# Estimating Carbon Emissions Throughout the Value Chain of Ammonia Using the Life Cycle Assessment Methodology

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# Preface

This bachelor's thesis was written by Jacob Ø. Sørvik and Sølve E. Bergheim from the Department of Mechanical and Marine Engineering at Western Norway University of Applied Sciences (*Høgskulen på Vestlandet, HVL*), as part of a Bachelor of Science degree in Energy Technology. The thesis's goal was set by Ocean Hyway Cluster, who also provided us with Mark Purkis, M.Sc., as our external industry supervisor. Professor Richard John Grant was our internal academic supervisor.

We would like to thank our supervisors Mark and Richard for their guidance and helpful insight throughout the project. Although a sudden change of external supervisor was made early in the project phase, the work was relatively unaffected. In addition, we would like to thank Håkon Hauan (EPD Norge) for valuable information regarding guidelines, requirements, and the verification process of a life cycle assessment.

Hopefully, the overall result will be an informative and interesting read.

- Jacob and Sølve



# Abstract

Ammonia is emerging as a potential new fuel for marine vessels due to having zero carbon emissions when consumed. This does not mean that the lifecycle of ammonia is emission free. Throughout the ammonia value chain, carbon emissions are being accumulated by raw material extraction, electricity generation, production, storage, and distribution.

The purpose of this thesis is to break down the value chain of ammonia and look at emissions in every step using the life cycle assessment (LCA) methodology. An LCA must be used to document the emissions of an alternative fuel across its value chain, according to new ferry contracts issued by the Norwegian Public Roads Administration. This methodology is a powerful tool that assesses every step of a product's processes, from raw material extraction to final use, or recycling.

It was found in the analysis that the production of hydrogen is by far the most energy demanding process of the ammonia chain and is, therefore, the main determining factor for the carbon intensity of the final product. Steam reforming of natural gas can utilise carbon capture technologies to dramatically reduce the carbon emissions, although a high degree of carbon capture rate (>90%) is necessary for it to be comparable to production from renewable energy, in terms of emissions.

Hydrogen production from electrolysis requires about 60-70 kWh/kg H<sub>2</sub>, with overall carbon emissions mostly dependent on the carbon intensity of the electricity that is used. Using electricity directly generated from wind, hydro, geothermal and nuclear is preferred as the alternatives to grid electricity, since grid electricity is a mixture of electricity from different sources, including fossil sources.

It was also found that for utilising ammonia as a marine fuel, the preferred method is expected to be the use of a direct ammonia-fed high-temperature fuel cell, although it is not yet commercially available. In comparison, the use of a low-temperature hydrogen-fed fuel cell requires an energy-demanding ammonia cracking unit to extract hydrogen from ammonia. The hydrogen fuel cell technology is, however, more mature. While ammonia can be used directly or as a supplement in a combustion engine, more research needs to be conducted to address the various challenges before it can be considered a viable technology for marine usage.

Note that a simplified Excel tool has been developed as part of the project. It can be used to estimate carbon emissions of ammonia in different scenarios and is a good tool to determine if a specific ammonia producer is worth pursuing.

## Sammendrag

Ammoniakk blir regnet som et potensielt nytt drivstoff for marine fartøyer, da det ikke har karbonutslipp ved forbruk. Dette betyr ikke at livssyklusen til ammoniakk er utslippsfritt. Gjennom verdikjeden akkumuleres karbonutslipp ved råstoffuthenting, elektrisitetsgenerering, produksjon, lagring og distribusjon. Dette utslippet må dokumenteres for å bekrefte at sluttproduktet er bærekraftig.

For å dokumentere utslippene til et alternativt hydrogenbasert drivstoff krever nye ferjekontrakter fra Statens Vegvesen en livssyklusvurdering (LCA). Metodikken ser på hver prosess i utviklingen av et produkt, fra råvareutvinning til endelig bruk eller resirkulering. Dette innebærer en målutviklingsfase og et omfang der perspektivet «well-to-wake» eller «brønn til vake» er foretrukket for ammoniakk som drivstoff. Dette omfatter prosessene for hydrogenproduksjon via dampreformering eller elektrolyse, samt nitrogengenerering, syntese, lagring, distribusjon, bunkring og forbruk i et fartøy.

Produksjon av hydrogen er den desidert mest energikrevende prosessen i verdikjeden til ammoniakk, og er derfor den viktigste avgjørende faktoren for karbonintensiteten til sluttproduktet. Dampreforming av naturgass kan benytte karbonfangstteknologier for å redusere karbonutslippene drastisk, men en høy grad av karbonfangst (>90 %) er nødvendig for å være sammenlignbart med produksjon fra fornybar energi når det gjelder karbonutslipp.

Hydrogenproduksjon fra elektrolyse krever ca. 60-70 kWh/kg H<sub>2</sub>, der det totale karbonutslippet er mest avhengig av karbonintensiteten til elektrisiteten som benyttes. Elektrisitet generert fra vind, vann, geotermisk og kjernekraft er foretrukket over elektrisitet fra strømnettet, da dette er en blanding av elektrisitet fra ulike kilder, deriblant fra fossile kilder.

Bruken av en direkte ammoniakkmatet høytemperatur brenselcelle forventes å være den foretrukne metoden for å utnytte ammoniakk som et marint drivstoff, selv om den ennå ikke er kommersielt tilgjengelig. Bruken av en lavtemperatur brenselcelle krever en «cracker»-enhet for å frigjøre hydrogen fra ammoniakk. Splittingen av amoniakk er en energikrevende prosess, men brenselcelleteknologien er derimot mer moden. Ammoniakk kan også brukes direkte eller som et supplement i en forbrenningsmotor, men forskning pågår fortsatt, og det er ulike utfordringer som må løses før det kan anses som en levedyktig teknologi.

Et forenklet Excel-verktøy for å estimere utslipp fra ammoniakk i forskjellige scenarioer er utviklet som en del av prosjektet. Dette kan brukes til å vurdere om forskjellige scenario er interessant å undersøke videre, men er ikke nok for en fullstendig LCA ettersom det kun tar hensyn til globalt oppvarmingspotensial i form av karbondioksidekvivalenter (GWP).

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# Nomenclature

Abbreviation	Description
AEC	Alkaline electrolysis cell
AFC	Alkaline fuel cell
BOG	Boil-of-gas
$^{\circ}C$	Degrees Celsius
CCUS	Carbon capture, utilization and storage
$CH_4$	Methane
СО	Carbon monoxide
$CO_2$	Carbon dioxide
$CO_2$ - $eq$	Carbon dioxide equivalents
EJ	Exajoule
EP	Eutrophication Potential
EPD	Environmental Product Declaration
η	Efficiency
GHG	Greenhouse gas
Gtonne	Gigatonne (metric)
GW	Gigawatt
GWP	Global Warming Potential
$\Delta H_f^\circ$	Change in enthalpy between reactants and products
$H_2$	Hydrogen
$H_2O$	Water
HBP	Haber-Bosch process
HFO	Heavy fuel oil
HHV	Higher heating value
HTFC	High-temperature fuel cell
ICCT	The International Council on Clean Transportation
ICE	Internal combustion engine
IEA	International Energy Organization
ISO	International Organization of Standardization
IMO	International Maritime Organization
kJ	Kilojoule
kWh	Kilowatt-hour
L	Liter
LCA	Life cycle assessment
LCI	Life cycle inventory analysis
LCIA	Life cycle impact assessment
LHV	Lower heating value
LNG	Liquified natural gas

