDs, the Commission adopted 2 delegated acts in June 2023 to supplement the RED II. Delegate acts, formally called Commission Delegated Regulations, are regulations adopted by the European Commission and directly applicable to all EU countries. The first delegated act sets additionality and imposes temporal and geographical correlation requirements to the renewable energy used in RFNBO production. The second delegated act defines a minimum threshold for GHG emission reductions of RFNBOs compared to a fossil fuel comparator and provides a methodology for calculating the GHG reductions.

The first delegated act CDR 2023/1184 established the conditions under which the electricity for both domestic and imported RFNBO production is considered fully renewable. There are 3 cases where the electricity used to produce RFNBO can be considered fully renewable. In the first case where the production of RFNBOs is directly connected to the renewable electricity generation facilities, the renewable electricity plants must come into operation not earlier than 36 months before RFNBO production sites start to operate. In the second case where the production of RFNBOs is powered by the grid, the renewable energy share of a bidding zone must be over 90% in the previous calendar year. In the third case where renewable electricity is purchased through a Power Purchase Agreement (PPA), the requirements regarding additionality, and temporal and geographical correlation must be fulfilled. The additionality principle requires that RFNBO manufacturers must sign PPAs with new renewable electricity plants, which are commissioned no more than 36 months before the operation of the RFNBO production sites and do not receive CAPEX or OPEX support. This requirement aims to avoid the highly increasing demand for renewable electricity for hydrogen plants causing more fossil-based electricity generation to cover conventional load. The temporal and geographical correlation includes requirements to ensure hydrogen should be produced at the location and time when renewable electricity is available. (CDR 2023/1184, 2023)

The second delegated act CDR 2023/1185 sets a minimum threshold for GHG emissions savings of recycled carbon fuels and provides methodological guidelines to calculate GHG emissions of RFNBOs used as transport fuels throughout their life cycle. Both RED II and RED III require that the minimum GHG savings of RFNBOs is 70% compared to fossil comparator of 94 g CO2 eq/MJ, meaning that the maximum GHG of RFNBOs could not exceed 28.2 g CO2eq/MJ. (CDR 2023/1185, 2023)

In addition, the production of green ammonia could be more economically viable when green hydrogen is more abundant in Europe. Hydrogen is now a priority of the European Union to decarbonize the economy, especially in energy-intensive industries and transportation. In 2022, hydrogen only represented under 2% of the total Europe's energy consumption. It was mainly used in chemical industries such as plastics and fertilizer production. Currently, several strategies and frameworks have been established to change the situation and increase the hydrogen proportion in the economy. According to the REPowerEU Strategy launched in 2022, European countries are expected to produce 10 million tonnes of hydrogen and import 10 million tonnes by 2030. By 2050, renewable hydrogen is expected to account for 10% of the total European energy consumption. (European Commission, 2025a)

2.1.2 Estonia's strategies and policies

A big opportunity for green ammonia production in Estonia comes from the European Hydrogen Backbone initiative launched in 2021, which initiated a plan to build a hydrogen transmission network of 40,000 km connecting 21 European countries by 2040. The construction of this transnational hydrogen network will help to promote hydrogen production and trading between the countries, hence, increasing the capacity of green hydrogen resources for ammonia production. Currently, 33 transmission network operators have participated in the initiative, including Elering, Estonia's transmission network operator. In addition, in 2022, a cooperation was established between Estonia, Finland, Latvia, Lithuania, Poland, and one German gas system operator to develop a hydrogen transmission pipeline from Finland through Estonia to Germany. Collaborative efforts at the regional level not only help to construct hydrogen transmission infrastructure but also foster information exchange between neighboring countries. (Eesti Vabariigi Valitsus, 2023)

The hydrogen industry is also one of the key aspects to help Estonia achieve ambitious goals regarding climate, environment, and energy aspects based on the long-term goals set in the European Green Deal and 'Estonia 2035'. 'Estonia 2035' is a development strategy to establish goals for people, society, the economy, the living environment, and governance of the country. These goals will also impact the financial management of the country (Eesti Vabariigi Valitsus, 2022). The strategy sets several targets for 2035. Compared to 2019, Estonia should reduce 42% of GHG emissions, improve the percentage of sustainable mobility from 38.7% to 55%, and raise the ranking from 10th place in 2019 in the Sustainable Development Goal Index (Eesti Vabariigi Valitsus, 2023). The country identifies hydrogen as an important step towards achieving several objectives in creating local socio-economic opportunities around new sustainable sectors, energy transition towards cleaner energy sources, and becoming a hydrogen technology exporter country (Eesti Vabariigi Valitsus, 2023).

Based on the ‘Estonia 2035’, the Estonia Hydrogen Roadmap has been developed by Estonia’s Ministry of Environment and Ministry of Economic Affairs and Communication. The roadmap describes the current state of hydrogen-related activities in Estonia and discusses plans until 2050 aiming to establish a hydrogen value chain based on demand and renewable energy. At the current state, there is no hydrogen market as well as commercial generation and use of hydrogen in Estonia. (Eesti Vabariigi Valitsus, 2023)

The objectives and activities of the roadmap will be re-evaluated every 3 years based on the actual development progress. The planning phase of the Estonia hydrogen roadmap includes 3 development stages: a pilot phase from 2021 to 2030, a scaling phase from 2030 to 2035, and an expansion phase from 2036 to 2050. The pilot phase (2021-2030) involves activities acting as the basis for future implementation of hydrogen such as the development of policies and standards, investments in research, and evaluations of the potential of hydrogen in terms of political and socio-economic objectives. It also contains the plan to gradually develop pilot projects on hydrogen production, distribution, tank storage, and usage, and develop hydrogen production technologies. It is expected that by 2030, the capacity of green hydrogen production in Estonia will be around 2,000 to 40,000 tonnes per year, depending on the developments of the hydrogen market and electricity facilities. In the scaling phase (2030-2035), the focus will be on constructing the value chain, resolving difficulties, and increasing the usage of renewable energy. It is expected that by this time, hydrogen projects will have zero emissions or much lower emissions than before throughout their life cycles. Besides, hydrogen applications should have the capability to achieve financial break-even without public incentives and within the availability of renewable energy capacity. The expansion phase (2036-2050) aims to build a zero-emission value chain of hydrogen from the abundant availability of affordable renewable energy. By this period, the installed offshore wind farm capacity is estimated at over 7 GW. Over time, the greater availability of green hydrogen will foster the development of transmission infrastructure and applications in different fields such as energy, transport, chemical industry, or hydrogen conversion to electricity and heat. (Eesti Vabariigi Valitsus, 2023)

Green hydrogen production is expected to help Estonia reduce its dependence on fossil fuels and encourage the growth of new industries such as ammonia, methanol, fertilizers, synthetic fuels, and polymers. In addition, hydrogen refueling stations will be installed every 100-200 km along the Trans-European Transport Network (TEN-T) core network. TEN-T is a seamless transport system connecting European countries, enabling efficient transportation of goods and people to encourage trade and economic growth across Europe (European Commission, 2025b). The production and storage capacity of each station is designed to be 2 tonnes of hydrogen per day at the minimum. To reach this target, Estonia has to build at least 3-5 hydrogen refueling stations per year, with a total hydrogen capacity of around 2000 tonnes of hydrogen. (Eesti Vabariigi Valitsus, 2023)

2.2 Production technologies and environmental impacts

This section describes some of the most popular technologies to produce hydrogen and nitrogen for ammonia production, and some alternative technologies used to synthesize ammonia in addition to the Haber-Bosch process.

2.2.1 Hydrogen production

Hydrogen can be produced from a wide range of feedstocks by using different technologies. Based on the feedstock sources, hydrogen production technologies can be categorized into 2 groups that are fuel processing, and non-reforming hydrogen production. Fuel processing technologies produce hydrogen from fossil-based materials such as gasoline, ammonia, and methanol. Some examples of fuel processing technologies are hydrocarbon reforming, pyrolysis, plasma reforming, aqueous phase reforming, and ammonia reforming. Non-reforming hydrogen production refers to other production methods that are not reforming processes, such as producing hydrogen from biomass or water. For hydrogen production from biomass, some current technologies are gasification, pyrolysis, liquefaction, and hydrolysis. A diverse biomass source can be used to produce hydrogen. These include animal wastes, municipal solid wastes, crop residues, sawdust, or waste paper. Hydrogen can also be produced by splitting water into hydrogen and oxygen. The technologies used in water splitting are electrolysis, thermolysis, and photoelectrolysis. (Holladay et al., 2009)

In large-scale hydrogen production, steam methane reforming (SMR) and water electrolysis are the two most popular processes to produce hydrogen. SMR belongs to hydrocarbon reforming technology, which produces hydrogen from hydrogen-containing hydrocarbon fuels. Hydrocarbon reforming technology also includes other processes such as partial oxidation, dry reforming, and auto-thermal reforming. Among the reforming processes, SMR is the oldest and most widely used process to produce H_2. The reactions to convert CH_4 to H_2 are shown in Equations 1 and 2 below. Because the reforming process produces a large amount of carbon monoxide (CO), a water-gas-shift reactor is commonly used to convert the CO produced to H_2. Equation 1 describes the reforming reaction and the second equation describes the water-gas-shift reaction. (Holladay et al., 2009; Meloni et al., 2020)

$$\mathrm{CH_4 + H_2O \leftrightarrow CO + 3H_2} \qquad \Delta\mathrm{H}\ 298 = 206\ (\mathrm{kJ/mol}) \qquad (1)$$

$$\mathrm{CO + H_2O \leftrightarrow CO_2 + H_2} \qquad \Delta\mathrm{H}\ 298 = 41\ (\mathrm{kJ/mol}) \qquad (2)$$

SMR produces a syngas mixture comprising H_2, CO, and CO_2. This technology is preferable to other reforming processes because it produces a gas mixture with a high H_2/CO ratio (around 3:1), compared to ratios of 1:1 or 2:1 of other reforming processes. The reforming reaction (Equation 1) is endothermic, which requires an external heat source of higher than 700°C. Nickel is commonly used as a catalyst for the reforming process. The water-gas-shift reaction can be carried out in a high-temperature reactor or low-temperature reactor. If the reactor operates at a high temperature (>350°C), the kinetics happen faster, but it can only convert a certain amount of carbon monoxide due to thermodynamics limitations. On the other hand, if the reactor operates at a lower temperature (210-330°C), a larger proportion of carbon monoxide will be shifted. An iron catalyst is commonly used in high-temperature reactors, and a copper catalyst is used in low-temperature reactors. (Holladay et al., 2009; Meloni et al., 2020)

Water electrolysis is a reaction that splits water into hydrogen and oxygen in an electrolyzer powered by electricity. The system efficiencies of water electrolysis range from 56 to 73%, and an electrolyzer produces around 70.1-53.4 kWh/kg H_2 at a condition of 1 atm and 25°C (Turner et al., 2008). Water electrolysis can produce high-purity hydrogen (Holladay et al., 2009). There are different technologies in water electrolysis such as alkaline water electrolysis, solid oxide electrolysis, microbial electrolysis cells (MEC), and polymer electrolyte membrane (PEM). Among those technologies, alkaline electrolysis is considered the most mature and cheapest. However, this technology has the lowest efficiency so its electricity consumption is also highest. An alkaline electrolyzer (AEL) has a current density of 100-300 mA cm^{-2} and efficiencies from 50-60% based on the lower heating value of hydrogen. (Holladay et al., 2009)

The main components of an AEL usually consist of electrodes, a microporous separator, and an aqueous alkaline electrolyte such as 30 wt% KOH or NaOH. The liquid electrolyte needs to be refilled after a period of time due to system losses during hydrogen recovery, although the electrolyte is not consumed in the production process. In each cell, there are two electrodes which are cathode and anode. The cathode material is commonly made of nickel with a catalytic coating such as platinum. The anode materials are commonly made of nickel or copper metals coated with metal oxides such as manganese, tungsten, or ruthenium. Equations 3, 4, and 5 describe the reactions that happen in an electrolyzer. On the cathode side, water is split into hydrogen and hydroxide ions (OH^-) (Equation 3). The hydroxide ions produced on the cathode side pass through the electrolyte to the anode side and form oxygen (Equation 4). The hydrogen produced on the cathode side remains in the alkaline electrolyte. After that, the solution will be processed in a gas-liquid separation unit to separate hydrogen from the alkaline electrolyte. (Holladay et al., 2009)

At cathode: $$2H_2O + 2e^- \rightarrow H_2 + 2OH^- \tag{3}$$

At anode: $$4OH^- \rightarrow O_2 + 2H_2O \tag{4}$$

Overall: $$2H_2O \rightarrow 2H_2 + O_2 \qquad \Delta H = -288\ (kJ/mol) \tag{5}$$

One drawback of water electrolysis is that it requires large amounts of water. From the stoichiometric of the equation, it requires 9 kg of water to produce 1 kg of H_2. However, according to some electrolyzer manufacturers, the water consumption per kg of H_2 could be higher depending on electrolyzer types, technologies, and manufacturers varying from 10.01 to 22.4 per 1 kg of H_2 (Shiva Kumar & Himabindu, 2019; Simoes et al., 2021). Based on the information of 5 electrolyzer manufacturers, namely Kraftanlagen München GmbH, Thyssenkrupp Uhde Chlorine Engineers GmbH, Hydrogenics, GreenHydrogen.dk and H-Tec Systems GmbH, the water usage of electrolyzers from these companies ranges from 10.00 to 11.11 per 1 kg of H_2, (Simoes et al., 2021). The high demand of de-ionized water for NH_3 production is a challenge in many places in the world where water depletion is a growing concern due to climate change.

One approach to increase the resilience of the water supply for hydrogen production is diversifying the water intake sources. A study by (Simoes et al., 2021) suggested the use of different water sources such as seawater, estuaries, surface water, groundwater, rainwater, tap water, and recycled water. In places where freshwater is in short supply or might become limited in the future, finding alternative water sources is important to ensure the water supply in the long term. To evaluate the suitability of a water source, the authors suggested considering some factors, such as the availability of the water sources in the short-term and long-term under the impact of climate change, the continuity of the water supply, competition with other water uses, volume of the water input, distance from the water source to the production site, feasibility of the water collection, complexity of permitting process, and social acceptance. One important thing is that AEL is very sensitive to the purity level of water. Therefore, water treatment processes such as desalination and demineralization must be conducted before the electrolysis, which could be very energy-intensive and cause damage to ecosystems (Bobbi Peterson, 2018).

Many LCA studies have shown that hydrogen via water electrolysis powered by renewable energy reduces GHG emissions significantly compared to other production pathways (Ghavam et al., 2021). Ammonia production from fossil fuels releases very high emissions, for example, at 2.81 kg CO_2-eq/kg NH_3 for SMR using natural gas (Arora et al., 2018). Ammonia production powered by wind is estimated to produce 0.12-0.53 kg CO_2-eq/kg NH_3 (Smith et al., 2020). The emission results from LCA studies could vary depending on many factors, such as the scope of the study, details of the models, location, etc. However, ammonia production from renewable energy is commonly found to produce less emissions than fossil-based production.

2.2.2 Nitrogen production

There are three main technologies to produce nitrogen from air separation: cryogenic distillation, pressure swing adsorption (PSA), and membrane separation. However, only cryogenic distillation and PSA are used for ammonia production as the purity of hydrogen produced from membrane separation is not high enough to be used in ammonia synthesis. 90% of the global nitrogen production comes from cryogenic distillation. Compared to other technologies, cryogenic distillation produces the highest purity level of nitrogen, with impurity concentrations in the parts-per-billion range, and this technology also has the lowest energy consumption. The PSA technology is more commonly used in small-scale production. The purity level of nitrogen from this technology can reach up to 99.99%. In applications powered by renewable energy with intermittent and fluctuating supply, one advantage of PSA is that it can reach the full production capacity within a few minutes. Cryogenic distillation, on the other hand, needs 2 hours to start the production. (Liu et al., 2020)

The process of cryogenic distillation is illustrated in Figure 1 below. This technology separates components of a gas mixture based on the differences in boiling points of air components through two main stages, liquefaction and distillation. In this case, nitrogen will be separated from the atmosphere using this method. The air comprises 78.084% of nitrogen, 20.9476% of oxygen, 0.934% of argon, and 0.04% of carbon dioxide (Anne Marie Helmenstine, 2024). First, the feeding air is pretreated in the air compression and aftercooling section to remove dust, impurities, water, carbon dioxide, and hydrocarbons. Then, the air is cooled down until it is liquefied. The liquid air is sent to the distillation column, which contains a number of trays or packing materials for vapor-liquid contact. In this distillation reactor, the temperature starts to rise. At -196°C, nitrogen turns into gas, and nitrogen gas is collected. If the temperature continues to rise, argon and oxygen can be collected at -186°C and -183°C, respectively.