LTFC	Low-temperature fuel cell
MJ	Megajoule
MPa	Megapascal
Mtonne	Megatonne (metric)
$N_2$	Nitrogen
$N_2/H_2$	Ration between N <sub>2</sub> and H <sub>2</sub>
NG	Natural gas
NH <sub>3</sub>	Ammonia
$NO_x$	Nitrogen oxides
NPRA	The Norwegian Public Roads Administration
PEMEC	Proton exchange membrane electrolysis cell
PEMFC	Proton exchange fuel cell
PV	Photovoltaic
SOEC	Solid oxide electrolysis cell
SOFC	Solid oxide fuel cell
SOFC-H	Proton conducting solid oxide fuel cell
SOFC-O	Oxygen-ion conducting solid oxide fuel cell
SMR	Steam-methane reforming
WGS	Water-gas shift conversion
WtW	Well-to-wake

## 1. Introduction

The Paris Agreement states that the goal is "to limit global warming to well below 2°C, preferably to 1.5°C, compared to pre-industrial levels" [1]. According to the International Council on Clean Transportation (ICCT), the shipping industry can emit a total of 10 and 17 Gtonnes to fulfil the Paris Agreement's global warming targets of 2°C and 1.5°C, respectively. [2].

About 90% of the world's trade is done through shipping. When compared with other methods of global transportation, such as air or road, ocean-going shipping is both the most cost and energy efficient, though it still carries responsibility to reduce the climate-hostile impact [3]. According to the Fourth IMO GHG Study 2020, the shipping industry emitted approximately 1.1 billion tonne carbon dioxide (CO<sub>2</sub>) in 2018, accounting for 2.89% of global GHG emissions [4] [5].

Based on 2008 emission levels, the 2018 initial GHG strategy by the International Maritime Organization (IMO) aims for a reduction in the carbon intensity of international shipping by at least 40% by 2030, with a target of achieving 70% by 2050. As per the strategy, the total annual GHG emissions from international shipping should also be halved by 2050, compared to 2008 levels [6].

## 1.1. Background

Modern ships are ranked high among "the most cost- and emission-effective transport means", but the demand for low carbon alternatives to traditional fossil fuels are increasing [7]. The use of ammonia as an energy carrier is looking very promising as an alternative transportation fuel in the marine shipping industry, which is currently dominated by heavy fuel oils (HFO) [8] [9]. Ammonia is a carbon-free chemical and has a great potential to contribute to the shipping sector as a CO<sub>2</sub>-neutral transportation fuel. Even if the fuel is labelled "zero-carbon," the carbon accumulated throughout the production chain may make it unsustainable.

Most of the ammonia produced today derives from natural gas, which generates a significant amount of  $CO_2$  emissions through the processing. To reduce emissions associated with natural gas reforming processes, different approaches, such as the use of carbon capture, utilization, and storage (CCUS), are required [10]. The hydrogen for the ammonia production can also be generated using water electrolysis, although this requires a renewable electricity source to be considered "low carbon".

In the new ferry contracts from the Norwegian Public Roads Administration, it is specified that energy carriers produced by other means than by electricity from the Nordic grid, must document that the entire production chain does not generate CO<sub>2</sub> emissions exceeding 130 grams CO<sub>2</sub>-eq per kilowatt-hour (kWh) delivered power. All the value chain steps must be accounted for, from raw material extraction to final consumption. Emissions must be documented using a Life Cycle Assessment (LCA) according to the following standards: ISO 14040 and ISO 14044. Such regulations and documentation of emissions for ferries are also expected to be introduced for other marine vessels as well, such as offshore vessels and bulk carriers.

#### 1.2. Aim

The aim of the thesis is to gain an understanding of what must be in place to document emissions throughout the value chain of ammonia to comply with regulations for use as marine fuel. Increased understanding of life cycle analyses related to emissions through the production and use of hydrogen and ammonia, as well as the ISO standards, is also of particular interest. Furthermore, if possible, to create a simplified model that can be used as an early-stage assessment of  $CO_2$  emissions throughout the production chain of ammonia.

#### 1.3. Objectives

To comply with the aim, the thesis has the following objectives:

- Break down the value chain of ammonia and look at the emissions associated with every step from feedstock to utilization.
- Analyse and describe the standards *ISO14040* and *ISO14044*
- Develop a simplified tool to determine emissions of the ammonia value chain in different scenarios.
- Write a technical report documenting the steps taken to reach the conclusion.

#### 1.4. Method

Throughout the work of the thesis, a large part of the time has been spent doing a thorough literature review. The literature search includes all relevant topics to achieve a high grade of completeness in the thesis, and most of the information and data is collected from previous scientific articles, reports, life cycle assessments, academic supervision, companies, and lecture notes. Most of the scientific articles and reports are found through Elsevier's ScienceDirect and Google Scholar, which both include a large database of revised scientific publications and e-books, which ultimately increases the credibility of the thesis. Otherwise, Google's search function has been widely used, where you may also have access to publications that include relevant and valuable information, but it is vital to evaluate the source's credibility.

While reading publications, there have been a variety of challenges in establishing the reliability and relevance of papers, particularly the article's published year. Even if a study was last modified 5-10 years ago, the data utilized may have been collected 5-10 years earlier. As a result, some data might be up to 20 years old, or even older in some instances, which ultimately affecting the thesis's validity. Processes, technologies, and environmental

requirements are constantly changing and improving, as well as companies nowadays have way more focus on global and local emissions, than 10-20 years ago. This causes a lot of this data to be inaccurate and irrelevant in today's global situation. Data may also be misinterpreted and thus lead to an inaccurate or invalid conclusion.

Various LCA software was utilized as a reference to figure out how to develop a simplified tool for estimating ammonia emissions, with openLCA and Sphera Gabi finally being the preferred ones. OpenLCA is open-source software that does not require a license, but it does come with a limited database inventory. In exchange, OpenLCA Nexus, an online repository for LCA data, NexusLCA offers the ability to import several free and purchasable databases, including ecoinvent [11]. Ecoinvent contains inventory data for international industrial processes such as energy supply, resource extraction, chemicals, waste management, and transport service, and is widely regarded as the most famous and extensive LCA database in the world [12]. Sphera Gabi is a software that can be acquired as an educational license, and since Ecoinvent is included, it was the obvious choice of software to use as a reference through the thesis. Understanding how an LCA software works took some time, as each process has its own set of emissions, inputs, outputs, and flows.

#### **1.5. Report outline**

The thesis is built up of 6 chapters, where Chapter 1 covers the introduction. Chapter 2 is a collection of relevant works that serves as a literature review about ammonia, its value chain, and the emissions associated with each step. Then continuing the literature review section with a breakdown of the standards ISO 14040 and ISO14044 to understand how an LCA is applied to research. In Chapter 3, "Guidance on performing an LCA on ammonia as marine fuel", the necessary steps that must be taken to complete an LCA to determine emissions of ammonia will be explained. Thereafter, in Chapter 4, "Simplified Excel tool to determine emissions", the development of the MS Excel spreadsheet will be explained and how to use it. I Chapter 5, a discussion of the findings is made before a conclusion and further work is given in the final chapter, Chapter 6.