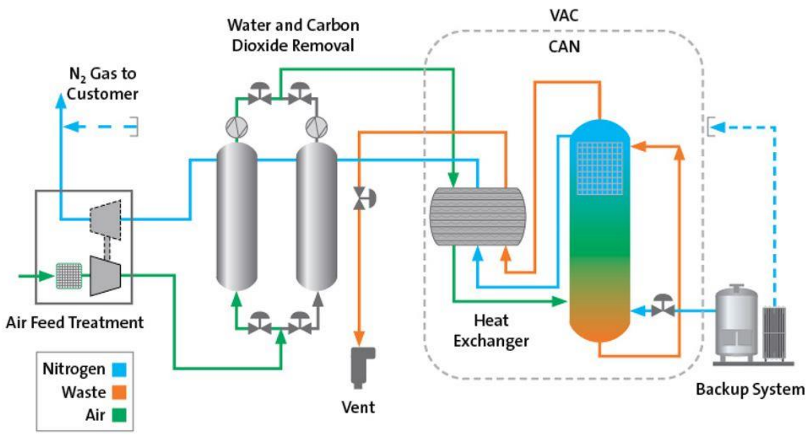

FIGURE 1. A diagram of the cryogenic distillation process (Murray, 2024)

The PSA process starts with feeding air passing through some filters to purify air from entrained oil and water as illustrated in Figure 2 below. Then, the air is sent to one of the two adsorption vessels, which are full of adsorbent materials such as carbon molecular sieves (CMS). The adsorption material is selected to capture the target gas on its solid surfaces at high pressure. In this case, the CMS will adsorb impurities such as carbon dioxide and moisture at the entrance of the adsorbent bed. When high pressure is applied in the vessel, the CMS will adsorb oxygen, and nitrogen at a high purity level can be collected. In the second vessel, the pressure will be reduced so that the CMS carrying the adsorbed oxygen can release the oxygen into the atmosphere. The utilization of both vessels helps the oxygen adsorption and desorption process of the adsorbent material happen continuously, enabling a more efficient nitrogen production process. (Ivanova & Lewis, 2012)

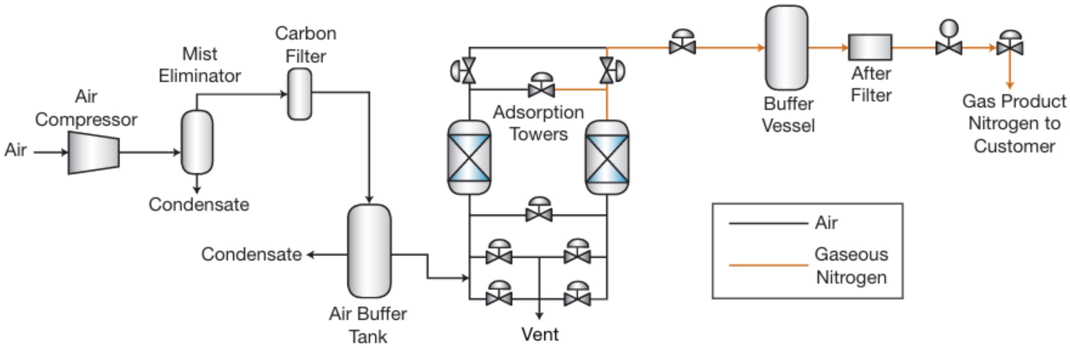

FIGURE 2. A diagram of a PSA system (Ivanova & Lewis, 2012)

The environmental impacts of cryogenic distillation and PSA technology mostly come from electricity usage. Other elements in the production phase, such as the construction of facilities and transportation, contribute very small proportions to the total impacts. It was suggested that the environmental performance of these processes could be improved by using renewable-based electricity and optimizing the unit structure and design. For the PSA process, the environmental burden could be significantly reduced by using activated carbon produced from renewable energy instead of fossil fuels. (Akbarian Shourkaei et al., 2018; Kohlheb et al., 2021)

2.2.3 Ammonia synthesis

In the 20th century, the discovery of the Haber- Bosch process has created a revolution in the global agricultural industry. In 1908, a German chemist Fitz Haber developed a method to synthesize ammonia from H_2 and N_2 under high pressure and temperature. This process was later applied to industrial production by Carl Bosch in 1911. This ammonia synthesis method was later named after them, known as the Haber-Bosch process. Fritz Haber and Carl Bosch were awarded Nobel Prize in Chemistry for their contributions in 1918 and 1931, respectively. Currently, this technology is the most popular method to produce ammonia.

Under the Haber-Bosch process, ammonia is produced through a reaction between hydrogen and nitrogen as shown in Equation 6 below:

$$\mathrm{N_2(g) + 3H_2 \leftrightarrow 2NH_3\ (g)} \qquad \Delta\mathrm{H} = 93\ (\mathrm{kJ/mol}) \tag{6}$$

This process operates at high pressure (10 MPa and 20 MPa) and high-temperature conditions (400-500°C), over an iron (Fe) based catalyst. Although the Haber-Bosch process is an exothermic process, the rate of reaction is very low at room temperature because the catalysts' activity is not high. Therefore, the Haber-Bosch process usually operates at high temperatures to increase the reaction rate and at high pressures to achieve a desired conversion rate.

Besides the dominance of the Haber-Bosch process in ammonia production, there are some other technologies that can produce ammonia in a sustainable way. One of the green ammonia production methods is electrochemical ammonia synthesis. This technology synthesizes ammonia from nitrogen and water at an ambient temperature and pressure. Therefore, it requires much less energy than the Haber-Bosch process and also reduces the need for hydrogen production through the direct use of water. Without the dependence on hydrogen production, this technology is expected to be highly flexible and scalable. However, electrochemical synthesis technology is still in the development phase. In order to achieve a higher synthesis rate and higher durability, better cathode and anode catalysts need to be developed. (Humphreys & Tao, 2024)

The electrochemical cell consists of 2 electrodes, a cathode and an anode, and a proton-conducting electrolyte. Nitrogen is fed to the cathode side, and the nitrogen reduction reaction happens (Equation 7). On the anode side, water is fed and oxidized with oxygen under an oxygen evolution reaction (Equation 8). Equation 9 shows the overall reaction of the electrochemical synthesis process. (Humphreys & Tao, 2024)

At cathode: $$\mathrm{N_2 + 6H^+ + 6e^- \rightarrow 2NH_3} \tag{7}$$

At anode: $$\mathrm{6H_2O \rightarrow 12H^+ + 3O_2 + 12e^-} \tag{8}$$

Overall: $$\mathrm{2N_2 + 6H_2O \rightarrow 4NH_3 + 3O_2} \tag{9}$$

Another sustainable ammonia production technology is photocatalytic ammonia synthesis. Similar to electrochemical technology, photocatalytic ammonia synthesis also uses nitrogen and water to produce ammonia at ambient temperature. The working principle of photocatalytic ammonia production is illustrated in Figure 3. When a semiconductor comes in touch with water in the presence of sunlight, the electrons in the semiconductor absorb photons and gain energy from the photons. If the energy in the photons is enough, which is usually over 1.137 eV, it will generate photoexcited electron-hole pairs. The process is called the oxygen evolution reaction (Equation 10). The generated electrons (e^-) can move freely from the valence band and react, while the holes stay in the valence band. The energy band gap is used to attract the moving electrons towards the conduction band. Therefore, this energy gap between the minimum energy of the conduction band and the maximum energy of the valence band has to be larger than 1.137 eV. On the conduction band, the nitrogen reduction reaction (Equation 11) occurs and ammonia is produced. (Joseph Sekhar et al., 2024)

The feasibility of applying this technology in large-scale industry is still a dispute among scholars due to its disadvantages such as low production rate, high production cost, and limited production of ammonia. (Joseph Sekhar et al., 2024)

$$2H_2O\ (l) \leftrightarrow O_2\ (g) + 4H^+ + 4e^- \qquad E^o = 1.229\ V \qquad (10)$$

$$N_2(g) + 6H^+ + 6e^- \leftrightarrow 2NH_3 \qquad E^o = 0.092\ V \qquad (11)$$

$$2N_2 + 6H_2O \rightarrow 4NH_3 + 3O_2 \qquad \text{Overall reaction} \qquad (12)$$

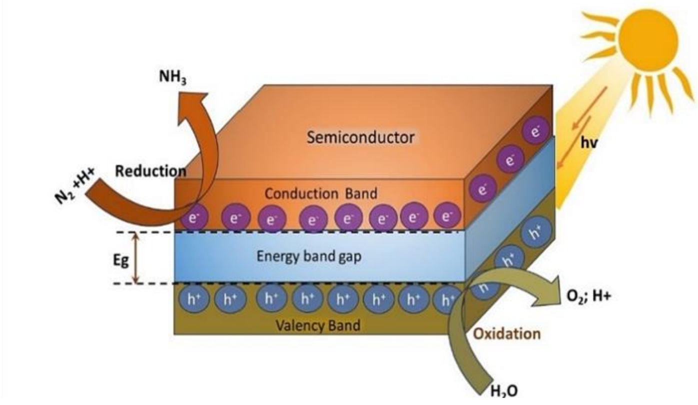

FIGURE 3. Ammonia production process through photocatalytic synthesis (Joseph Sekhar et al., 2024)

Besides the environmental impacts resulting from hydrogen and nitrogen inputs, the Haber-Bosch process also affects the environment through energy consumption due to the demanding operational conditions at high temperatures and pressures. If the process is powered by fossil fuel-based electricity, it will passively contribute to higher GHG emissions, compared to the process powered by renewable-based electricity.

Several efforts have been made to reduce the energy consumption of the ammonia synthesis process. One solution is to develop more effective catalysts for the process, which can help achieve good reaction rates at lower temperatures and pressures. Operating the production in less demanding conditions not only reduces energy consumption but also improves the conversion per pass of the process. Because the Haber-Bosch reaction is exothermic, the increase in operational temperature harnesses the overall conversion of the process. In the most current ammonia production plants via the Haber-

Bosch process, the conversion per pass is around 20%. In addition, when the operational condition is less extreme, the system designs for production could be less demanding. New catalysts are also expected to maintain their activities in the presence of higher oxygen and oxygenate impurities. In cases where hydrogen is produced from water, it carries some amount of oxygen and moisture. The improvement in the catalyst's tolerance to oxygen and oxygenate impurities will help reduce the need for energy-demanding purification processes. (Humphreys & Tao, 2024)

Fused-iron catalysts are the most developed catalysts for ammonia synthesis and they are popularly used in ammonia production plants around the world. Their designed characteristics such as stability, structural integrity, and activity are achieved using support from promotors. Some conventional promotors are alumina, potassium oxide, and silica, which can help to reach ammonia conversions of 15-20% per converter pass at a condition of 425°C and 15 MPa. In recent years, there have been some improvements in the promotor materials. Lithium hydride was discovered as an excellent promotor for iron catalysts at temperatures around 300°C and above (Wang et al., 2017). Barium hydride was found to not only perform well in normal ammonia synthesis production but also work excellently in a chemical looping synthesis system at lower temperatures and ambient pressure (Gao et al., 2018). Although newly developed catalysts can work more effectively than conventional ones, their applications in industrial plants are still challenging due to their complex synthesis method and lower tolerance to oxygen and moisture. (Humphreys & Tao, 2024)

Electrochemical ammonia production technology has some advantages over the Haber-Bosch process from technical and environmental perspectives. It has higher energy efficiency due to operating at lower temperatures and pressures. The technology also has higher selectivity which helps to reduce the requirements for the purification process. However, the downsides of this technology are that it has low production rates, which are around 10-13 to 10-18 mol s^{-1} cm^{-2}, and unstable operations of the acidic electrolyte membrane. (Ghavam et al., 2021)

The environmental impacts of the photocatalytic ammonia synthesis process have not been studied in depth. The technology is still in development phase and has not been applied in industrial production.

2.3. LCA on ammonia production

2.3.1 LCA methodology

LCA is defined as “the compilation and evaluation of the inputs, outputs, and the potential environmental impacts of a product system throughout its entire life cycle” (ISO, 2006a). The advantage of LCA is its life cycle aspect, which considers the environmental impacts of a product throughout different stages during its lifetime such as development, production, usage, disposal, and recycling applications. From an LCA study, decision-makers can have an overall understanding of the environmental burdens that are generated throughout the life span of a product or process, and search for solutions to improve the environmental performance. Besides, LCA can be applied to evaluate and compare the impacts between alternative options of a product or process, or between products within the same categories.

To reduce the subjectivity of LCA studies, a series of standardized methodologies for LCA has been established by the International Organization for Standardization (ISO) with the aim of increasing the credibility and usefulness of LCA results. These ISO standards are ISO-14040, Life Cycle Assessment Principles and Framework (ISO, 2006a), and ISO-14044, Life Cycle Assessment Requirements and Guidelines (ISO, 2006b).

The structure of an LCA study primarily comprises 5 phases that are (1) goal and scope definition, (2) LCI analysis, (3) life cycle impact assessment (LCIA), (4) Improvement analysis, and (5) Interpretation. Each phase is interconnected to the others. The relationship between the phases in an LCA study is illustrated in Figure 4 below:

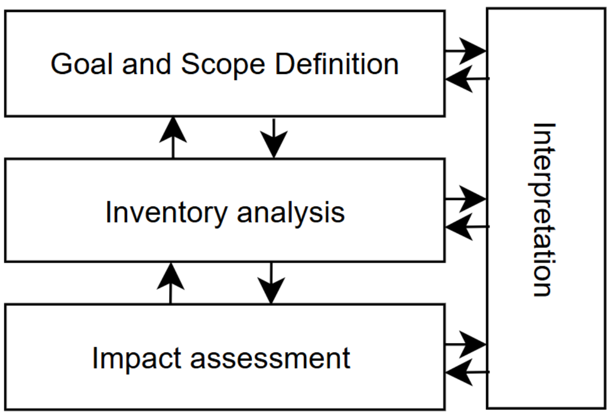

FIGURE 4. LCA framework according to ISO 14040

Goal and Scope Definition is the first phase in LCA studies. Goals is defined in terms of the intended applications of the study, the importance of the study, for whom the LCA is addressed, and the publication of the study. The scope of a study defines what is be included and what is excluded in the study. The first element of scope definition is system boundary, which determines the inclusion of materials and processes under the scope of the LCA study. Besides, a functional unit is also defined to quantify the emissions of materials and processes within the system boundary based on this reference unit. (Lozanovski A et al., 2011).

The second phase, inventory analysis, involves the collection of data regarding quantifiable inputs and outputs of a product or process under the system boundary defined in the previous phase. The data collected is often the quantity of mass and energy flows into a system, and some traced emissions. (Klöpffer & Grahl, 2014)

Impact assessment is the third phase of an LCA study. In this phase, the LCI collected data will be used to evaluate the magnitude and significance of the potential environmental impacts of the product or process under study. It is necessary to emphasize that the results of the impact assessment do not indicate the actual impacts that will occur in the environment, but only show the potential connections between the activities and environmental impacts. Hence, it is different from an environmental risk assessment, which concerns the concentration of compounds at the site of impact. According to ISO 14040 and 14044, the structure of impact assessment consists of mandatory and optional elements. Mandatory parts include the selection of impact categories, category indicators, and characterization models. It is followed by the assignment of LCI results (classification) and the calculation of category indicator results (characterization). Optional parts include the calculation of category indicator results against reference information (normalization), grouping, and weighting.

In the mandatory part, a few important terminologies are impact category and impact category indicator. The term impact category refers to environmental issues that the life cycle inventory analysis results will be assigned to. The impact category indicator refers to the quantifiable representation of an impact category. For example, climate change is an impact category and it is quantified by the amount of GHGs per functional unit. The selection of impact categories depends on the goal and scope of the study. (Klöpffer & Grahl, 2014)

The conversion of LCI results to the units of impact category indicators will be done based on some characterization models that are internationally accepted. This conversion involves 2 main processes: classification and characterization. Figure 5 below illustrates the processes of classification and characterization.

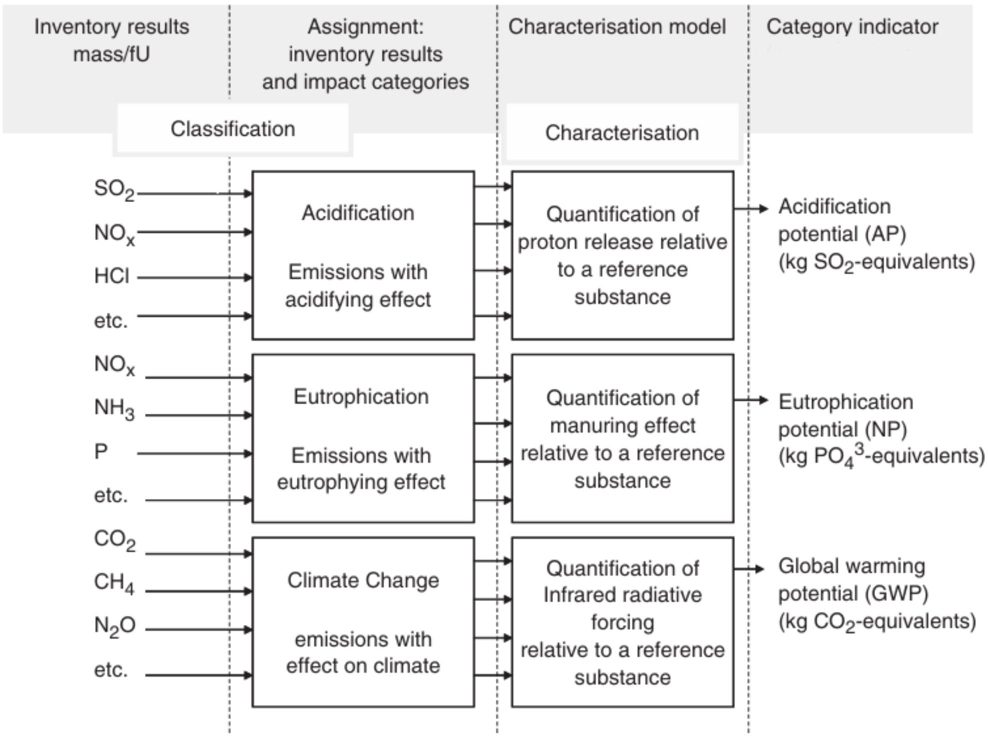

FIGURE 5. Principle of classification and characterization in LCIA (Klöpffer & Grahl, 2014)

Classification refers to the assignment of inventory results to impact categories. For example, as illustrated in Figure 5, acid-forming gases such as SO_2, NO_x, and HCl are assigned to the impact category of acidification, and GHGs such as CO_2, CH_4, and N_2O are assigned to the impact category of climate change. In the classification process, not only the emissions released from the technosphere into the environment are assigned to impact categories but inputs from the environment into the environment are also assigned to relevant impact categories. For example, fossil fuel consumption is assigned to the impact category of resource demand. According to ISO 14044, there should be a distinction between inventory results that can be assigned to only one impact category and those that can be assigned to more than one impact category. In the latter case, the relationship between different impact categories should be distinguished. For example, as can be seen in Figure 5, NO_x can be considered either an acid-forming gas or a gas with a eutrophication effect, which represents a parallel impact mechanism. On the other hand, NO_x can be considered an acid-forming gas after it forms photo oxidants in the summer smog, which indicates a serial impact mechanism. Characterization is a process that converts the LCI results to common units and aggregates the converted results into a numerical indicator called a category indicator by using the characterization factor. For example, the material inputs and outputs per functional unit of a product first are assigned to the impact category climate change through the classification process. These flows will be multiplied with a specific characterization factor. For example, under the climate change category, the global warming potential (GWP_{100}) for each GHG (kg CO_2-eq/kg gas) equals 1 for CO_2, 25 for CH_4, and so on. The characterization factor is obtained from characterization models developed based on scientific research. The results of the category indicator are calculated automatically using LCA software. However, these are the underlying methodologies used to conduct the impact assessment. (Klöpffer & Grahl, 2014)

Optional parts of the impact assessment include normalization, grouping, and weighting. Normalization is a process that divides the category indicator results by some reference values to understand the relative magnitude of the product system. A reference value could be the total category indicator result of a geographical system boundary such as the European Union, North America, and the Organization for Economic Co-operation and Development (OECD) as international reference values. For example, a product system produces 500 kg of CO_2-eq per functional unit (GWP_{100} = 500 kg), and its geographical system boundary is located in Germany. The normalization of this climate change indicator result is calculated relative to the annual release of CO_2-eq in Germany, which was 1 017 916 500 t in 2003. It is noted that the reference year should be similar to the year of conducting the study. The normalized value of 4.91E-10 is obtained by dividing the emissions caused by the product system per functional unit by the annual corresponding emission in Germany. Besides, a reference value could also be the category indicator result per capita population or a comparable measure, for example, the annual CO_2-eq emissions of 1 inhabitant in Germany. In the Environmental Footprint 3.1 method, the reference value is a global average of one person's emissions in a year (Malbar, 2023).

Grouping refers to the process of dividing the impact categories into one or more groups that are pre-determined in the goal and scope section, for example, based on characteristics of inputs and output flows, or regional and local spatial scales. Grouping might also include sorting and/or ranking of the impact categories based on some pre-defined criteria. Weighting is defined as a conversion of category indicator results using numerical factors based on value choices and may include the process of aggregation of the weighted indicator results, which is called a single-point method. The weighting factor is not decided based on scientific findings but rather on value-based decisions. Therefore, the use of weighting is not recommended by ISO standards. (Klöpffer & Grahl, 2014)

For example, Table 1 shows the weighted impacts of different impact categories in the Environmental Footprint 3.1 method.

Table 1. *Weighted impacts of 16 impact categories in the Environmental Footprint 3.1 method (Malbar, 2023)*

Impact category	**Weighted impact**
Acidification	6.20%
Climate change	21.06%
Ecotoxicity, freshwater	1.92%
Particulate matter formation	8.96%
Eutrophication, marine	2.96%
Eutrophication, freshwater	2.80%
Eutrophication, terrestrial	3.71%
Human toxicity, cancer	2.13%
Human toxicity, non-cancer	1.84%
Ionizing radiation	5.01%
Land use	7.94%
Ozone depletion	6.31%
Photochemical ozone formation	4.78%
Resource use, fossils	8.32%
Resource use, minerals and metals	7.55%
Water use	8.51%

The last phase, interpretation, ensures that the LCA model fulfills the goals and quality requirements of the study and produces robust conclusions and recommendations for future improvements. Three techniques that could be used to increase the reliability of LCA results are completeness check, sensitivity check, and consistency check. A completeness check ensures all the data needed to cover the goal and scope of the study is included. For example, it concerns the inclusion of all processes at each life-cycle stage and all the inflows and outflows of each process. A sensitivity check is used to estimate the result variations resulting from different methodology choices, such as the selections of data, cut-off criteria, and allocation rules. It involves the comparison between the main model and other scenarios modeled with altered parameters. Consistency check ensures that the predefined assumptions, methods, and data are applied consistently throughout the entire study and consistent with the study's goal and scope. (Klöpffer & Grahl, 2014)

2.3.2 LCA studies on ammonia production

This section reviews five LCA studies on ammonia production. The studies were selected based on the diversity in plant locations, the relatively recent published years, and the inclusions of both ammonia production systems via renewable energy and SMR. Table

2 below summarizes some information about the LCA studies regarding the objective of the studies, system boundaries, selection of methods and impact categories, and plant details. Table 3 describes the green ammonia systems with hydrogen production via electrolysis powered by renewable energy in the LCA studies. These are not all the green ammonia systems modeled by the studies. The selection limited the review to 8 green ammonia systems, prioritizing the systems powered by wind and solar electricity or fully renewable energy. In the study by Boero et al., 2021 where there were 8 wind-based ammonia production systems, the selected system 'Wind-GB' is the one that has a production capacity of approximately 20,000 tons of NH_3/ year and is located in the UK. Table 4 summarizes 6 ammonia production systems via SMR in the literature. In the study by Boero et al., 2021, there were 3 SMR systems. The selected system 'SMR-GB' has a capacity of 20,000 tons of NH_3 and is located in the UK. The environmental impacts of the green and SMR-based ammonia systems in the study by Singh et al., 2018 are shown in Table 5. The impacts of the other green ammonia systems are summarized in Table 6, and the impacts of the other ammonia systems via SMR are summarized in Table 7. The study of Singh et al., 2018 used the CML 2001 and Eco-indicator 99 method, and the other studies used the ReCIPe 2016 Midpoint Hierarchist method. The impact categories and impact categories indicators are different between these three methods, therefore, the results from the Singh et al., 2018 study are shown separately from other studies.

Table 2. *Overview of the LCA studies on ammonia production*

Reference	Objective	System boundary	Impact Categories	Plant details
Singh et al., 2018	Evaluate and compare the environmental impacts of various ammonia production routes	Cradle-to-grave	CML 2001 method: (1) abiotic depletion, (2) acidification, (3) eutrophication, (4) global warming, (5) human toxicity, and (6) freshwater aquatic eco-toxicity. Eco-indicator 99 method: (1) carcinogens, (2) climate change, (3) eco-toxicity, (4) acidification/eutrophication, (5) minerals, and (6) fossil fuels	NA
Vinardell et al., 2023	Evaluates the potential environmental and economic impacts of green ammonia production in Spain	Cradle-to-gate	ReCIPe 2016 Midpoint Hierarchist: (1) global warming, (2) fossil resource scarcity, (3) freshwater eutrophication, (4) mineral resource scarcity, (5) stratospheric ozone depletion, (6) terrestrial acidifica-tion, and (7) land use	The ammonia plant under the study was designed to produce 430 kt of ammonia per year. It operated 8000 h/ year with a utilization factor of 0.92. Located in Spain.
Chisalita et al., 2020	Evaluate and compare the environmental impacts of various ammonia production routes	Cradle-to-gate	ReCIPe 2016 Midpoint Hierarchist: (1) global warming, (2) freshwater eutrophication, (3) ozone depletion, (4) fossil fuel depletion, (5) freshwater ecotoxicity, (6) Human toxicity, (7) mineral depletion, (8) photochemical oxidant formation, and (9) terrestrial ecotoxicity	Life time of the plant is 25 years. Located in Germany
Ochoa, 2023	Evaluate and compare the environmental impacts of various ammonia production routes	Cradle-to-gate	ReCIPe 2016 Midpoint Hierarchist: (1) global warming, (2) water use, (3) freshwater ecotoxicity, (4) ionizing radiation. Cumulative energy demand	NA
Boero et al., 2021	Evaluate and compare the environmental impacts of various ammonia production routes, especially on the environmental performance of ammonia-based electricity generated in a combined heat and power cycle	Cradle-to-gate	ReCIPe 2016 Midpoint Hierarchist: (1) global warming, (2) freshwater eutrophication, (3) ozone depletion, (4) fossil fuel depletion, (5) photochemical oxidant formation, (6) terrestrial ecotoxicity, and (7) ionizing radiation	Small-scale production: 20,000 t of NH_3 per annum. Medium-scale production: 100,000 t of NH_3 per annum. Located in UK, Morocco, Australia, Chile, Brazil, Iceland, and the United Arab Emirates

Table 3. *Green ammonia production systems in the literature*

Case code	Case description	System boundary	Reference
Wind-NA	Electricity from wind. The plant's location is not specified.	Cradle-to-grave: H_2 via electrolysis, N_2 via cryogenic distillation, ammonia synthesis, plant construction, electrical energy, ammonia storage, facility decommissioning, recycling facility, and waste management	Singh et al., 2018
Solar-NA	Electricity from solar PV. The plant's location is not specified.		Singh et al., 2019
Wind-ES	Electricity from wind. The plant is located in Spain. Capacity of 430 kt of NH_3 per year.	Cradle-to-gate: H_2 via PEM electrolyzer, N_2 production via cryogenic distillation, ammonia synthesis, lithium-ion battery for storing renewable electricity, and hydrogen storage system	Vinardell et al., 2021
Solar-ES	Electricity from solar PV. The plant is located in Spain. Capacity of 430 kt of NH_3 per year.		Vinardell et al., 2022
Mix-ES	Electricity from solar PV (50%) and wind (50%). The plant is located in Spain. Capacity of 430 kt of NH_3 per year.		Vinardell et al., 2023
Mix-DE	Electricity from Germany's grid mix of renewable energy sources. The plant is located in Germany.	Cradle-to-gate: H_2 via electrolysis, N_2 via cryogenic distillation, ammonia synthesis	Chisalita et al., 2020
Wind-FI	Electricity from wind. The plant is located in Finland.	Cradle-to-gate: H_2 via electrolysis, N_2 via cryogenic distillation, ammonia synthesis	Ochoa, 2023
Wind-GB	Electricity from wind. The plant is located in the UK. Capacity of 20 kt of NH_3 per year.	Cradle-to-gate: facility construction, H_2 via electrolysis, N_2 via air separation, ammonia synthesis	Boero et al., 2021

Table 4. *Ammonia production systems via SMR in the literature*

Case code	Case description	System boundary	Reference
SMR - NA	The plant's location is not specified. The source of the electricity input is not mentioned.	Cradle-to-grave: H_2 via SMR, N_2 via cryogenic distillation, ammonia synthesis, plant construction, electrical energy, ammonia storage, facility decommissioning, recycling facility, and waste management	Singh et al., 2018
SMR - ES	The plant is located in Spain. Capacity of 430 kt of NH_3 per year.	Cradle-to-gate: H_2 via SMR, N_2 production via cryogenic distillation, ammonia synthesis	Vinardell et al., 2023
SMR - DE1	The plant is located in Germany. Acid gas (CO_2) removal method is chemical absorption by MDEA. No external electricity.	Cradle-to-gate: H_2 via SMR, N_2 production via cryogenic distillation, ammonia synthesis, CO_2 capture, CO_2 compression, transportation and storage, solvent and oxygen carrier degradation and disposal	Chisalita et al., 2020
SMR - DE2	The plant is located in Germany. Acid gas (CO_2) removal method is chemical absorption by chilled ammonia. No external electricity. No external electricity.		Chisalita et al., 2021
SMR - FI	The plant is located in Finland. Electricity used in the plant is from wind power.	Cradle-to-gate: H_2 via SMR, N_2 production via cryogenic distillation, ammonia synthesis	Ochoa, 2023
SMR - GB	The plant has small capacity of 20 ktpa. It is located in the UK. Electricity used in the plant is electricity generation mix in the UK	Cradle-to-gate: facility construction, H_2 via SMR, N_2 production via air separation, ammonia synthesis, wastewater treatment	Boero et al., 2021

Table 5. *Environmental impacts of the ammonia systems in the study by Singh et al., 2018*

Calculation method	Impact category	SMR - NA	Solar - NA	Wind - NA
CML 2001	Abiotic depletion (kg Sb-eq/ tNH_3)	26.49	8.54	3.4
	Acidification (kg SO_2-eq/ tNH_3)	3.62	5.81	2.2
	Eutrophication (kg PO_4-eq/ tNH_3)	1.33	3.76	1.44
	Global warming (kg CO_2-eq/ tNH_3)	3032.26	1277.45	495.66
	Human toxicity (kg1,4-DB-eq/ tNH_3)	138.93	1366.73	598.22
	Freshwater aquatic eco-toxicity (kg1,4-DB-eq/ tNH_3)	192.29	753.65	314.04
Eco-indicator 99	Climate change (DALY/ tNH_3)	4.6E-04	2.5E-04	9.7E-05
	Carcinogens (DALY/ tNH_3)	1.4E-04	1.3E-03	2.2E-04
	Fossil fuels (MJ surplus/ tNH_3)	4263.3555	1102.3114	400.18669