# 2. Literature review

#### Global Warming Potential

Global warming potential (GWP) is a unit that measures the greenhouse gas (GHG) potential of a gas relative to carbon dioxide, hence  $CO_2$  has a GWP of 1. It is a way of measuring of how much energy 1 tonne of greenhouse gas emissions will absorb over a given time period, usually 20 or 100 years, in comparison to 1 tonne of carbon dioxide emissions [13]. GWP values from the Third Assessment Report (TAR) are presented in Table 2.1 [14]. The report will be referring to GWP and  $CO_2$ -equivalents.

Gas	Chemical symbol	Global warming potential (TAR)
Carbon dioxide	$CO_2$	1
Carbon monoxide	CO	1.9
Methane	CH <sub>4</sub>	23
Nitrous oxide	N <sub>2</sub> O	296
Sulphur hexafluoride	CF <sub>6</sub>	22 200

Table 2.1: GWP of different gasses. Third assessment report (TAR) [14]:

The term *carbon intensity* refers to the amount of carbon dioxide emissions, or carbon dioxide equivalents, associated with a product, energy carrier, or electricity.

## 2.1. Introduction to Ammonia

Ammonia consists of nitrogen and hydrogen and is denoted by the chemical formula  $NH_3$ . About 180 million tonne of ammonia is produced annually at a global scale, of which 80% of the production is used to develop agricultural fertilizer. It is also a key element in the production of AdBlue, a chemical used for reducing both  $NO_x$  and  $CO_2$  emissions in diesel-fuelled transport vehicles [15].

Ammonia is usually synthesized through the Haber-Bosch process (HBP). The entire production process from raw materials to pure ammonia is highly energy-intensive and consumed around 8.6 EJ of energy globally in 2020 [16]. Regarding carbon emissions, ammonia production contributes with about 450 Mtonne of CO<sub>2</sub> each year, making it the most carbon-emitting chemical industry process as well as being the world's 16<sup>th</sup> most carbon emitting industry process [17] [16].



Figure 2.1: Comparison of energy density of different marine fuels [18]

With an energy density of 18.8 MJ/kg (LHV) and a boiling point of -33.43°C, ammonia has a great advantage compared to other potential maritime energy carriers such as hydrogen [Figure 2.1]. The chemical properties of ammonia is presented in *Table 2.2* [19] [20]. Ammonia in liquid phase is more energy dense than liquid hydrogen. While hydrogen must be stored at cryogenic temperatures below -252.8°C in liquid state or at a high pressure of up to 700 bar in a gaseous state, ammonia storage requires regular refrigeration below -34°C or a pressure of at least 10 bar [21]. Although ammonia is hazardous to handle and the chemical being very corrosive, it is much less flammable than hydrogen.

Compared to commercial marine fuels, such as heavy fuel oil (HFO) or liquified natural gas (LNG), ammonia does not contain carbon, resulting in the inability to produce  $CO_2$  when combusted [18]. The chemical can also be transported and stored in similar fashion to other marine fuels, as well as having an already established and extensive infrastructure. The transport sector is therefore significantly skilled with handling of the chemical.



Chemical formula	NH <sub>3</sub>
Boiling point (1 atm)	-33.43°C
Condensation pressure at 25°C	9.90 [atm]
Density (liquid)	682 [kg/m <sup>3</sup> ]
Gravimetric energy density (LHV)	18.8 [MJ/kg] / 5.22 [kWh/kg]
Hydrogen content (% by mass)	17.8
Hydrogen density	121 [kg H <sub>2</sub> /m <sup>3</sup> ]
Energy to extract $H_2$	30.6 [kJ/mol - H <sub>2</sub> ]

Ammonia is referred to by colour, like hydrogen, depending on the hydrogen component's production method. The most frequent types of ammonia are gray, blue, and green ammonia, which are explained in *Figure 2.2* [24].



Figure 2.2: Common colours of ammonia/hydrogen [24].

Although the final utilization of ammonia as a fuel is defined as a "carbon-free process", the processes of production and distribution of the chemical for final utilization are not. It makes little sense to use a "carbon-neutral" fuel if the total emissions associated with its production have a greater global impact than the original carbon-based fuel. One can argue for developing technology with higher overall emissions, especially during the start-up phase, but emissions must be reduced in the long run. The value chain of ammonia will be examined in the following chapters, from raw material acquisition to final consumption for propulsion, referred to as a well-to-wake (WtW) perspective through LCA-terminology.

#### 2.2. Value chain analysis of ammonia

A value chain is the collection of actions required to create a final product or service, and it includes all steps from raw material extraction to final use [26].





The most common value chains for low-carbon ammonia as marine fuel are depicted in *Figure* 2.3, which includes the method of production, storage, distribution, and utilization. Because ammonia is produced by the reaction of atmospheric nitrogen with pure hydrogen, the question is how the hydrogen is produced. Natural gas is the major source of hydrogen in today's market, but it can also be made from coal, biomass, and electrolysis. The thesis will only cover hydrogen produced from natural gas and electrolysis, as well as the emissions generated by these pathways.

### 2.2.1. Hydrogen production

Hydrogen is an energy carrier that is rarely found naturally in its pure form, mostly because it is highly reactive and binds easily to other elements. It must be extracted from other materials or other chemical compounds, such as fossil fuels, water, biomass, and ammonia [28]. The total global hydrogen production accounted for approximately 53 Mtonne in 2015, with the distribution of production methods displayed in *Figure 2.4* [29].



Global hydrogen production by source

Figure 2.4: Global hydrogen production by source [29] [30]

Around 40% of all hydrogen produced today is generated as a by-product of processes in which hydrogen is not the primary or intended product. The remaining 60% produces hydrogen as the main product, referred to as *dedicated* hydrogen production. Natural gas is the absolute dominant method of production in today's market, followed by oil, coal, and electrolysis. Hydrogen production from biomass is not common today, but as technology advances, it may become more common and relevant in the future [31].

With current technology it is already viable to dramatically decrease the carbon emissions from hydrogen production, and the drawback being that the processes are more expensive than the alternatives.

There are mainly two pathways to low carbon hydrogen which are SMR with CCUS and electrolysis using renewable electricity. Hydrogen production from coal with CCUS and

hydrogen from biomass might also have a role to play in the years to come, but the report does not take these into consideration.

A report from SINTEF estimates that electrolysis produced  $H_2$  with electricity generated by around 95% renewable power sources it is comparable to natural gas reforming with the use of CCUS measures at a 94% carbon capture rate from the SMR process [32].

#### Hydrogen production from natural gas

Natural gas, mostly consisting of methane, is, as mentioned, the primary source of hydrogen today. To produce hydrogen this way, methane must go through a process of steam-methane reforming (SMR), which consists of several steps, including desulphurization, methane-reforming, shift-conversion, and purification [Figure 2.5].