Table 6. *Environmental impacts of green ammonia production systems in the literature*

Impact category	**Vinardell et al., 2023**			**Chisalita et al., 2020**	**Ochoa, 2023**	**Boero et al., 2021**
	Wind-ES	**Solar-ES**	**Mix-ES**	**Mix-DE**	**Wind-FI**	**Wind-GB**
Global warming (kg CO_2-eq/ tNH_3)	300	800	600	149.14	177	280
Fossil resource scarcity (kg oil eq/ tNH_3)	80	220	160	36.06	-	68
Land use (m^2*a crop eq/ tNH_3)	20	320	170	-	-	-
Mineral resource scarcity (kg Cu-eq/ tNH_3)	0.26	0.15	0.2	-	-	-
Ozone depletion (kg CFC11-eq/ tNH_3)	1.5E-04	3.8E-04	2.6E-04	2.6E-09	-	1.7E-05
Terrestrial acidification (kg SO_2-eq/ tNH_3)	1.4	3.4	2.4	-	-	1.51
Freshwater eutrophication (kg P-eq/ tNH_3)	0.32	0.46	0.39	4.1E-03	-	0.25
Photochemical ozone formation (kg NMVOC/ tNH_3)	-	-	-	0.48	-	1.2
Terrestrial ecotoxicity (kg 1,4-DB-eq/ tNH_3)	-	-	-	0.07	-	-
Mineral depletion (kg Fe-eq/ tNH_3)	-	-	-	36.75	-	-
Ionizing radiation (kBq Co-60-eq/ tNH_3)	-	-	-	-	22	-
Ionizing radiation (kg U235-eq/ tNH_3)	-	-	-	-	-	7.93
Freshwater ecotoxicity (kg 1,4-DB-eq/ tNH_3)	-	-	-	0.19	34	-
Human Toxicity (kg 1,4-DB-eq/ tNH_3)	-	-	-	31.61	-	-
Water consumption (m^3/ tNH_3)	-	-	-	-	1060	-

Table 7. *Environmental impacts of ammonia production systems via SMR in the literature*

Impact category	**Vinardell et al., 2023**	**Chisalita et al., 2020**		**Ochoa, 2022**	**Boero et al., 2021**
	SMR - ES	**SMR - DE1**	**SMR - DE2**	**SMR - FI**	**SMR - GB**
Global warming (kg CO_2-eq/ tNH_3)	2000	2794.82	2804.69	1883	2600
Fossil resource scarcity (kg oil eq/ tNH_3)	880	913.9	915.04	-	1220
Land use (m^2*a crop eq/ tNH_3)	0	-	-	-	-
Mineral resource scarcity (kg Cu-eq/ tNH_3)	0.04	-	-	-	-
Ozone depletion (kg CFC11-eq/ tNH_3)	4.80E-04	3.47E-09	3.48E-09	-	1.67E-04
Terrestrial acidification (kg SO_2-eq/ tNH_3)	0.7	-	-	-	1.86
Freshwater eutrophication (kg P-eq/ tNH_3)	0.02	0.003	0.003	-	0.068
Photochemical ozone formation (kg NMVOC/ tNH_3)	-	1.55	1.56	-	2.31
Terrestrial ecotoxicity (kg 1,4-DB-eq/ tNH_3)	-	7.9E-03	8.1E-03	-	-
Mineral depletion (kg Fe-eq/ tNH_3)	-	3.29	3.18	-	-
Ionizing radiation (kBq Co-60-eq/ tNH_3)	-	-	-	18	-
Ionizing radiation (kg U235-eq/ tNH_3)	-	-	-	-	286.42
Freshwater ecotoxicity (kg 1,4-DB-eq/ tNH_3)	-	0.35	0.35	22	-
Human Toxicity (kg 1,4-DB-eq/ tNH_3)	-	29.77	29.86	-	-
Global warming (kg CO_2-eq/ tNH_3)	-	-	-	1090	-

The studies in the literature found that ammonia production from renewable energy significantly reduces the environmental impacts of climate change, resource use of fossil fuels, and water use compared to the traditional SMR method. However, green ammonia production increases the environmental burdens on some other environmental impact categories such as ozone depletion, resource use of minerals and metals, and land use. The environmental impacts of green ammonia production on acidification, freshwater eutrophication, freshwater ecotoxicity, and photochemical ozone formation could be higher or lower than the impacts of ammonia production via SMR, depending on the sources of electricity. There were some differences in the findings of the impacts of green ammonia and SMR-based ammonia on human toxicity. The ionizing radiation category is most important for nuclear-based ammonia, whereas green ammonia production contributes little to this category. A more detailed description of the environmental impacts of green ammonia production is summarized below.

The results of all the studies in the literature showed that ammonia production via renewable energy had much less impact on global warming compared to ammonia production via SMR. Ammonia produced from renewable energy was shown to achieve a reduction from 40% to 95% in GWP (Boero et al., 2021; Chisalita et al., 2020; Ochoa, 2023; Singh et al., 2018; Vinardell et al., 2023). Specifically, green ammonia helps avoid direct GHG emissions by using renewable electricity in the production system, therefore, it is expected to have positive improvements in climate change and air quality. However, if hydrogen production via water electrolysis is powered by fossil-based sources, this ammonia production system will result in the highest air, water, and soil emissions (Chisalita et al., 2020).

Acidification is the reduction in pH in soil and water bodies due to the emissions of acidic gases such as nitrogen oxides and sulfur oxides. Vinardell et al., 2023 found that the production of ammonia using renewable energy increases the environmental impacts on terrestrial acidification compared to the traditional SMR method (Vinardell et al., 2023). On the other hand, the study of Singh et al., 2018 found that ammonia produced from wind has a lower acidification impact than ammonia via SMR whereas solar-based ammonia has more impact on this category than ammonia via SMR.

Freshwater eutrophication is related to the emissions of nutrients such as nitrogen (N) and phosphorus (P) into freshwater environments such as ponds, lakes, rivers, swamps, or reservoirs. The emissions of phosphates come from the waste treatment processes of copper, hard coal, and lignite mining (Boero et al., 2021). The comparison results of the environmental impacts between green ammonia and traditional SMR production varied between the studies. The studies of Chisalita et al., 2020 and Vinardell et al., 2023 found that the freshwater eutrophication impact of green ammonia production is higher than the impact of ammonia via

SMR. In ammonia systems powered by renewable energy, the contribution to freshwater eutrophication is from electricity production whereas in the SMR-based system, the impacts on freshwater eutrophication come from wastewater treatment (Chisalita et al., 2020). On the other hand, Singh et al., 2018 found that solar-based ammonia has a higher impact on freshwater eutrophication while wind-based ammonia systems had slightly less impact than SMR-based systems. Boero et al., 2021's result showed that the impacts of wind-based systems in freshwater could be higher or lower than the SMR systems, depending on the size and location of the plants. The only solar PV-based system in the Boero et al., 2021 study was found to have a higher impact than the SMR systems.

Freshwater ecotoxicity potential concerns the adverse effects of hazardous substances on aquatic ecosystems. The study by Chisalita et al., 2020 showed that the impact of green ammonia powered by renewable mix electricity on freshwater ecotoxicity is lower than the impact of ammonia production via SMR. The sources of emissions in this category are similar to the freshwater eutrophication category, which are wastewater treatment for SMR and electricity generation for green ammonia production. In the study of Ochoa, 2023 where green ammonia is powered by wind electricity, the impact on freshwater ecotoxicity is lower than SMR-based ammonia. The source of impact from wind electricity is from the processing of scrap copper, which is waste from the production of large wind turbines. This process releases incompletely combusted metals and chemical substances that may cause negative impacts on the ecosystems, as well as on human health (Ochoa, 2023).

Human ecotoxicity potential concerns the impacts of hazardous substances on human health. The study by Chisalita et al., 2020 found that green ammonia had similar impacts as ammonia production via SMR in this category. However, the study by Singh et al., 2018 showed that the impact on human toxicity of the wind-based system is 3 times higher than the SMR system and the impact of the solar PV-based system is 7 times higher than the SMR system. The ammonia system powered by solar PV in the study was found to also have significantly higher impacts in acidification and eco-toxicity categories compared to other ammonia production methods. These high impacts were due to the material components used to manufacture a PV cell and for cleaning, such as hydrochloric acid, sulfuric acid, nitric acid, hydrogen fluoride, 1,1,1-trichloroethane, and acetone. The amount of these chemicals used depends on the type of cell used. For example, thin film PV cells have more toxic materials than traditional cells. Besides, many hazardous compounds are used to manufacture batteries for energy storage.

Ozone depletion potential is associated with the emissions of chlorodifluoromethane (HCFC-22) and bromochlorodifluoromethane (Halon 1211), which are released during the natural gas extraction and transport processes, and from the manufacturing process of PV cells (Boero et al., 2021). It can also come from wastewater treatment, which treats all the water used for the ammonia production phase (Chisalita et al., 2020). It was found that green ammonia production contributes less impact to ozone depletion compared to the SMR method (Boero et al., 2021; Chisalita et al., 2020; Vinardell et al., 2023). However, if the electricity for water electrolysis is produced from fossil fuel sources, the impact on ozone depletion is 3 times higher than production via SMR (Chisalita et al., 2020).

Photochemical ozone formation potential is related to the formation of tropospheric ozone under the effect of sunlight on nitrogen oxides (NO_x, NO) and reactive hydrocarbons, commonly referred to as 'smog' (Boero et al., 2021). The impact of ammonia produced from renewable energy on photochemical ozone formation is 30.82% higher than ammonia produced by SMR (Chisalita et al., 2020). The main contributor to this impact category mostly comes from the electricity supply for electricity-based ammonia, and natural gas supply for ammonia produced from SMR. The study by Boero et al., 2021 found that the implementation of wind-based systems could increase or decrease the impact on photochemical ozone formation compared to SMR systems based on the sizes and the locations of the wind-based plants. The only solar-based system in this study was shown to have a higher impact than the SMR systems in this category. In addition, the study by Chisalita et al., 2020 found that when electricity is produced from biomass, the impact on photochemical ozone formation is higher than the original system using the German electricity grid mix which consists of wind (23.59%), lignite (20.05%), nuclear (13.7%), natural gas (10.53%), solar PV (9.8%), hard coal (9.47%), biomass (8.62%), hydropower (3.82%), oil (0.29%), and waste (under 1%). It is due to high NO_x and NMVOC emissions from biomass-fired power plants.

The resource use of fossil fuels is related to the use of natural gas, coal, or coal. Ammonia production via SMR has higher impacts than green ammonia in this category due to the consumption of natural gas. Regarding green ammonia production, the environmental impacts on resource use of fossils were shown to reduce significantly when green ammonia was powered by renewable energy (Boero et al., 2021; Chisalita et al., 2020; Vinardell et al., 2023). In the study by Chisalita et al., 2020, the reduction was 97.7% when changing the electricity grid mix to fully renewable electricity.

The impact of ammonia production via renewable energy on the resource use of minerals and metals was found to be 10-11 times higher than the impacts of the ammonia produced by SMR (Chisalita et al., 2020; Vinardell et al., 2023). The scarcity of mineral resources and metals due to green ammonia production is from the manufacture of PV panels, wind turbines, and Li-ion batteries (Vinardell et al., 2023). Wind power had the highest impact on the mineral resource scarcity category due to the high usage of common metals such as iron, aluminum, copper, and rare earth elements in constructing wind energy systems (Vinardell et al., 2023).

Ochoa, 2023 found that 1 kg of ammonia produced through SMR consumes 1.09 m^3 of water, slightly higher than the water consumption for ammonia production through water electrolysis at 1.06 m^3. In the SMR pathway, water is utilized in fossil fuel extraction, transportation, and refining processes. Some more studies are reviewed to understand the water consumption of the SMR method. An LCA study on hydrogen production via SMR mentioned that the water consumption of an H_2 production plant is around 19.8 liters/ kg H_2, equivalent to 0.0198 m^3/ kg H_2, in which 95.2% is used for the plant operation, 3.6% is used for the construction and decommissioning of the site, and 1.3% is used for natural gas production and transport (Spath & Mann, 2000). Another LCA study on hydrogen production showed that the hydrogen production pathway via SMR consumes 5.77 m^3 of water/ kg H_2 in its life span, in which water consumption during the operational phase is 21.869 kg/ kg H_2, equivalent to 0.021869 m^3/ kg H_2 (Mehmeti et al., 2018). In this study, the water use as an operational resource for SMR is even higher than for water electrolysis (PEM technology), which is around 18.04 kg/ kg H_2.

Green ammonia production was shown to have higher environmental impacts on land use due to huge land requirements for building renewable energy production plants (Vinardell et al., 2023). In addition, land conversion for energy plant construction can contribute to higher CO_2 emissions if vegetation on the land is cleared. It was suggested that the environmental impacts on land use can be reduced by improving the efficiency of the renewable energy systems. For example, solar PV panels with higher efficiency will require fewer cells and a smaller area of land to produce the same amount of electricity (Singh et al., 2018).

Ionizing radiation is associated with the emissions of radioactive materials that cause adverse effects on human health, depending on the level of exposure. This impact category is most relevant for ammonia production powered by nuclear electricity. In ammonia production via SMR or electrolysis, small amounts of ionizing radiation could be released during the oil refining process, for example for electricity production or transportation (Ochoa, 2023).

Besides, wind-powered ammonia production was found to have less environmental impact than solar PV-powered ammonia systems in general (Singh et al., 2018; Vinardell et al., 2023). Vinardell et al., 2023 found that solar-based systems had higher impacts than wind-based systems on global warming, fossil resource scarcity, land use, stratospheric ozone depletion, terrestrial acidification, and freshwater eutrophication. In the Singh et al., 2018 study, the Eco-indicator 99 method is used to combine all the emissions into a single score. The result showed that ammonia from SMR has the highest single score of 0.19 millipoints (mPT) for 1 kg of ammonia. The single score for ammonia from PV is 0.135 mPT, and for ammonia from wind is around 0.05 mPT.

3. MATERIALS AND METHODS

3.1 Description of a case study

The planned ammonia production site is located in a coastal area in the North-East of Estonia. It is designed to produce 100,000 tons per annum (100 ktpa) of ammonia from 20,000 tons of hydrogen (20 ktpa) and nitrogen from air separation. Electricity sources for the site are from the 250 MW solar farm distributed through private connections and supported by a 330 kV grid connection with a 260 MW onshore wind farm through a PPA. With the hydrogen production capacity of 20 kt per year, the plant requires around 493 m^3 of water per day. It is planned to collect surface water from a nearby river, approximately 500 meters from the area, to meet the water demand for the production. The water abstraction from this source requires applying for a permit as the surface water extraction is limited to 30 m^3 per day.

3.2 LCA model development

The LCA methodology used in the thesis is based on the ISO 14040 and ISO 14044 standards. In this section, the details of the LCA study on the case study are described regarding the study's goal and scope, LCI, and the selection of a calculation method and impact categories.

3.2.1 Goal and scope

The main objective of the thesis is to understand the environmental impacts of the ammonia production system from renewable energy in Estonia. The thesis will identify the most relevant impact categories related to the case study, as well as the most environmentally impactful elements among life cycle stages and single processes in the system. The target groups of the thesis are the company that carries out the project, and general readers who are interested in this topic.

In this thesis, the functional unit of this ammonia production system is chosen to be "1 kg of ammonia produced at the site". The scope is cradle-to-gate, which includes the environmental impacts of material flows from the phase of raw material extraction to the completion of ammonia products at the factory gate. Phases after the production of ammonia such as transportation, usage, and end-of-life are not included in the system boundary because the project is in the development phase at the time of writing. The ammonia production system is divided into 4 main life cycle stages: the manufacture of the AEL, operational resources for hydrogen production, nitrogen production through cryogenic distillation, and other inputs for ammonia synthesis through the Haber-Bosch process. The system boundary of the ammonia production in the case study is illustrated in Figure 6 below.

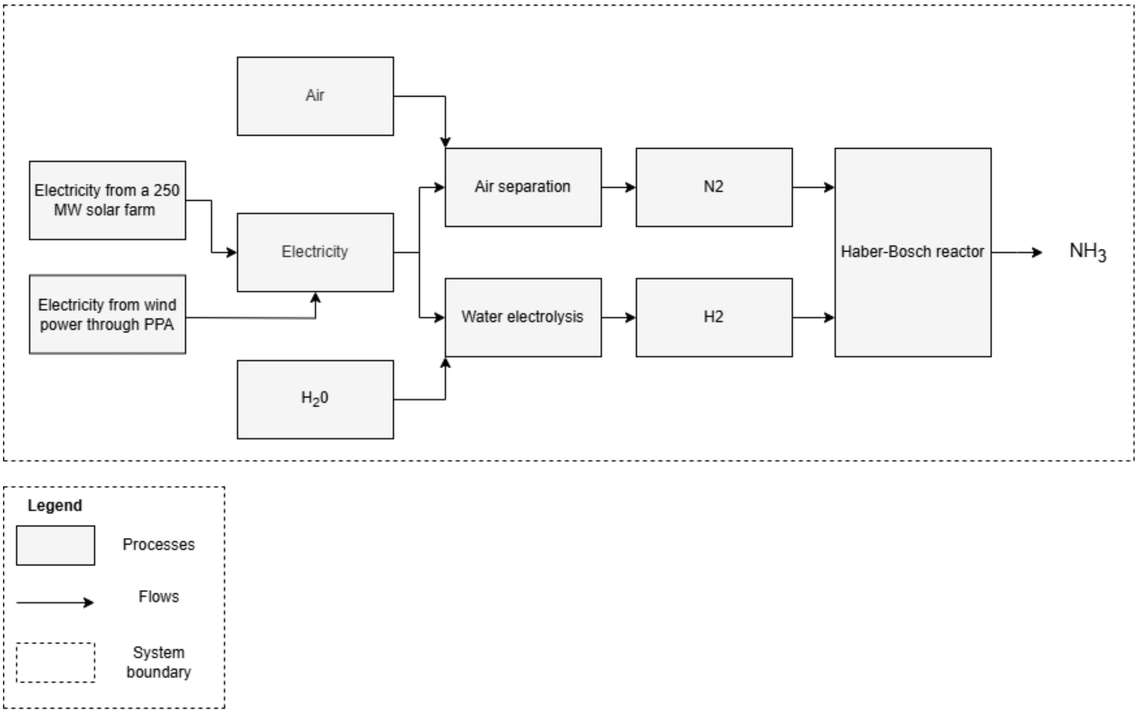

FIGURE 6. The system boundary of the ammonia production system

3.2.2 Life cycle inventory

The data collected for the life cycle inventory (LCI) mostly came from a literature review, and some information about the plant capacity and electricity sources was provided by DGE Group, an environmental consultancy working with the site selection of potential hydrogen facilities in Estonia. The LCA model was calculated using the LCA software SimaPro 9.6.0.1. Background processes were selected from the ecoinvent v3.10 database, which is a commonly used database for scientific-based LCA. Because the project is located in Estonia, the locations of background processes for operational resources for ammonia production, such as electricity and water consumption, were selected based on this priority order: data from Estonia (EE), the average data for European countries (RER), and average global data (GLO). On the other hand, the manufacture of other electrical components, such as electrolyzers or solar panels, was assumed to happen in China. Therefore, the locations of the background processes for these components were selected based on this order: data from China (CN), average global data (GLO), or the rest of the world (RoW). The section below describes the inventory used in the thesis in more detail.

Hydrogen production process

At the time of writing, the AEL model for the case study has not been decided. Therefore, the AEL used in the LCA model is modeled based on the study by Koj et al., 2017. The AEL in this paper is a pressurized 6 MW, which has the same production capacity with the AEL needed for the case study's plant. The total hydrogen production of this AEL is nearly 98,000 tons of ammonia per year, which is relatively close to the expected production capacity of the case study's plant at 100,000 tons of ammonia per year. The AEL in the study by Koj et al., 2017 was projected based on commercially available 3.5 MW AELs and scientific research. Some technical characteristics of this electrolyzer are shown in Table 8 below.

Table 8. *Characteristics of the AEL (Koj et al., 2017)*

Parameter	Unit	Value
Capacity	6	MW
System lifetime	20	years
Stack lifetime	10	years
Stacks per AEL system	4	pieces
Annual operation	8300	hours
Hydrogen production rate	118	kg H_2/h
Life-time hydrogen production	$1.95*10^7$	kg H_2 / 20 years

The electrolyzer contains four cell stacks. Each cell stack has 139 cells. The structure of a cell consists of electrodes, a membrane, a cell frame, and a gasket. The diameter of each cell is 1.6 meters. An illustration of a cell in the AEL is shown in Figure 7. (Koj et al., 2017)

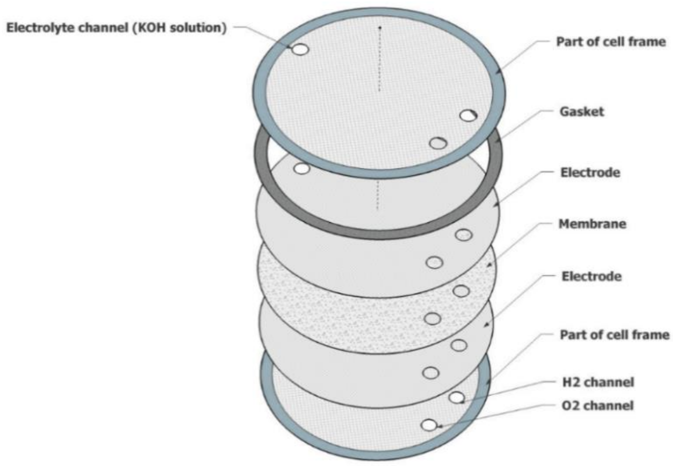

FIGURE 7. The structure of a cell in the AEL (Koj et al., 2017)

The inventory for hydrogen production includes the manufacture of the AEL and operational resources to produce H_2 at the site. Table 9 lists the materials and energy inputs for the manufacture of the original 6 MW AEL, and the operational resources to produce 1 kg of H_2 provided by the reference study Koj et al., 2017.

Table 9. *The inventory of hydrogen production using a 6 MW AEL (Koj et al., 2017)*

Process	Input	Value	Unit
Cell stack framework	Copper	2000	kg
	Unalloyed steel	200000	kg
Cells	Nickel	19000	kg
	Aluminum	450	kg
	Calendered rigid plastic	780	kg
	Polytetrafluoroethylene	78	kg
	Acrylonitrile butadiene styrene	160	kg
	Polyphenylene sulfide	340	kg
	Polysulfones	260	kg
	N-Methyl-2-pyrrolidone	1300	kg
	Aniline	49	kg
	Acetic anhydride	54	kg
	Terephthalic acid	88	kg
	Nitric acid	33	kg
	Hydrochloric acid	130	kg
	Graphite	430	kg
	Lubricating oil	0.48	kg
	Zirconium oxide	1100	kg
	Carbon monoxide	150	kg
	Decarbonized water	11000	kg
	Deionized water	86000	kg
	Industrial machine production	0.16	kg
	Plaster mixing	780	kg
	Electricity	36	GJ
	Heat	88	GJ
	Steam	700	MJ
Operational resources for 1 kg H2	Electricity	180	MJ
	Deionized water	10	kg
	Nitrogen	0.29	g
	Potassium hydroxide	1.9	g
	Steam	0.11	kg

Table 10 below shows the inventory for hydrogen production used in the case study's LCA model.

Table 10. *LCI for 1 kg of H_2*

Process	Inputs	Value/ kg H_2	Unit
Cell stack framework	Copper	1.03E-04	kg
	Unalloyed steel	1.03E-02	kg
Cells	Nickel	9.74E-04	kg
	Aluminum	2.31E-05	kg
	Calendered rigid plastic	4.00E-05	kg
	Polytetrafluoroethylene	4.00E-06	kg
	Acrylonitrile butadiene styrene	8.21E-06	kg
	Polyphenylene sulfide	1.74E-05	kg
	Polysulfones	1.33E-05	kg
	N-Methyl-2-pyrrolidone	6.67E-05	kg
	Aniline	2.51E-06	kg
	Acetic anhydride	2.77E-06	kg
	Terephthalic acid	4.51E-06	kg
	Nitric acid	1.69E-06	kg
	Hydrochloric acid	6.67E-06	kg
	Graphite	2.21E-05	kg
	Lubricating oil	2.46E-08	kg
	Zirconium oxide	5.64E-05	kg
	Carbon monoxide	7.69E-06	kg
	Decarbonized water	5.64E-04	kg
	Deionized water	4.41E-03	kg
	Plaster mixing	4.00E-05	kg
	Electricity	1846.15	J
	Heat	4512.82	J
	Steam	35.90	J
Operational resources for 1 kg H_2	Electricity	180	MJ
	Deionized water	10	kg
	Nitrogen	0.29	g
	Potassium hydroxide	1.9	g
	Steam	0.11	kg

The purposes of each material input in the hydrogen production inventory are explained in Table 16 in the Appendix. In the operation of the AEL, a potassium hydroxide solution (KOH) of 25% w/w is utilized. It is assumed that the KOH solution will have a life span of 10 years, and during this period, the solution is used in the AEL without being changed. Besides hydrogen products, AEL also generates oxygen as a by-product. In this LCA model, the oxygen product is assumed to be released into the air, which is a common practice in industrial applications. In addition, it is assumed that the AEL operates 95% of the total hours in a year, which equals 8300 hours per year. The electrolyzer also has

5 run-ups per year. This AEL used Zirfon-based membranes, considering that recent AELs are using polymer-based membranes due to the former asbestos membranes have been prohibited by the regulation (EC) No 1907/2006 (REACH, 2006).

In the case study, the total H_2 production is expected to be 20 ktpa (kilotons per annum), which equals 20,000 tonnes of hydrogen per year. To acquire the inventory for 1 kg of H_2 in the case study as shown in Table 10, the material and energy consumption to produce stacks and cells of the 6 MW electrolyzer (Koj et al., 2017) was divided by the total hydrogen produced by the electrolyzer during the system life span of 20 years, which is $1.95*10^7$ kg of H_2. The information needed for the calculation of total hydrogen production can be seen in Table 8. The selection of background processes from the ecoinvent database for the material and energy inputs is listed in Table 17 in the Appendix. Compared to the original model in the Koj et al., 2017 study, there are a few differences in the inventory of the thesis's model. The polytetrafluoroethylene input is replaced by tetrafluoroethylene, and the material input for industrial machine production is omitted because the background processes for these inputs can't be found in ecoinvent.

Ammonia production process

The inventory for ammonia production is referenced from the study by Chisalita et al., 2020. The inventory for the Haber-Bosch process is relatively similar between studies in the literature but the model from Chisalita et al., 2020 also includes the water consumption for reactor cooling and specifies the composition of the iron-based catalyst.

In this model, ammonia is produced through the Haber-Bosch process using nitrogen obtained from a cryogenic distillation in an air separation unit and hydrogen produced from water electrolysis in the previous stage. The catalyst used in the ammonia production process contains 96% of Iron (Fe), 1% of Potassium hydroxide (KOH), and 3% of Aluminum oxide (Al_2O_3). Table 11 summarizes the inventory used in the LCA model to produce 1 kg of NH_3 via the Haber-Bosch process.

Table 11. *LCI for 1 kg of NH_3 (Chisalita et al., 2020)*

Process	**Inputs**	**Value/ kg NH_3**	**Unit**
NH_3 synthesis	Hydrogen from water electrolysis	0.188	kg
	Nitrogen from ASU	0.874	kg
	Electricity for H_2 and N_2 compression	1.709	MJ
	Water for reactor cooling	0.381	kg
	Ammonia synthesis catalyst	0.0002	kg
Catalyst's composition	Iron (Fe) - 96%	0.000192	kg
	Potassium hydroxide (KOH) - 1%	0.000002	kg
	Aluminium oxide (Al_2O_3) - 3%	0.000006	kg

Electricity sources

According to the information provided by DGE, the assumed sources of electricity in the case study are from 250 MW solar through internal connections and from 260 MW onshore wind through PPAs. It is estimated that the actual energy output of the solar farm is 250 GWh per year, and the wind farm is 750 GWh per year. Based on this information, the electricity profile of the plant in the LCA model is assumed to consist of 25% of solar and 75% of wind electricity.

Regarding the solar farm in the case study, only the environmental impacts from manufacturing solar panels are taken into account due to the lack of information about the electrical system constituting the solar farm. PV panels chosen for the thesis are single-crystalline silicon (sc-Si) panels. Silicon-based solar technology is the most common and mature technology in the industry. Overall, this technology has good chemical and mechanical properties compared to other solar PV technologies based on different semiconductor materials (Muteri et al., 2020). Sc-Si panel has higher commercial efficiency, around 16-22%, compared to multi-crystalline silicon (mc-Si) panels, which are around 15-18% (Muteri et al., 2020).

The unit of the background process selected for solar PV panels from ecoinvent is the total surface area of the panels, in m^2. The total panel surface required to produce 250 GWh of solar power in the case study is calculated using Equation 13:

$$E = I * \eta_{panel} * \eta_{system} * A_{panel} \quad (13)$$

Whereas:

E: electrical power output of the panels (kWh)

I: solar irradiance, the amount of sunlight received in 1 unit of area (kWh/m^2)

η_{panel}: efficiency of solar panels

η_{system}: efficiency of the solar system

A: the total surface area of the solar panels (m^2)

The solar farm in the case study has a production capacity of 250 MW or 250 GWh. The annual solar irradiation at the site is around 1027.5 kWh/m^2 (Global Solar Atlas, 2025). The efficiency of the sc-Si module is assumed to be 19.5%, based on the data from the product SunPower E Series E20 327 module (IEA, 2020). The system efficiency is assumed to be 92%, which is due to energy losses in electrical components, shading losses, or due to dirt on the module surface (Khan et al., 2024). From the information above, the total surface area of the panels required for a 250 MW solar farm is estimated at 3.7 km^2.

3.2.3 Impact assessment

There are various impact assessment methods. Some of the methods that are available in SimaPro 9.6.0.1 are CML 2001, Environmental Footprint, LC-IMPACT, IMPACT World, ReCiPe 2016, BEES+, and TRACI 2.1. In this thesis, the Environmental Footprint 3.1 method will be used to calculate the impact assessment of the ammonia system. This method contains 16 impact categories in total.

The five LCA studies on ammonia production in the literature review had highly varying selections of impact categories. Therefore, in this thesis, the impact assessment is carried out in 2 parts. The first part will analyze the environmental impacts of all the impact categories that were covered in the LCA studies in the literature. The second part is the analysis of the normalization and weighting results to identify the most relevant impact categories to the case study. The aim is to identify the five most impactful categories from the normalization and from the weighting results, then aggregate the findings. These most relevant impact categories will be used in further analysis to identify the most environmentally impactful life cycle stages and single processes in the ammonia production system. Based on the literature review, 13 impact categories that will be used for the first part of the impact assessment are (1) acidification, (2) climate change, (3) freshwater ecotoxicity, (4) freshwater eutrophication, (5) human toxicity, cancer, (6) human toxicity, non-cancer, (7) ionizing radiation, (8) land use, (9) ozone depletion, (10) photochemical ozone formation, (11) resource use, fossils, (12) resource use, minerals and metals, and (13) water use. Table 12 summarizes the overview of the impact categories used in this thesis, including the category impact indicators and their units, the description of the impact categories, and the models behind the Environmental Footprint method.