Figure 2.5: Block diagram of process from natural gas to hydrogen [33]

Desulphurization is performed to avoid any catalyst poisoning of the methane gas during the reforming stage. Through the reforming stage, methane reacts with high-temperature steam, typically around 700°C-1000°C and a pressure at around 3-25 bar, with the presence of a catalyst [34] [35]. Subsequently, an exothermic ( $\Delta H_f^{\circ} < 0$ ) water-gas shift (WGS) conversion is done to maximize the yield of hydrogen and remove biproducts from the reforming. Although the overall

reaction of steam-methane reforming is endothermic ( $\Delta H_f^{\circ} > 0$ ), the necessary energy in the reformation process will be covered by the heat excess created by WGS, as well as by combusting a portion of the methane feedstock [36] [35] [37]. The chemical reactions in SMR and WGS is shown in *Equation 2.1* and *Equation 2.2*.

Equation 2.1: Reaction equation in SMR [38]

 $CH_4 + H_2O \rightarrow CO + 3H_2$ ,  $\Delta H_f^{\circ} = 206.10 \text{ kJ/mol}$ 

Equation 2.2: Reaction equation in WGS [38]

$$CO + H_2O \rightarrow CO_2 + H_2$$
,  $\Delta H_f^{\circ} = -41.15 \text{ kJ/mol}$ 

Since the hydrogen that is produced is not pure enough for either ammonia synthesis or direct utilization in fuel cells, the gas must be purified through methanation or pressure swing absorption [39]. By the second method, the purity of the hydrogen can be nearly 99.99%.

Based on the theoretical demand from *Equation 2.1*. and *Equation 2.2*, the overall process consumes 4.5L of water, although the real amount is higher. This is due to the release of large amounts of energy through the processes, which requires a significant amount of water for steam and system cooling and will thus impact the water consumption [40]. Furthermore, the stochiometric amount of carbon emissions through the processes is 5.5 kg of  $CO_2$  per kg of hydrogen produced.

Input	Value
Water	16.30 L
Electricity	0.49 MJ
Natural gas	3.04 kg
Output	
$H_2$	1.00 kg
$CO_2$	9.21 kg
$CH_4$	$0.0560 \text{ kg} = 1.29 \text{ CO}_2\text{-eq}$

Table 2.3: Inputs and outputs for steam-methane reforming [41] process.

Regarding the actual inputs and outputs for steam-methane reforming of natural gas, E. Budsberg et al. found that for every kg of hydrogen that is produced, the process requires 3.04 kg natural gas, 16.3 L water and 0.490 MJ of electricity as shown in *Table 2.3* The report also estimated that for every kg of produced hydrogen, 9.21 kg of CO<sub>2</sub> is generated, as well as having a fugitive

loss of 0.0560 kg CH<sub>4</sub> [41]. Another article states that an SMR plant of Praxair generates 9.30 kg of CO<sub>2</sub> per kg of hydrogen produced, equal to 0.28 kg of CO<sub>2</sub> per kWh of hydrogen production in terms of energy [42]. A. Elgowainy et al. conducted a literature review of the total emission ratio of CO<sub>2</sub> per kg H<sub>2</sub> in SMR facilities in the United States, which showed an average emission ratio of 9.01 [43].

These different articles and reports do not account for construction and decommissioning of production plants, which also contributes to total carbon emissions through natural gas processing. When considering construction and decommissioning, E. Cetinkaya et al. found that the total emissions were approximately 11.90 kg CO<sub>2</sub>-eq/kg H<sub>2</sub> [44]. It demonstrates that this part of the process has a significant environmental impact, especially when viewed from a life cycle perspective.

Steam reforming of natural gas is an economical process for hydrogen production compared to other technologies. The overall efficiency is usually between 65%-75%, which generates among the highest yield of hydrogen [39] [45]. The cost of operation is often limited by the price of natural gas, with high gas prices resulting in high cost and vice versa. Natural gas is a convenient hydrogen source with a high hydrogen-to-carbon ratio and a well-developed infrastructure, but the reforming produces a significant amount of CO<sub>2</sub>.



Figure 2.6: Carbon capture, utilization, and storage (CCUS) [46]

To reduce carbon emissions, carbon capture, utilization, and storage (CCUS) is a necessary system that needs to be implemented. The technology is based on capturing CO<sub>2</sub> from various industrial processes and power generation processes and is a valuable and important solution to combat climate changes and GHG emissions. Carbon is captured and either utilized for different purposes or transported and permanently stored in geological formations, most commonly saline aquifers beneath the seabed [Figure 2.6]. Permanent storage is a very sensible solution to the climate problem because there are plenty of storage locations around the world, and former oil and gas reservoirs do also meet all requirements to be used for this purpose [47].

Although CCUS is efficient and solves a complex problem of reducing carbon emissions, the technology is expensive [48]. There are currently 20 carbon capture facilities around the globe, accounting for a captured quantity of approximately 43.7 Mt CO<sub>2</sub> [47]. A vast number of capture facilities and networks for large scale carbon capture are in development, e.g., *Langskip* and *Northern Lights* in Norway. The latter will become the first "cross-border, open-source CO<sub>2</sub> transport and storage infrastructure network" when completed [49]. As the technology evolves and large-scale CCUS facilities are developed, it will contribute to a reduction of production costs in the coming years and decades [50]. This will also make the concept of carbon capture much more realistic to implement around the globe.

#### Hydrogen production by electrolysis

Water, H<sub>2</sub>O, is the most abundant source of hydrogen [51]. It can be split to hydrogen and oxygen by the process of electrolysis, where a current is passed through water [52][Equation 2.3]. As of 2020, the global electrolysis capacity is about 0.3 GW, accounting for only 4% of the global hydrogen production. A dramatic increase is projected towards the goal of net zero emission by 2050 [53].

Equation 2.3: Reaction equation of water electrolysis [54]

 $2H_2O \rightarrow 2H_2 + O_2$ ,  $\Delta H^\circ = 285.84 \text{ kJ/mol}$ 

The international energy agency (IEA) is expecting an electrolysis capacity of 180 GW by 2030. In the scenario where Net Zero Emissions by 2050 is achieved, a capacity of 850GW and nearly 3600 GW by respectively 2030 and 2050 is required [55]. This is a scenario in which hydrogen is almost entirely produced using low-carbon technology, with electrolysis accounting for more than 60% of total hydrogen production and natural gas with integrated CCUS accounting for the remaining part.



Figure 2.7: Schematic displayed proton exchange membrane electrolysis (PEMEC) [142]

The process of electrolysis requires both water and electricity; with approximately 9 kg of water producing 1 kg H<sub>2</sub> and 8 kg O<sub>2</sub>, see *Table 2.4*, which is the same for all electrolysis technics. For the operation, a continuous supply of high purity, pre-treated water is required to limit the chances of catalyst poisoning in the electrochemical cell [56]. There are a variety of different water electrolysis cells, including alkaline (AEC), proton exchange membrane (PEMEC) and solid oxide electrolysis cell (SOEC). PEMEC, shown in *Figure 2.7*, is widely regarded as one of the most promising techniques, considering its great efficiency and purity of the hydrogen produced [57].