Table 12. *Overview of the 13 impact categories used in thesis's LCIA (Andreasi et al., 2023)*

Impact category	Indicator	Unit	Description	Underlying LCIA method
Climate change	Radiative forcing as Global Warming Potential (GWP100)	kg $CO2_{eq}$	This indicator refers to the rise in the average global temperatures due to GHG emissions.	Bern model - Global warming potential (GWP) over a 100-year time horizon based on IPCC 2021 (Forster et al., 2021).
Ozone depletion	Ozone Depletion Potential (ODP)	kg C FC-11_{eq}	This indicator refers to destruction of the stratospheric ozone layer due to airborne emissions.	EDIP model based on the ODPs of the World Meteorological Organisation (WMO) over an infinite time horizon (WMO 2014 + integrations)
Photochemical ozone formation, human health	Tropospheric ozone concentration increase	kg $NMVOC_{eq}$	This indicator refers to potential human health impacts due to the formation of photochemical ozone in the lower atmosphere (smog).	LOTOS-EUROS model (Van Zelm et al., 2008) as applied in ReCiPe 2008.
Acidification	Accumulated Exceedance (AE)	mol $H+_{eq}$	This indicator refers to the potential acidification of soil and water due to the emissions of gases such as nitrogen oxides and sulfur oxides.	Accumulated Exceedance (Seppälä et al. 2006, Posch et al., 2008)
Eutrophication, freshwater	Fraction of nutrients reaching freshwater end compartment (P)	kg P_{eq}	This indicator refers to the eutrophication of freshwater due to phosphorus containing compounds.	EUTREND model (Struijs et al., 2009) as implemented in ReCiPe 2008.
Water use	User deprivation potential (water consumption)	m^3 world eq. deprived water	This indicator refers to relative amount of water consumption depending on regional water scarity factors.	Available WAter REmaining (AWARE) model (Boulay et al., 2018; UNEP 2016)

Resource use, minerals and metals	Abiotic depletion resource (ADP ultimate reserves)	kg Sb_{eq}	This indicator refers to the depletion of natural non-fossil resources.	van Oers et al., 2002 as in CML 2002 method, v.4.8
Resource use, fossil	Abiotic depletion resource – fossil fuels (ADP-fossil)	MJ	This indicator refers to the depletion of natural fossil resources.	van Oers et al., 2002 as in CML 2002 method, v.4.8
Human toxicity, cancer	Comparative Toxic Unit for humans (CTUh)	CTUh	This indicator refers to the impacts on human health due to substances that might increase the risks of cancers.	Based on USEtox2.1 model (Fantke et al. 2017, Rosenbaum et al. 2008), as in Saouter et al. (2018)
Human toxicity, non-cancer	Comparative Toxic Unit for humans (CTUh)	CTUh	This indicator refers to the impacts on human health due to substances that might cause non-cancerous health issues.	Based on USEtox2.1 model (Fantke et al. 2017, Rosenbaum et al. 2008), as in Saouter et al. (2018)
Ionising radiation, human health	Human exposure efficiency relative to U235	kBq U235	This indicator refers to the potential ionizing radiation exposure causing adverse impacts on human health	Human health effect model as developed by Dreicer et al. (1995) and published in Frischknecht et al. (2000).
Ecotoxicity, freshwater	Comparative Toxic Unit for ecosystems (CTUe)	CTUe	This indicator refers to the releases of harmful compounds to freshwater ecosystems.	Based on USEtox2.1 model (Fantke et al. 2017, Rosenbaum et al. 2008), adapted as in Saouter et al. (2018)
Land use	Soil quality index	Dimensionless (pt)	This indicator refers to changes in soil quality regarding 4 soil properties: biotic production, erosion resistance, mechanical filtration, and groundwater regeneration.	Soil quality index based on LANCA model (De Laurentiis et al. 2019) and on the LANCA CF version 2.5 (Horn and Maier, 2018)

4. RESULTS

4.1 Environmental impacts of the case study

The environmental impacts of 1 kg of ammonia produced in the case study are summarized in Table 13 below.

Table 13. *Characterization results of the case study*

Impact category	Unit	Total
Acidification	mol H+ eq	0.01
Climate change (Total)	kg CO_2 eq	0.92
Ecotoxicity, freshwater	CTUe	11.05
Eutrophication, freshwater	kg P eq	5.8E-04
Human toxicity, cancer	CTUh	1.4E-08
Human toxicity, non-cancer	CTUh	3.7E-08
Ionizing radiation	kBq U-235 eq	0.16
Land use	Pt	4.99
Ozone depletion	kg CFC11 eq	4.3E-08
Photochemical ozone formation	kg NMVOC eq	3.6E-03
Resource use, fossils	MJ	13.10
Resource use, minerals and metals	kg Sb eq	4.6E-05
Water use	m^3 depriv.	0.97

1 kg of ammonia production is estimated to produce 0.01 mol H^+ eq contributing to acidification in soils and water, and 0.92 kg of CO_2 eq contributing to global warming potential. The production of 1 kg of NH_3 also releases $5.8*10^{-4}$ kg P eq of substances into the environment potentially causing freshwater eutrophication. Regarding the toxicity categories, the environmental impact of 1 kg of NH_3 on freshwater toxicity is estimated at 11.05 CTUe. The Comparative Toxic Unit for Ecosystems (CTUe) is calculated by integrating the potentially affected fraction of species over time and volume, per unit mass of a chemical released (Malbar, 2023). The impact of 1 kg of NH_3 on human toxicity (cancer) is $4.3*10^{-8}$ CTUh and on human toxicity (non-cancer) is $3.7*10^{-8}$ CTUh. The Comparative Toxic Unit for Humans (CTUe) is measured by considering the effect on mortality of the total human population per unit mass of chemicals released.

The human health impact from ionizing radiation exposure created by the production of 1 kg of NH_3 is estimated at 0.16 kBq U-235 eq. 1 kg of NH_3 produced releases $4.3*10^{-8}$

kg CFC11 eq contributing to ozone depletion potential, and 3.6*10^{-3} kg NMVOC eq contributing to photochemical ozone formation. The production of 1 kg of NH_3 also consumes 13.1 MJ of fossil fuel resources and 4.6*10^{-5} kg Sb eq. In addition, it contributes to 0.97 m^3 of water deprived in the site area. This water volume is not only the water consumed to produce 1 kg of NH_3 but it is the amount of water missing after the water consumption, which is related to the water scarcity situation of the location. The land use impact of 1 kg of NH_3 is 4.99 points, which is an indicator of soil quality loss due to ammonia production.

4.2 Most relevant impact categories

The normalization and weighting results will be used to identify the most relevant impact categories. Figure 8 below shows the normalization results, which indicate the contributions of the impact categories in the case study relative to a reference unit, which is the global average emissions of 1 person per year. According to the normalization results, the case study contributes the biggest proportions to these five impact categories: human toxicity (cancer), resource use (minerals and metals), freshwater eutrophication, human toxicity (non-cancer), and resource use (fossils). Figure 9 illustrates the weighting results to support the identification of the most relevant impact categories associated with the case study. Figure 9 shows that the ammonia production system contributes the highest proportions to these five impact categories: resource use (minerals and metals), climate change, human toxicity (cancer), resource use (fossils), and freshwater eutrophication. Combining the normalization and weighting results, the most relevant impact categories of the ammonia production system are resource use (minerals and metals), resource use (fossils), climate change, human toxicity (cancer), human toxicity (non-cancer), and freshwater eutrophication. The contributions of the ammonia production system to these 6 impact categories will be analyzed further in the following sections to identify the most impactful life cycle stages and the most impactful single processes in the ammonia production system.

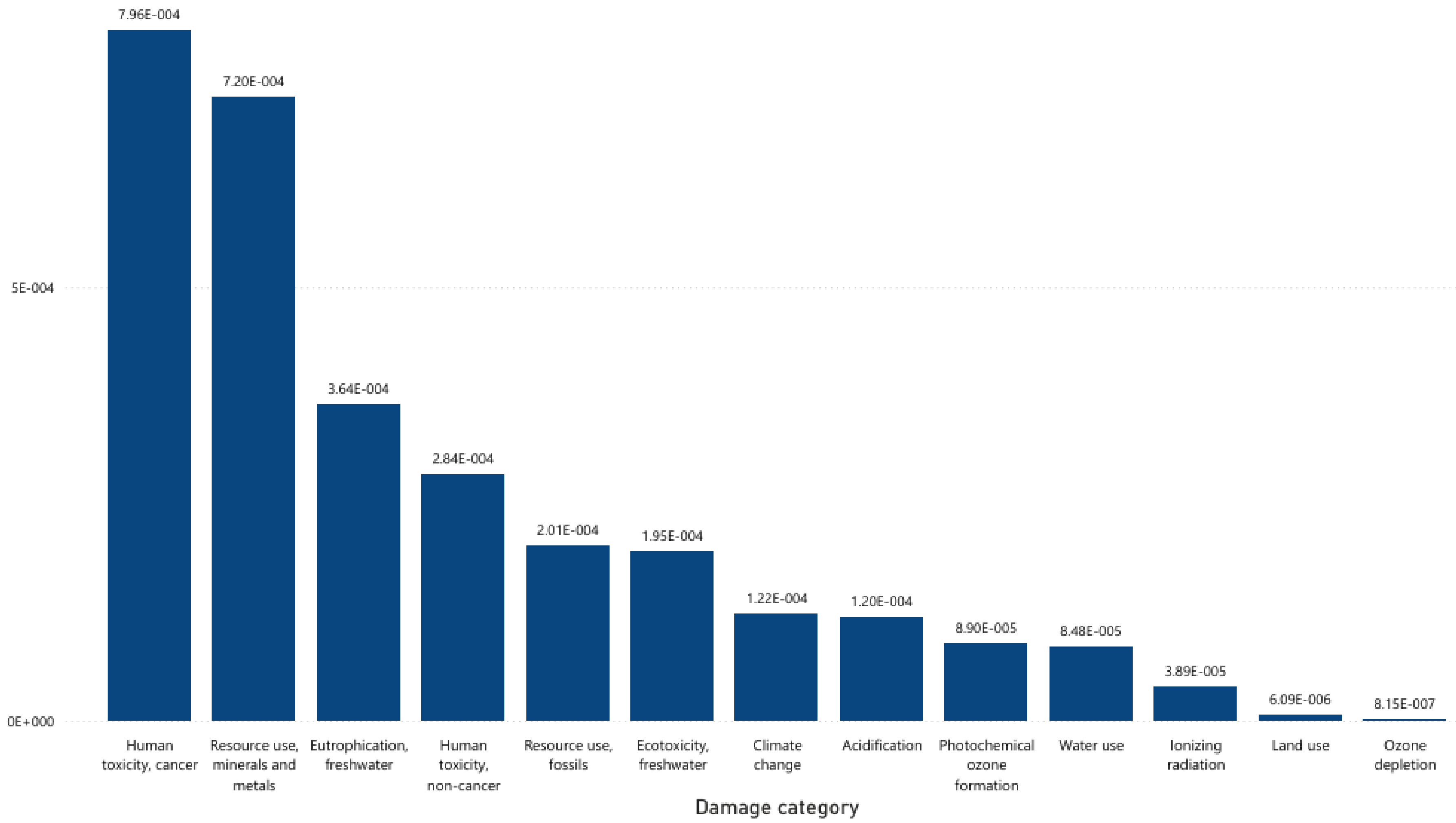

FIGURE 8. A comparison of environmental impact categories based on normalization results

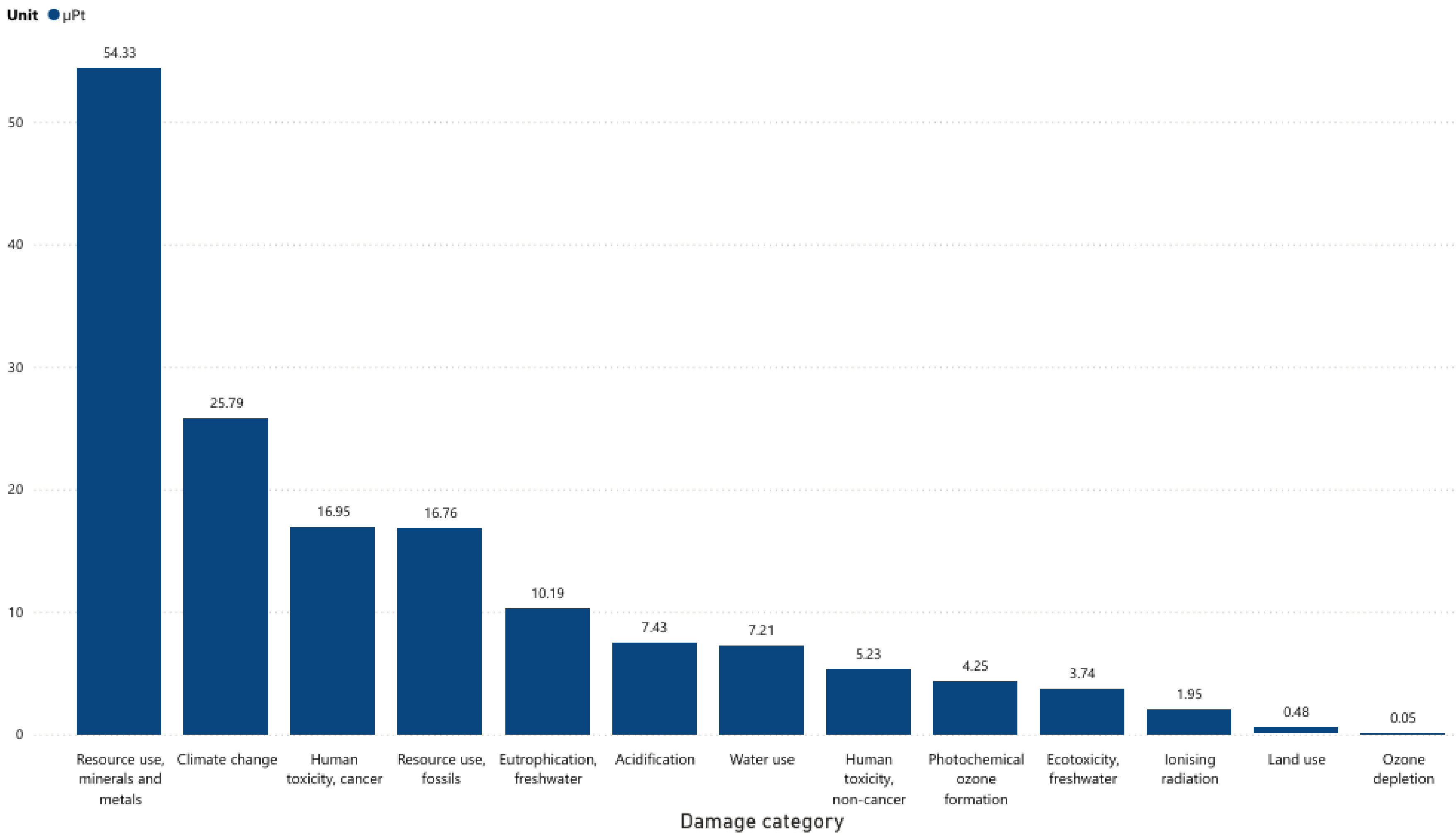

FIGURE 9. A comparison of environmental impact categories based on weighting results

4.3 Most impactful life cycle stages

This section will identify the most impactful life cycle stages in the ammonia production system. Four life cycle stages of the ammonia system are (1) AEL construction, (2) operational resources for hydrogen production, (3) nitrogen production, and (4) other inputs for ammonia synthesis such as electricity, water for reactor cooling, and catalyst for the reaction. Figure 10 shows the contribution of these life cycle stages to 6 impact categories that are resource use (minerals and metals), resource use (fossils), climate change, human toxicity (cancer), human toxicity (non-cancer), and freshwater eutrophication.