Table 2.4: Inputs and outputs of electrolysis of water

Input	Value
Water	9 kg
Electricity	39kWh/ $\eta_{el}$
Output	
$H_2$	1 kg
$O_2$	8 kg

The electrolysis efficiency varies depending on the technology, but generally from 60-80%, while PEM can operate at an energy efficiency of 80-90%. Despite its high energy efficiency, electrolysis for hydrogen generation is struggling to be economically viable due to its high energy consumption and limited hydrogen evolution rate [57]. If, theoretically, an electrolyzer

were to be 100% effective, it would require 141.7 MJ (HHV) or 39.4 kWh of electricity to produce 1 kg of hydrogen [58]. At 80% efficiency, the same product quantity of hydrogen would require 56.3 kWh, and 49.3 kWh at 70%. Hence, the hydrogen produced has an energy value of respectively 80% and 70% of that of the electricity used to split the water molecule into hydrogen and oxygen.

Table 2.5: Energy requi	red to produce I	kg H2 and	different ef	fficiency levels	[58]
-------------------------	------------------	-----------	--------------	------------------	------

Efficiency	Energy required to pro	oduce 1 kg H <sub>2</sub>	
$\eta = 100\%$	141.7 MJ	39.4 kWh	
(theoretical)			
$\eta=80\%$	177.1 MJ	49.2 kWh	
$\eta=70\%$	202.4 MJ	56.2 kWh	
$\eta = 60\%$	236.2 MJ	65.6 kWh	

GHG emissions from electrolysis are almost exclusively determined by the carbon intensity of the electricity that is used. The global average carbon intensity of electricity generation was 475 g CO<sub>2</sub>/kWh (IEA) in 2018 and 230 g CO<sub>2</sub>/kWh for the European Union in 2020 [59] [60]. Only 43 g CO<sub>2</sub>/kg H<sub>2</sub> is emitted during the production of the electrolysis units [Figure 2.8] [61].



Fig. 8. Share of GWP (970 g CO2 eq/kg H2) in wind electrolysis.

Generating renewable electricity production releases zero carbon in the process itself but constructing and operating the facilities is a carbon-intensive process, at least with most technology used today, as seen in *Figure 2.8*. Luckily for hydroelectric plants, wind farms, solar farms, geothermal plants, and nuclear plants, the lifetime is so long and the production of electricity so large that this only accounts for a small amount. This is again largely dependent on the source of materials, size, environment, and other factors. For example, for the construction of photovoltaic farms about 84% of the total energy consumption was from producing PV modules.

Figure 2.8: Share of GWP from wind electrolysis with alkaline electrolysis [61]

If a tracker system was also to be installed the total energy consumption was to increase by over 65%. A plethora of LCA studies on renewable electricity has been done, and the spread between studies is large, with the varying data mostly dependent on the size of different plants.

Electricity source	Life Cycle GHG Emissions	Life Cycle GHG Emissions
	spread [g CO <sub>2</sub> -eq/kWh]	median [g CO2-eq/kWh]
PV	9.4 -218	52.0
Hydropower	2.2 - 162	8.0
Geothermal	16.9 - 142	20.0
Concentrated solar	14.2 - 203	25.0
power		
Wind power offshore	6.2 - 46.0	12.0
Wind power onshore	1.0 - 82.0	12.0
Wave energy	3.0 - 22.5	7.5
Nuclear	1.0 - 220	15.0
Coal	650 - 1700	980

#### Table 2.6: Comparison of renewable electricity sources [62] [63].

As mentioned, for every kg H<sub>2</sub> produced by electrolysis, about 8 kg oxygen is also generated. The oxygen is primarily a by-product, and if it is not utilized further, it is also regarded as a waste product. On the other hand, oxygen is an important contribution in various applications and industrial processes and can therefore derive from electrolysis with an economical advantage. G. Maggio et al. concluded that the use self-produced oxygen from electrolysis "should be considered as an economically feasible route for hospitals and medical centers", in which it will be used for different medical situations [64]. In another technical report, H. Mohammadpour et al. found that utilizing the oxygen from electrolysis as a replacement for the air that is now used in centralised wastewater treatment facilities, can reduce the total cost of hydrogen production by up to 30% [65]. Other industries that can utilize the waste product from electrolysis, include space industry and fish farming [66] [67].

#### 2.2.2. Compression, storage, and transport of hydrogen

If ammonia is to be synthesized at a different location than where the hydrogen is produced it must be transported. The report will not go into detail of transporting and storing hydrogen, but some key aspects are important to note. *Table 2.7* contains data from an article published in "Journal of Cleaner Production" where various hydrogen transport options are compared from an LCA perspective [33].

OPTION		GWP TRANSPORT [KG CO2-EQ /KG H2]	GWP STORAGE [KG CO2-EQ /KG H2]
COMPRESSION TO 500 BAR	Transport by	1.25 @ 100 km	0.03
COMPRESSION TO 100	Transport by	3.06 @ 400 km 0.35 @ 10 t/day	0.03
BAR	pipeline	0.15 @ 10 / day 0.16 @ 40 //day	0.03
LIQUID ORGANIC	Transport by	0.17 @ 80 t/day (400km) 3.40 @100 km	0.03
HYDROGEN CARRIER (LOHC)	truck	4.28 @ 400 km	

Table 2.7: Comparison of transport and storage methods of hydrogen [68]

#### 2.2.3. Haber-Bosch process

Global ammonia production is mostly based on the Haber-Bosch process, which has been one of the most successful and impactful inventions in human history, because it made it possible to produce "bread from air", as the chemical is mainly used to produce fertilizers [69]. It facilitated the dramatic increase in the world population and made sure the growing population could be sustained. Although the process was and still is, important to society, it accounts for about 1.6% of the global CO<sub>2</sub> emissions, mainly because natural gas is the primary feedstock for the process in today's market [59] [70].

The process was fully developed in early 1900 by Fritz Haber and by Carl Bosch, and is still the leading production method of ammonia, although lots of adjustments and efficiency improvements are done. In the 1930s, the process required an energy magnitude of about 100 GJ/ton NH<sub>3</sub> and has since been optimized to only consume 26-36 GJ/ton NH<sub>3</sub> [32] [71] [56]. Of the various methods of producing ammonia, the Haber-Bosch process is the only method of production that will be discussed in the thesis [15].



Figure 2.9: Simplified schematic of the Haber-Bosch process. Illustration by author.

The synthesis of ammonia is done by reacting nitrogen from cryogenic air separation and hydrogen from either SMR or electrolysis over several rows of iron-based catalysts. In general, the synthesis efficiency is heavily influenced by the reaction rate and the equilibrium reaction that follows the principle of Le' Châteliers [72][Equation 2.41].

Equation 2.41: Ammonia synthesis

 $N_2 + 3H_2 \rightarrow 2NH_3, \Delta H = -92.0 \text{ kJ}$ 

To maximize the yield of ammonia, the synthesis is performed at a temperature between 350-500°C and a pressure of about 10-30 MPa [Figure 2.9]. For the reaction to be efficient enough, the presence of an oxide-promoted magnetite iron-catalyst and the high temperatures, are needed [70] [72]. The high temperature and pressure have the disadvantage of facilitating for a low equilibrium pass conversion, where the efficiency of each pass is around 15%. Recycling of unreacted hydrogen and nitrogen is therefore a necessity, which eventually alters the overall conversion to 99% of the supplied hydrogen energy [32] [73][27].

Electricity-based HBP has and estimated power consumption of about 1 MWh/t-NH<sub>3</sub>, which includes a hydrogen compressor (182 kWh/t-NH<sub>3</sub>), N<sub>2</sub>/H<sub>2</sub>-mixture compressor (416 kWh/t-NH<sub>3</sub>) and the mixture heating (403 kWh/t-NH<sub>3</sub>). The nitrogen generator is estimated to have a power consumption of about 200 kWh/t-NH<sub>3</sub> [32].

#### 2.2.4. Storage and distribution

Due to ammonia being one of the most used chemicals globally, the infrastructure for production and distribution is already mature and extensive. It also has the potential to be adapted for a wide range of new and exciting applications. However, the infrastructure will need to evolve as the chemical's production volume, as well as its distribution, are set to grow rapidly in years to come [74]. It is still worth mentioning that there are some challenges because of the chemical's properties.

Anhydrous (waterless) ammonia, commonly known as pure ammonia, can induce stress corrosion in steel tanks. This is referred to as "ammonia stress corrosion cracking," and it can typically be avoided by adding a small amount of water (0.2%) to the chemical concentration [75].

Cleaning ammonia tanks may be required before a transport vehicle or vessel is returning either with or without cargo, or with a different chemical or gas. Apart from washing tanks with freshwater, which has an assumed negligible energy consumption, no information or data on this issue was available. It has therefore not been included the thesis.

#### Storage

There are essentially two methods of storing ammonia in its liquid phase. Either pressurized or refrigerated below -33.43°C with atmospheric pressure. Although the storage tanks of ammonia are insulated when it is refrigerated, an amount of heat is transferred from the environment, which ultimately in vapor formation and increased pressure. This is referred to as boil off gas (BOG). The pressure must be released to avoid structural damage and is usually released to a separate container where it can be recycled back into the original tank. Insulated ammonia tanks are designed to keep a low BOG rate. A daily rate of 0.01% of total energy is lost which is significantly lower compared to LNG [76].

#### Distribution by truck

When transported by truck, ammonia is usually pressurized in steel tanks built to withstand pressures up to 18 bar. The weight constraints of roadways are the limiting factor for tank size. A truck and trailer combination is limited to 60 tons per EU standards. Trucks typically have a capacity of 13-56 m<sup>3</sup>, with the most frequent size being between 30-45 m<sup>3</sup> [77] [78].

Based on an average load of 80% of maximum and 25% empty runs, 62.0 g CO2/tonne-km is utilized as a carbon emission estimate for truck transportation [79]. Empty runs, also known as *deadhead mileage*, is when a vehicle returns from a site without a cargo load.

#### Distribution by rail

Most of the ammonia is today moved on rails in tank cars. In the same way as trucks, pressurized tanks are used, but usually with a larger capacity, specifically up to 130 m<sup>3</sup> [77] [78]. Emission factors for rail distribution varies greatly between countries due to differences in carbon intensity of electricity and the use of fossil-powered trains. Global rail distribution emissions are estimated to be around 22g CO<sub>2</sub> /tonne-km. [79].

### Distribution by ship

For ship transport, ammonia is usually refrigerated during the voyage, using large, spherical tanks are with a capacity of between 15 000-85 000 m<sup>3</sup> gas. These carriers are usually equipped with systems for reliquefying boil-off gas during the voyage. For shorter voyages, pressurized tanks or semi-refrigerated ships can be used, which have a capacity of up to 5000 m<sup>3</sup> gas [32] [27].

Emission factors for seaborne transport is estimated to be 16.0 g CO<sub>2</sub>/tonne-km for short-sea shipping and 8.4 g CO<sub>2</sub>/tonne-km for deep-sea shipping [79]. Intercontinental routes are regarded as deep-sea shipping.

### Distribution by pipeline

Pipelines carrying liquid ammonia are normally pressured at roughly 13 bar. Although liquid ammonia pipelines have been in operation for almost 70 years, they are not widely used outside of the United States. Only one pipeline in Europe is longer than 25 kilometres and has a capacity of 900 tonnes per day and is in Italy. Nustar Energy, for example, has a 2000-mile pipeline system that carries 1.5 million tonnes of ammonia per year [80] [81].

In terms of the emission factor for pipeline distribution of ammonia, data on pipeline transit was insufficient. The estimated quantity is 5 g CO2/tonne-km, however the real amount is likely lower, depending on distance [79].

### Bunkering

A fuel must first be loaded in a vessel's tank before it can be utilized for propulsion. The infrastructure for ammonia bunkering is currently inadequate and will continue to remain so until the technology evolves. Bunkering of ammonia is expected to be similar to that of LNG, shown in *Figure 2.11*, but less energy intensive to retain in liquid state [82]. While ammonia has roughly half the energy density of LNG, this does not imply that ammonia tanks require twice the capacity to store the same amount of energy [Figure 2.1 on page 5].



Figure 2.11: The four different bunkering methods for LNG [138]

Because of the toxicity of ammonia, specific precautions must be taken to ensure that it is handled safely. Although ammonia venting or leakage has no direct impact on GWP, due to ammonia not being a GHG, it is toxic for both ecosystems and humans, and may be fatal.

The required energy for the process of bunkering is assumed to be exclusively considered as the energy for pumps and reliquification at 80kWh/t-NH<sub>3</sub> [32].

#### 2.2.5. Ammonia as marine fuel

The final stage of the ammonia value chain as a marine fuel is the utilization for propulsion of a vessel. There are mainly three ways to utilize ammonia, with advanced fuel cells serving as the alternatives to combustion engines with the chemical as fuel. Every solution has its own set of advantages and disadvantages, with one of the most significant being that using a fuel cell rather than a combustion engine is better for the environment as it does not generate environmental-hostile emissions. The system has an efficiency factor that specifies how much fuel is required to deliver 1 kWh of energy in each of the technologies. As ammonia's energy density (LHV) is 5.22 kWh/kg, a 70% efficient system would require approximately 0.27 kilogram of ammonia for every kWh of supplied energy [Table 2.2: Properties of ammonia ].

A fuel cell is based on converting chemical energy to electrical energy in the same way as a battery. The operational process of a fuel cell is regarded as a reversed electrolysis and unlike a battery, the fuel cell can produce electricity continuously while fuel is available and supplied continuous [83]. Furthermore, compared to internal combustion engines (ICE), it requires significantly less maintenance, as a fuel cell has no moving parts that are subjected to heavy loads, in addition to operating at a higher thermodynamic efficiency [84]. The overall efficiency of a fuel cell is therefore much greater than that of an ICE.

Fuel cells are frequently divided into two categories based on the temperature at which they operate, where low-temperature fuel cells (LTFC) operate at temperatures below 200°C, while high temperature fuel cells (HTFC) operate at temperatures up to 1100°C [85]. Alkaline (AFC), proton exchange membrane (PEMFC), and solid oxide fuel cells (SOFC) are the most common types of fuel cells, and differ in their properties and preferred parameters, and thus in their applications.

### Low-temperature fuel cell and cracking

The main LTFCs are AFC and PEMFC, which both have a drawback of only being able to use hydrogen gas as the feedstock fuel. Both fuel cells are extremely sensitive to contaminants, necessitating a high level of purity. In the case of PEMFC, platinum is mostly used as a catalyst due to its high reduction activity and stability [86] [87]. Although the average amount of platinum is between 30-60 g per fuel cell, depending on the manufacturing, platinum is a very expensive material, resulting in a high cost of production compared to AFC [88] [89].