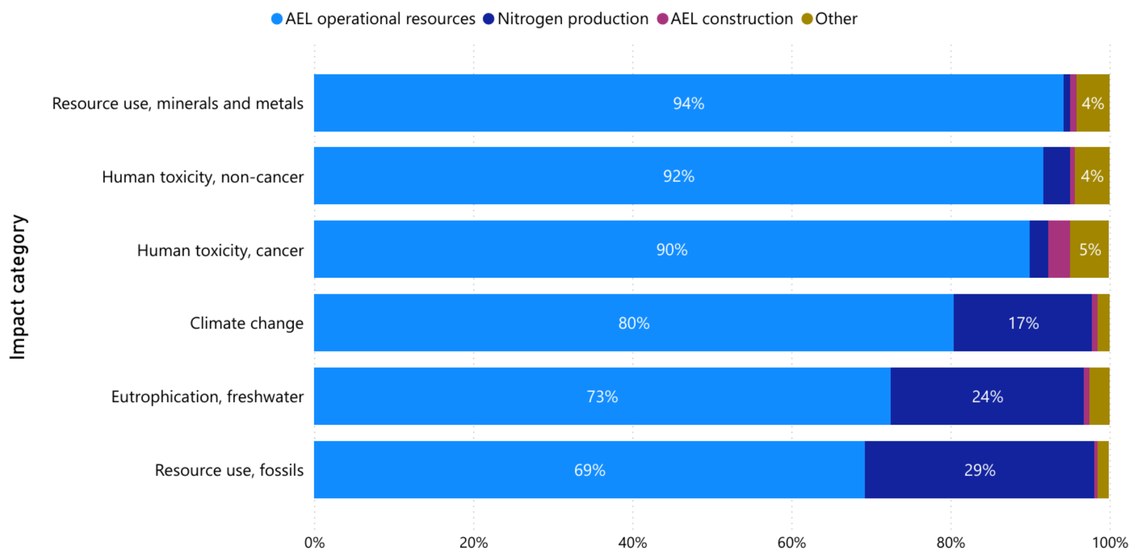

FIGURE 10. Contributions of life cycle stages to environmental impacts

From Figure 10, it was shown that hydrogen production, including the AEL construction and operational resources, makes up 70-95% of the total impacts of the whole system, highest in resource use of minerals and metals (95%). Nitrogen production is the second largest contributor to environmental impacts, accounting for 1-29% of the total impacts of the ammonia system. It affects the highest on resource use of fossils (29%) and freshwater eutrophication (24%). The environmental impacts of the remaining inputs for the Haber-Bosch process, including electricity for H_2 and N_2 compression, water for reactor cooling, and catalyst for the synthesis, account for less than 5% combined in every impact category.

In hydrogen production, the majority of environmental impacts come from the operational phase of the ammonia plant, which contributes 69%-94% to the total impacts. It is the biggest contributor to the impacts on resource use of minerals and metals (94%). The construction of the AEL contributes much less environmental impact than the operational resources for hydrogen production. Overall, it accounts for less than 3% of the total impacts in all impact categories.

4.4 Most impactful single processes

Figure 11 illustrates the contributions of the ammonia production system to the impact categories on the level of single processes.

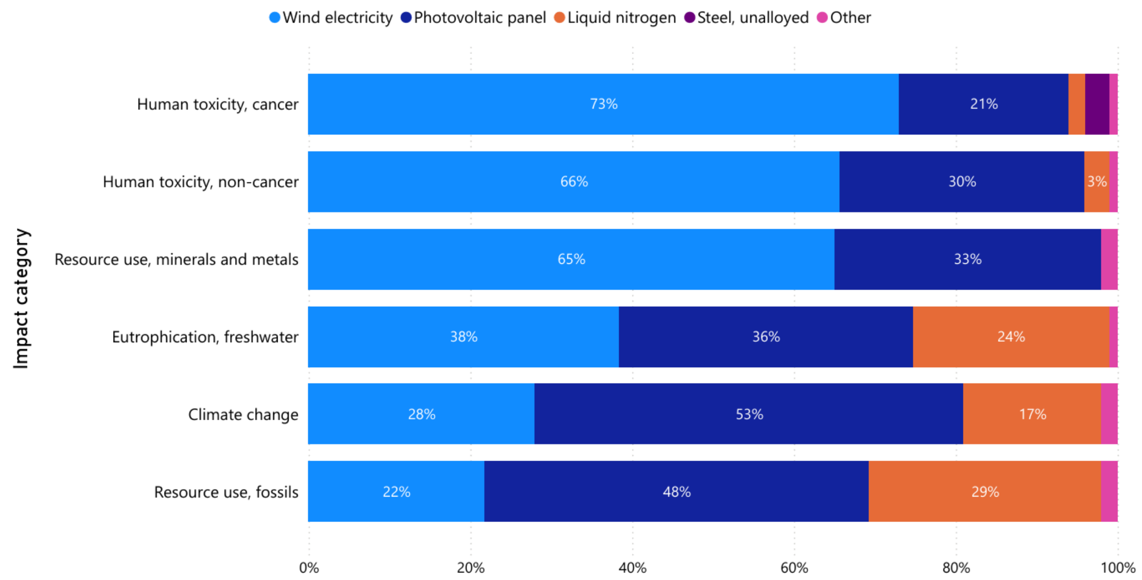

FIGURE 11. Contributions of single processes to environmental impacts

It is shown that the environmental impacts of ammonia production mostly come from 3 processes: PV panel production, wind power production, and nitrogen production. The combined impacts of solar and wind electricity production make up 70%-94% of the total impacts. The production of wind electricity is the largest source of impacts in 4 out of 6 impact categories, except for the impacts on climate change and resource use (fossils). Electricity production from wind has the most adverse effects on human toxicity (cancer) (73%), human toxicity (non-cancer) (66%), and resource use of minerals and metals (65%). The production of PV panels is the second largest source of impacts, highest in climate change (53%) and resource use (fossils) (48%). Nitrogen production causes the most environmental impacts on resource use of fossils (29%), freshwater eutrophication (24%), and climate change (17%). Nitrogen production contributes very small proportions to the other impact categories, under 4% in each of the other categories. Besides these three processes, steel consumption for AEL construction has a small contribution to the environmental impact on human toxicity (cancer), at 3%. All remaining processes combined have less than 3% impact on every category.

Regarding the sources of electricity, the ammonia system in the case study has an electricity profile consisting of 25% solar PV and 75% wind energy. It is reasonable that the environmental impacts of wind electricity are higher than solar electricity in general.

4.5 Environmental impacts on climate change

Climate change is an important impact category that is concerned in many legislative frameworks such as the European Green Deal and Estonia 2035. Therefore, this section focuses on analyzing the environmental impacts of the ammonia production system on climate change.

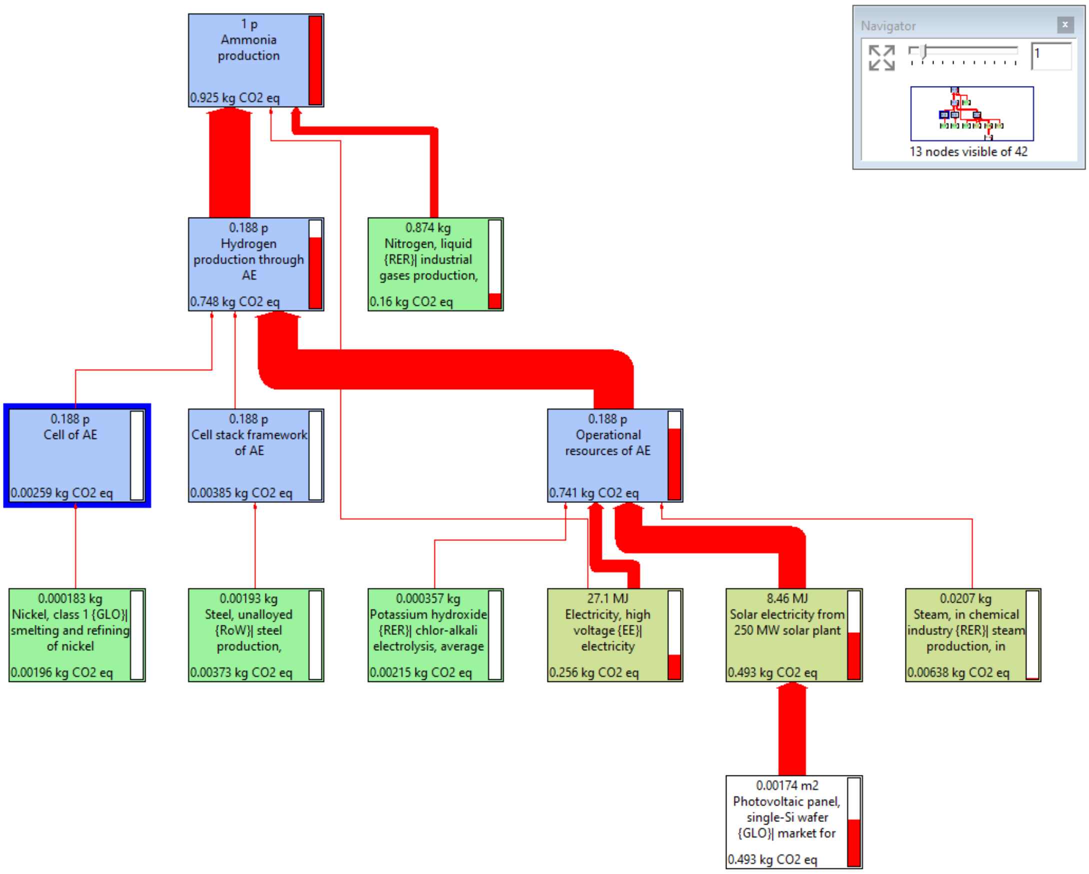

FIGURE 12. Impacts of the ammonia production system on climate change

Figure 12 shows that the production of 1 kg of ammonia will produce 0.925 kg CO_2-eq. Around 80% of the total CO_2-eq emissions come from hydrogen production and 20% come from nitrogen production. 99% of the emissions from hydrogen production are from the electricity used in water electrolysis. The emission of electricity from solar PV is

0.0582 kg CO_2-eq per MJ, 6 times higher than the emission of wind electricity, which is around 0.0094 kg CO_2-eq per MJ. Other processes contribute much less to the impacts of climate change compared to electricity consumption.

5. DISCUSSION

5.1 Comparisons with other studies on green ammonia

In this section, the characterization results of the thesis's study will be compared with 8 other green ammonia production systems in the literature to understand the significance of the environmental impacts of the case study compared to other similar systems. The description of the systems used in the comparison is summarized in Table 3 above.

It is noted that the calculation method used in the thesis is different from the methods used in the studies in the literature. Most of the studies used the ReCIPe 2016 Midpoint Hierarchist method, and the study by Singh et al., 2019 used the CML 2001 and Eco-indicator 99 method. The impact categories in these 3 methods have different impact category indicators. Therefore, the comparison is limited to 2 impact categories that are climate change and freshwater eutrophication. The impact indicators of these 2 impact categories in the Environmental Footprint 3.1 method are similar to those in the ReCIPe 2016 Midpoint Hierarchist and/or CML 2001 method. Figure 13 below shows the comparison between the environmental impacts of the thesis's case study and other green ammonia systems in the literature.

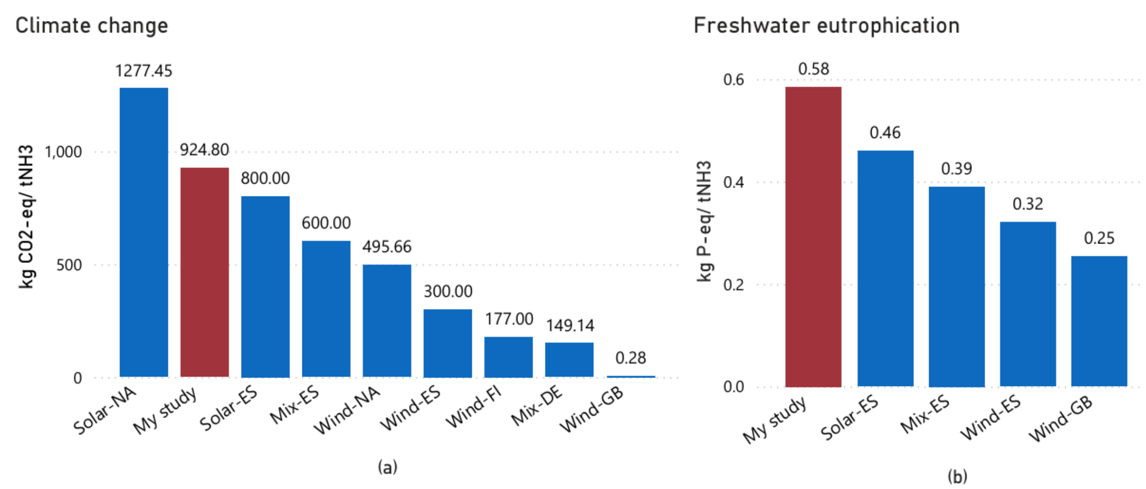

FIGURE 13. Comparisons of the environmental impacts between the thesis's system and other green ammonia systems in 2 impact categories: (a) climate change and (b) freshwater eutrophication

Figure 13 shows that the ammonia production system in this thesis has relatively high environmental impacts compared to other systems. It has the highest impact indicator values in freshwater eutrophication and the second highest value in climate change. The result of climate change impact of the thesis's case study could be relatively high in general. The case 'Solar-NA' by Singh et al., 2018 showed a higher climate change impact. However, the system boundary of the study is cradle-to-grave, which consists of more life-cycle stages than in the thesis's case. The case also used 100% solar power, which may contribute more to climate change than the electricity mix of wind and solar power used in the thesis. Another system in the study by Singh et al., 2018 'Wind-NA' also has the system boundary from cradle-to-grave. However, it has lower results than the thesis's case study, at around 0.5 t CO_2-eq/t NH_3. The case study also has higher CO_2 emissions than other systems that have more components in their system boundaries. For example, the systems 'Wind-ES', 'Solar-ES', and 'Mix-ES' from the study by Vinardell et al., 2023 include lithium battery and hydrogen storage system, and the 'Wind-GB' system by Boero et al., 2021 includes facility construction. However, these systems also have lower impacts on climate change than the thesis's system. In addition, the LCA study by Boero et al., 2021 contained 7 scenarios for ammonia production via water electrolysis, varying by different plant capacities (small/ medium capacity), electricity sources (wind/ solar), and countries where the plants were located. The study showed that the emissions of all ammonia production scenarios through water electrolysis based on renewable energy was below 0.7 t CO_2-eq/t NH_3, and the emissions from wind-based electrolysis were around 0.24-0.54 t CO_2-eq/t NH_3, which is much lower than the case study's emissions. The high emissions of the case study could be due to the inclusion of the solar farm in the system boundary or a more detailed inventory for the AEL.

The system in the case study has the second highest impact indicator value in freshwater eutrophication. The high environmental impacts of the case study on freshwater eutrophication could be due to higher water consumption in the plant leading to more wastewater sent to wastewater treatment facilities, or the use of solar panels in the system.

The differences in the results between the thesis's case study and other green ammonia production systems could be due to many factors such as different system boundaries, geographical locations, sources of material inputs, databases, calculation methods, and a different set of assumptions. The comparison of environmental impacts between the thesis's work and other studies is used to illustrate the relative magnitude of how impactful ammonia production can be on a more general scale. Each LCA study has its own system boundaries and assumptions, therefore, a proper comparison cannot be achieved. Besides, the inventory of some systems in the literature is unknown, therefore, it is uncertain if the reasons mentioned above are the actual causes of the higher environmental impacts on climate change and freshwater eutrophication of the case study compared to other systems in the literature.

The thesis's findings align with other studies in the literature that the major impact of ammonia production comes from hydrogen production. The thesis's result showed that hydrogen production is responsible for 70-95% of the total impacts of the ammonia production system, depending on the impact categories. Other studies have shown that the hydrogen production from water electrolysis could be responsible for 90%-94% of the total carbon emissions of the ammonia synthesis system in the impact category of climate change (Boero et al., 2021; Chisalita et al., 2020). The thesis also has a similar result to the study of Chisalita et al., 2020 in a point that electricity for water electrolysis is the biggest source of environmental impacts in hydrogen production. Singh et al., 2018 study comparing the ammonia production systems powered by solar PV and wind electricity concluded that ammonia production from solar PV panels causes more environmental damage than wind-based production. The thesis's result shows that electricity from wind has overall more environmental impact than electricity from solar PV panels in the impact categories chosen in the thesis. However, the comparison between the environmental impacts of wind and solar electricity in the thesis is not compatible with the study by Singh et al., 2018 because the thesis's case study consumes 75% wind and 25% solar electricity.