In the combination ammonia and a low-temperature fuel cell, the process of utilizing ammonia's hydrogen content is mainly carried out in two steps. Ammonia must first be decomposed and divided through a cracking process, in which nitrogen and hydrogen are produced. The ammonia cracking is considered as the reverse reaction of the ammonia synthesis, and the hydrogen is then used as feedstock for the fuel cells [90] [91] [19]. The cracking is an energy-intensive process with a loss of about 12,4%, according to a SINTEF report [32]. The process also requires about

400 kWh/t NH<sub>3</sub> cracked, and renewable electricity will hence be the preferred source of energy [92].

#### High temperature fuel cell

The solid oxide fuel cell is the most widely researched HTFC, operating at temperatures ranging from 500 to 1000°C. The high temperature-operation enables the injected fuel to reform internally in the electrochemical cell, which is a significant benefit for this fuel cell compared to other LTFC [93] [94] [95]. This removes the need for a precious-metal catalyst at the cathodes, reducing costs and allowing the use of a wide variety of fuels, including ammonia [85]. At temperatures above 1200°C, a phenomenon known as *thermal NO<sub>x</sub>* can lead to NO<sub>x</sub> formation, but this has not been considered by the report, although it is worth noting [96] [97].

HTFC are some of the most efficient fuel cells for generating electrical energy, with electrical efficiencies usually ranging from 60-70% [90] [91]. This indicates that approximately 1.67-1.43 kWh of fuel must be consumed for every 1 kWh of electrical power delivered.

Solid oxide fuel cells are often characterized as either SOFC-H or SOFC-O, depending on whether it is hydrogen or oxygen that is transported through the fuel cell membrane. A. Afif et al. found through a comprehensive review of ammonia-fed SOFCs, that the efficiency of ammonia-fed SOFC-H is about 10% higher than that of the SOFC-O, as well as having a much greater equilibrium potential. The review also stated that the SOFC-H have up to 30% higher peak power density than that of SOFC-O, and concluded, based on the findings, that the ammonia-fed SOFC-H is the "most promising energy source for next-generation fuel-cell technology" [98]. However, the technology is not yet ready for commercialization with the lack of maturity, since further research is needed to resolve remaining problems before it can be implemented in practical applications. To advance the technical maturity, cost reduction, enhanced operational control, and increased durability must all be achieved [99].

#### Combustion

Ammonia used in combustion engines has lately seen an increase in attention. It is not a new phenomenon since ammonia was already used to power buses in Belgium during World War 2 [100]. Ammonia is not as potent for combustion as fossil fuels, meaning the energy content of ammonia is much lower, as well as having a very narrow flammability range. Due to ammonia's nitrogen content, the release of NOx-exhaust gases from combustion must be considered. Generally, combustion engines have an efficiency of 20-40% depending on the type of engine and fuel used, as it is produced by combusting nitrogen and oxygen.

"The most efficient combustion engine" that is commercially available has an efficiency of just over 50 percent [101]. Ammonia is not commonly used in combustion engines, and no data is
available, thus accurate efficiency estimates are not available. This is expected to change in the coming years as the field is seeing increased interest and research [102].

#### 2.3. Life cycle assessment description

A life cycle assessment (LCA) is a methodology used to address both the real and potential environmental impact of a product or service throughout its life cycle [103] [104]. The assessment includes every aspect of a product's life cycle and is based on the fact that all the steps in the cycle can affect the environment in many ways, from the acquisition of raw material through production, the usage phase and finally what happens to the p3roduct when it is no longer in use [103] [105]. The different stages of a product's life are shown in *Figure 2.12*.



Figure 2.12: Different stages of a product's life cycle [105].

#### 2.3.1. LCA Perspectives

The assessment method is most often applied in a cradle-to-grave perspective, but also as cradle-to-gate, cradle-to-cradle, gate-to-gate, or gate-to-grave perspective, depending on what the analysis is accounting for or what the objective is [106]. *Figure 2.13* illustrates the different perspectives.



Figure 2.13: The different perspectives for a product life cycle [107].

The cradle-to-grave perspective is defined as a full LCA, from the resource extraction, "cradle", to the use phase and eventually the disposal phase, "grave" [108]. As for ammonia as a marine fuel, the "cradle"-phase would be the hydrogen extraction from natural gas and/or water through respectively steam reforming and/or water electrolysis. The "grave"-phase would then be defined as the consumption of ammonia as the fuel for marine vessels.

A cradle-to-cradle assessment has an alternative cradle-to-grave perspective where it is also accounted for recycling. The recycling is here done as the end-of-life disposal step of a product or service, and the method is commonly used to minimize the environmental impact of the product, in addition to ensuring a sustainable production, operation, and disposal [109] [110].

When conducting an LCA, the partial LCA methods of cradle-to-gate and gate-to-gate, often results in a full and comprehensive LCA report if each step is linked in their appropriate production chain [111]. Cradle-to-gate only addresses the life cycle of a product from raw material to the factory gate, the step before the product is transported to consumer. A gate-to-gate LCA only account for one value-added process in the entire production chain [112].

The International Organization for Standardization (ISO) provides principles and framework through ISO 14040 and guidelines and requirements through ISO 14044 [103] [104]. Regardless of how the LCA is conducted or which approach is used, the assessment should always include, as shown in *Figure 2.14*, the four phases [103]:

- 1. Goal and scope definition
- 2. Life cycle inventory analysis (LCI) phase
- 3. Life cycle impact assessment (LCIA) phase
- 4. Interpretation



Figure 2.14: Phases of LCA [103].

The life cycle assessment can be applied in a variety of cases, and as described in ISO 14040, a LCA can assist in [103]:

- identifying opportunities to improve the environmental performance of products at various points in their life cycle,
- informing decision-makers in industry, government, or non-government organizations,
- the selection of relevant indicators of environmental performance, including measurement techniques, and
- marketing

#### 2.3.2. Goal and scope definition

The goal and scope definition is the first stage of a LCA, and it's in this section that the studied system and the purpose of the study is described. The goal states what the intended application of the assessment is, why it is studied, and to whom the results are intended for [103].

After the assessment goal is stated, the scope should be defined. The scope includes all the relevant information regarding the data of the studies and that it is "sufficiently well defined to ensure that the breadth, depth, and detail of the study are compatible and sufficient to address the stated goal" [103].

The functional unit and system boundary are important modelling specifications that need to be determined through the scope. All other data of products or services in the system whose impact is assessed is compared to the functional unit [113]. To fulfill the intended function, it is important to determine the reference flow in each product system, with the system boundary constituting all the unit processes that are included in the evaluated system, see *Figure 2.15*. All assumptions, limitations, and restrictions throughout the system will also need to be stated in the scope section [103] [113].



Figure 2.15: Example of a product system, including the elementary product flows and the system boundary [103].

## **2.3.3.** Life cycle inventory analysis (LCI)

The life cycle inventory analysis is the second phase of an LCA, and it involves gathering, identifying, and quantifying all the data in a product system as inputs and outputs. The inputs include all resources that is used, such as energy, electricity and raw material, and the outputs will be the products, by-products, and various emissions that are generated from the system, products and co-products, waste, and other environmental aspects throughout the system [103] [114] [115]. The various inputs and outputs, as well as the processes in between, are displayed in *Figure 2.16*.