5.2 Comparisons with other LCA studies on SMR

In this section, the characterization results of the thesis's case study are compared with 6 other ammonia production systems in the literature, in which hydrogen is produced via SMR. This comparison will help to understand the differences in the environmental impacts of ammonia production via renewable energy, which is usually considered a more sustainable pathway, compared to the traditional production method based on the use of natural gas. Table 4 above describes the SMR systems that are used in the comparison.

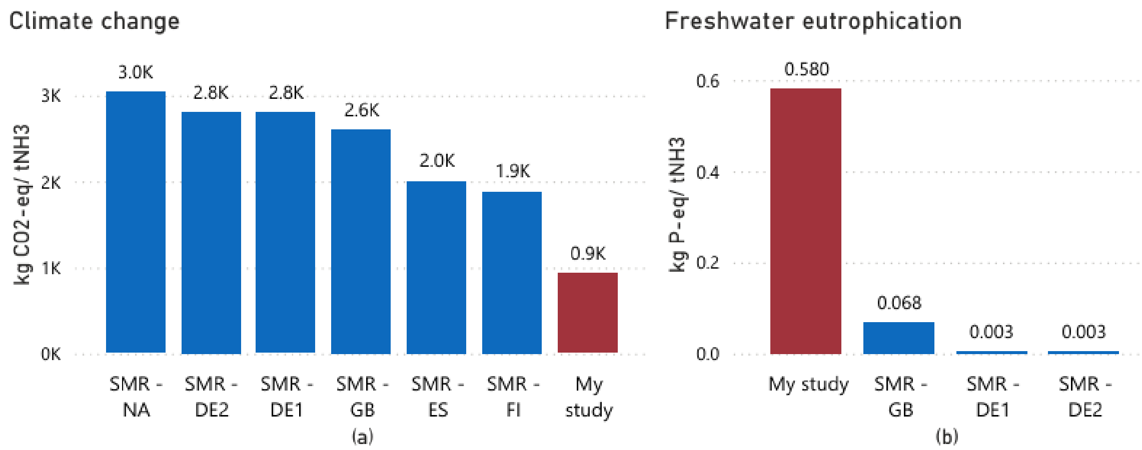

FIGURE 14. Comparisons of the environmental impacts between the thesis's system and other studies on ammonia via SMR in 2 impact categories: (a) climate change and (b) freshwater eutrophication

Figure 14 shows that ammonia production from renewable energy can reduce the CO_2-emissions by 50%-70% compared to the production via SMR. The result is aligned with the other studies in the literature, which found that green ammonia could reduce the impacts on climate change by 40% to 95%. However, green ammonia production increases the environmental impacts on freshwater eutrophication significantly, which is similar to the findings in the studies of Chisalita et al., 2020 and Vinardell et al., 2023.

5.3 Sensitivity analysis

As shown in the result section, electricity consumption for water electrolysis is a major source of environmental impacts. Therefore, a sensitive analysis is done to assess how the environmental impacts will change based on the selection of AELs that have more or less specific system energy consumptions than the AEL used in the case study. The typical specific system energy consumption of commercialized AELs is around 4.2-4.8 kWh/Nm^3 H_2, which equals 168.22-192.25 MJ/ kg H_2 (David et al., 2019). Three scenarios will be used to compare the variations in environmental impacts of AELs with different specific system energy consumptions, summarized in Table 14. The base scenario is the current model used in the thesis. The Min scenario is the model of a commercialized AEL that has a minimum energy consumption of 168.22 MJ/ kg H_2, and the max scenario is for an AEL having a maximum energy consumption of 192.25 MJ/ kg H_2. The results of the comparison are shown in Figure 15 below.

Table 14. *Three scenarios in the sensitivity analysis*

Scenarios	Specific system energy consumption
Base scenario	180 MJ/ kg H_2
Min scenario	168.22 MJ/ kg H_2
Max scenario	192.25 MJ/ kg H_2

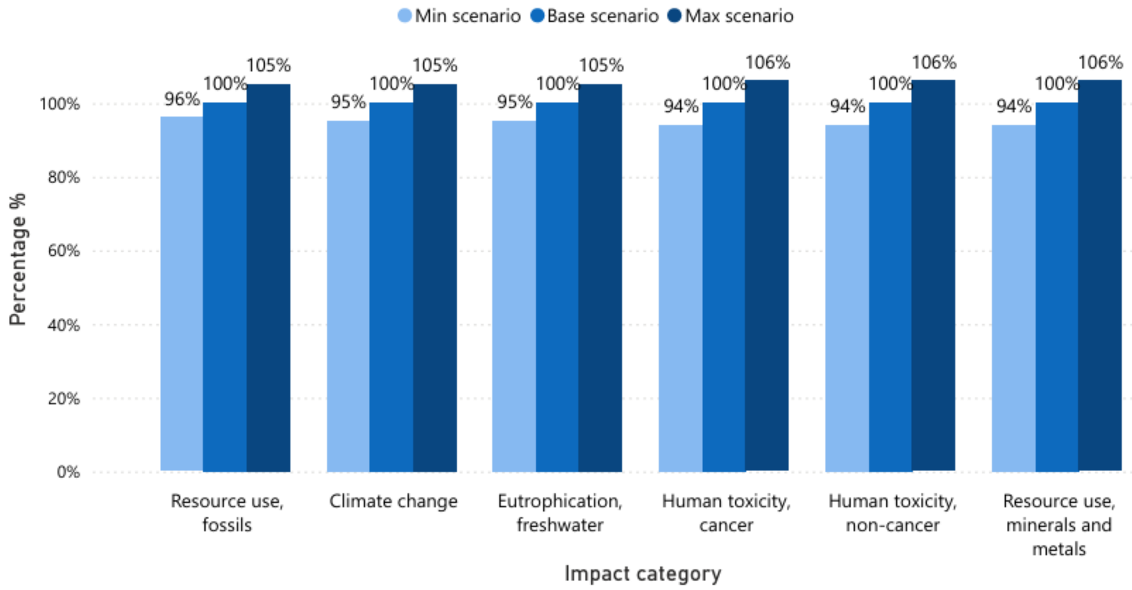

FIGURE 15. Comparisons of the environmental impacts between 3 scenarios

From Figure 15, it is shown that by selecting the highest energy efficiency AEL among those that are commercialized, the environmental impacts can be reduced by 4%-6%. By using the least energy-efficient AEL, the impacts on the environment increase by 5%-6%. Table 15 summarizes the environmental impacts of the 3 scenarios.

Table 15. *Results of the sensitivity analysis*

Impact category	Unit	Min scenario	Base scenario	Max scenario
Climate change	kg CO2 eq	0.88	0.92	0.97
Eutrophication, freshwater	kg P eq	6.1E-05	6.4E-05	6.7E-05
Human toxicity, cancer	CTUh	1.3E-08	1.4E-08	1.5E-08
Human toxicity, non-cancer	CTUh	3.4E-08	3.7E-08	3.9E-08
Resource use, fossils	MJ	12.51	13.10	13.71
Resource use, minerals and metals	kg Sb eq	4.3E-05	4.6E-05	4.9E-05

In the future, an LCA study for the case study could be modeled with the actual AEL and real data for operational resources from the plant to get a more accurate result. Also, it would be more accurate to include other elements in the production phase and even the use phase and the end-of-life into the system boundary when the plant design is finished and the plant comes into operation.

6. CONCLUSION

One aim of the thesis is to understand the legislative policies that encourage the development of green ammonia in Estonia. The green ammonia industry in Estonia is affected by the objectives and requirements of RED III and the two delegate acts supporting RED II, which are applied to the production of hydrogen and hydrogen derivatives. In addition, the European Hydrogen Backbone initiative, which planned to build a hydrogen transmission network of 40,000 km connecting 21 European countries by 2040, and the long-term development strategies set in 'Estonia 2035' also encourage green ammonia development in the country. The Estonia Hydrogen Roadmap was established to assist the development of hydrogen supply chains and infrastructure. It aims to produce abundant and zero-emission hydrogen by 2050, which assures a green hydrogen source for ammonia production.

The second aim of the thesis is to evaluate the environmental impacts of green ammonia production in Estonia by using LCA. The LCA results are used to identify the most relevant impact categories associated with green ammonia production and the biggest contributors to the total impacts in the level of life cycle stages and single processes. The results show that the most relevant impact categories to green ammonia production are resource use (minerals and metals), resource use (fossils), climate change, human toxicity (cancer), human toxicity (non-cancer), and freshwater eutrophication. Under these impact categories, hydrogen production contributes the majority of the total impacts, followed by the production of nitrogen. Most of the impacts of hydrogen production come from the use of electricity for water electrolysis. At the level of single processes, the production of solar PV panels and wind electricity accounts for the majority of environmental impacts. In the case study which has the electricity profile of 25% solar PV and 75% wind energy, solar power is found to be less impactful than wind power. Regarding the impacts on climate change, 1 kg of ammonia produced releases 0.925 kg CO_2-eq to the environment, of which 80% is from hydrogen production and 20% is from nitrogen production.

The discussion section compared the thesis's results with other green ammonia systems and ammonia production systems via SMR. In the comparison with other green ammonia systems, the case study in the thesis was found to have higher environmental impacts on climate change and freshwater eutrophication than other green ammonia systems. However, a deeper analysis is needed to investigate the reasons behind the differences between the results of the thesis and other studies in the literature. In the comparison with other SMR systems, the thesis agreed with the studies in the literature that green ammonia can reduce CO_2-eq emissions compared to the SMR method. The impact of the case study system on freshwater eutrophication is higher than SMR-based systems, which is similar to the findings of 2 studies in the literature.

In the future, an LCA study could be carried out for the case study using the actual data from the plant to increase the accuracy of the model. Besides, the system boundary could be expanded based on the plant design and cover more activities of the plant.

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APPENDIX

Table 16. *The purposes of each material input in the hydrogen production inventory (Delpierre, 2019; Koj et al., 2017)*

Process	Input	Purpose
Cell stack framework	Copper	Manufacture of the cell stack framework
	Unalloyed steel	Constituent of the framework
Cells	Nickel	Raney Nickel cathodes
	Aluminum	Constituent of the Raney Nickel cathodes
	Calendered rigid plastic	Plastic cell frames or used for the anode/cathode as a catalyst layer or as a sealant
	Polytetrafluoroethylene	Used as gasket material/diaphragm
	Acrylonitrile butadiene styrene	Constituents for gasket manufacturing
	Polyphenylene sulfide	Membrane production
	Polysulfones	Membrane production
	N-Methyl-2-pyrrolidone	Membrane production
	Aniline	Input for aramid fibres (for gasket manufacturing)
	Acetic anhydride	Input for aramid fibres (for gasket manufacturing)
	Terephthalic acid	Input for aramid fibres (for gasket manufacturing)
	Nitric acid	Input for aramid fibres (for gasket manufacturing)
	Hydrochloric acid	Input for aramid fibres (for gasket manufacturing)
	Graphite	Constituents for gasket manufacturing
	Lubricating oil	Constituents for gasket manufacturing
	Zirconium oxide	Membrane production
	Carbon monoxide	Manufacturing of the Raney Nickel cathodes
	Decarbonized water	Likely used as cooling water

	Deionized water	Likely used as cooling water
	Industrial machine production	Construction phase
	Plaster mixing	Construction phase
	Electricity	Construction phase
	Heat	Likely for heat exchanger
	Steam	Unclear role, likely for BOP element
Operational resources for 1 kg H2	Electricity	Reactant
	Deionized water	Reactant
	Nitrogen	Cleaning purposes
	Potassium hydroxide	Electrolyte
	Steam	Used during the run-up to heat up the system

Table 17. *Background processes selected from Ecoinvent 3.10 database*

Input	Ecoinvent process
AEL construction	
Copper	Copper-rich materials {GLO}| copper, anode to generic market for copper-rich materials | Cut-off, S
Unalloyed steel	Steel, unalloyed {RoW}| steel production, converter, unalloyed | Cut-off, S
Nickel	Nickel, class 1 {GLO}| smelting and refining of nickel concentrate, 16% Ni | Cut-off, S
Aluminum	Aluminium alloy, AlLi {GLO}| market for aluminium alloy, AlLi | Cut-off, S
Calendered rigid plastic	PVC calendered sheet E
Polytetrafluoroethylene	Tetrafluoroethylene {RoW}| tetrafluoroethylene production | Cut-off, S
Acrylonitrile butadiene styrene	Acrylonitrile butadiene styrene (ABS)/EU-27
Polyphenylene sulfide	Polyphenylene sulfide {GLO}| polyphenylene sulfide production | Cut-off, S
Polysulfones	Polysulfone {GLO}| polysulfone production, for membrane filtration production | Cut-off, S
N-Methyl-2-pyrrolidone	N-methyl-2-pyrrolidone {RoW}| N-methyl-2-pyrrolidone production | Cut-off, S
Aniline	Aniline {RoW}| aniline production | Cut-off, S
Acetic anhydride	Acetic anhydride {RoW}| acetic anhydride production, acetaldehyde oxidation | Cut-off, S
Terephthalic acid	Purified terephthalic acid {RoW}| purified terephthalic acid production | Cut-off, S
Nitric acid	Nitric acid, without water, in 50% solution state {RoW}| nitric acid production, product in 50% solution state | Cut-off, S
Hydrochloric acid	Hydrochloric acid, without water, in 30% solution state {RoW}| hydrochloric acid production, from the reaction of hydrogen with chlorine | Cut-off, S
Graphite	Graphite {RoW}| graphite production | Cut-off, S
Lubricating oil	Lubricating oil {RoW}| lubricating oil production | Cut-off, S
Zirconium oxide	Zirconium oxide {RoW}| zirconium oxide production | Cut-off, S
Carbon monoxide	Carbon monoxide {RoW}| carbon monoxide production | Cut-off, S
Decarbonized water	Water, decarbonised {RoW}| water production, decarbonised | Cut-off, S
Deionized water	Water, deionised {RoW}| water production, deionised | Cut-off, S
Plaster mixing	Cement plaster {RoW}| cement plaster production, hand-mixed on site | Cut-off, S
Electricity	Electricity, high voltage {CN-HB}| electricity production, hard coal | Cut-off, S
Heat	Heat, district or industrial, other than natural gas {CN-HB}| treatment of blast furnace gas, in power plant | Cut-off, S

Steam	Steam, in chemical industry {RoW}| ammonia production, steam reforming, liquid | Cut-off, S
AEL operational resources	
Electricity	Electricity, high voltage {EE}| electricity production, wind, >3MW turbine, onshore | Cut-off, S
	Photovoltaic panel, single-Si wafer {GLO}| market for photovoltaic panel, single-Si wafer | Cut-off, S
Deionized water	Water, deionised {Europe without Switzerland}| water production, deionised | Cut-off, S
Nitrogen	Nitrogen, liquid {RER}| industrial gases production, cryogenic air separation | Cut-off, S
Potassium hydroxide	Potassium hydroxide {RER}| chlor-alkali electrolysis, average production | Cut-off, S
Steam	Steam, in chemical industry {RER}| steam production, in chemical industry | Cut-off, S
Ammonia synthesis	
Nitrogen from ASU	Nitrogen, liquid {RER}| industrial gases production, cryogenic air separation | Cut-off, S
Water for reactor cooling	Tap water {Europe without Switzerland}| tap water production, conventional treatment | Cut-off, S
Potassium hydroxide (KOH)	Potassium hydroxide {RER}| potassium hydroxide production | Cut-off, S
Aluminium oxide (Al2O3)	Aluminium oxide, non-metallurgical {IAI Area, EU27 & EFTA}| aluminium oxide production | Cut-off, S
Iron (Fe)	Cast iron {GLO}| market for cast iron | Cut-off, S