Figure 2.16: Inputs/outputs from LCI displayed schematic [116]

Validation of the collected data, as well as the source, is essential when using the LCI. This is due to the data's accuracy and the assessment's overall thoroughness and comprehensiveness. The data quality is also important to the person or company who acquires or requires the results of the life cycle assessment, particularly regarding the report's strength [103].

The allocation of flows and releases is of great importance in the LCI, as "few industrial processes yield a single output or are based on a linearity of raw material inputs and outputs. In fact, most industrial processes yield more than one product, and they recycle intermediate or discarded products as raw materials" [104].

#### 2.3.4. Life cycle impact assessment (LCIA)

After the LCI, comes the LCIA. This is where the results from the life cycle inventory are analysed for potential environmental impacts, by converting the results into understandable impact indicators [117]. The impact assessment consists of several steps, where the selection of impact categories, category indicators and characterization models, and classification for indicator results are mandatory. There is also the optional elements of normalization, grouping and weighting, indicated in *Figure 2.17* [103]. These elements are usually conducted and simplified through a LCA software, where it is only necessary to select impact categories and category indicators.



#### LIFE CYCLE IMPACT ASSESSMENT

Figure 2.17: Elements of the LCIA phase

The impact assessment considers the actual impact on humans, ecosystem, and resources, rather than only account for specific quantities, such as amounts of emissions to air/soil/water or fuel consumed through a process [118]. The LCIA can be conducted using a variety of well-developed impact assessment methods, such as CML, ILCD, ReCiPe, and TRACI. Each of these

methods often use different impact categories, indicators, classification, and characterization through the assessment, and may therefore contribute to different LCA results [119]. Acidification, global warming, and human toxicity are typical impact categories that are often assessed.

### 2.3.5. Interpretation

It is in the interpretation phase that the results from the LCI and LCIA are evaluated and finally summarized. According to ISO 14040 and ISO 14044, the interpretation phase should include the following; identifying significant issues based on the LCI and LCIA results, evaluation of the completeness, sensitivity and consistency, as well as reaching conclusions, defining limitations and provide recommendations [103] [104]. An important aspect of the interpretation phase is that the LCI and LCIA results shall be interpreted in accordance with the goal and scope of the study.

# 3. Guidance on performing an LCA of ammonia

One of the issues with LCA studies is that there lacks a common ground for which impact areas that should be addressed. Data sets from different LCA practitioners include different impact categories. The only impact category that seems to be used by all studies is GWP. The European platform on LCA has therefore developed the International Reference Life Cycle Data System (ILCD) handbook, which aims to provide an in-depth guide on performing LCA studies [120]. However, the handbook is extremely broad and little of which is relevant or important in terms of performing an LCA on ammonia as a fuel.



Figure 3.1: Life cycle perspectives for marine transportation fuels - well-to-wake, well-to-tank, tank-to-wake [121].

As mentioned in *Chapter 2*, the results from the analysis are dependent on the life cycle perspective that is chosen. For marine transportation fuels, one often uses the perspectives of well-to-wake, well-to-tank and tank-to wake as respectively cradle-to-grave, cradle-to-gate and gate-to-grave for marine fuels as shown *Figure 3.1*. Well-to-wake include all steps from harvesting of raw resources and primary energy production, through production, conversion, distribution, storage, and bunkering, and finally the propulsion of the marine vessel [121]. This will be the relevant perspective to use in a life cycle assessment of ammonia as a marine fuel, as well as being the chosen perspective for the report.

The following sections aim to give a simplified understanding of the necessary steps that should be done to complete an LCA regarding ammonia as a marine fuel.

## **3.1. Preparation for the analysis**

- Get familiar with LCA methodology
- Get familiar with ammonia and various production methods
- Review similar studies
- Decide which LCA software to use

Before conducing an LCA, a familiarity to the methodology should be acquired as well as the topic at hand. Similar research should be explored as well. A recommended read for ammonia production is *"Environmental Life Cycle Assessment of Ammonia-Based Electricity*", an article published in *Energies 2021* [108]. More information about this study is shown in Appendix (A1).

For LCA software there are several available software that can be purchased with included databases. OpenLCA is an open-source alternative, although it lacks usable databases and has a limiting graphical interface. Even with the use of purchasable databases, they are limited, and knowledge of the software, processes and flows is required. The user must be able to understand and if necessary, edit inputs and outputs of the different processes.

## **3.2. Define the goal**

When defining the goal, the aim of the study must be set. A specific goal for "Well-to-Eake analysis of ammonia" is shown below in *Figure 3.2* 

#### Goal

• To provide a holistic examination of environmental impacts for ammonia for use as fuel in a specific marine vessel

Figure 3.2 Specific goal for an LCA of ammonia

In addition to this, the following must be included:

- Intended applications
- Method, assumptions, and impact limitations
- Reasons for carrying out the study
- Target audiences
- Which results, if any, is intended to be disclosed to the public

## **3.3. Define the scope**

When defining the scope all parts that will be considered must be clearly explained. This phase is important to do thoroughly as it defines the depth and the breadth of the study, and any errors will have consequences on the results. The functional unit and system boundary will determine if the results can be easily compared to other studies. The scope-phase includes the following:

- Function, functional unit and reference flow
- Life cycle inventory modelling
- System boundary and cut-off criteria
- Life cycle impact assessment methods and categories
- Type and sources of required data and information
- Data quality requirements
- Comparisons between systems
- Identification of critical review needs
- Intended reporting

Specifically for ammonia [Figure 3.3]:

#### Scope

- Primary energy production  $\rightarrow$  NH<sub>3</sub> synthesis  $\rightarrow$  Distribution  $\rightarrow$  Bunkering  $\rightarrow$  Consumption
- Functional units: Impact equivalents per kilowatt hour of energy and per kilogram of ammonia

e.g.: [g CO<sub>2</sub>-eq / kWh], [g CO<sub>2</sub>-eq / kg NH<sub>3</sub>]

• System boundary Figure 3.4 and Figure 3.5

Figure 3.3: Specific scope for LCA of ammonia

## 3.3.1. System boundary

When creating the boundary, it is important to consider every single part of the value chain. The boundary must be drawn to reduce the complexity of the analysis while taking all aspects into consideration.

For an ammonia study, the system boundary is limited to the production and distribution of the feedstock, as well as the production, distribution, and utilization of the produced fuel. As the hydrogen for production of ammonia is produced by different methods, the boundary includes two different scenarios: hydrogen produced from natural gas and by electrolysis. The different scenarios are displayed in *Figure 3.4* and *Figure 3.5*.



 $Figure \ 3.4: System \ boundary \ scenario \ 1 \ - hydrogen \ produced \ from \ natural \ gas. \ Illustration \ by \ author$ 



Figure 3.5: System boundary scenario 2 - hydrogen produced by electrolysis. Illustration by author.

## **3.4. Life Cycle Inventory analysis**

Data must be collected in accordance with the goal, scope and system boundaries. The standard approach is as follows:

- Identifying processes within the system boundary
- Planning data collection
- Data collection
- Validation of Data
- Reference of Data to a Functional Unit
- Compilation of data to a "Life Cycle Inventory"

Figure 3.6 shows what the LCI for a "Well to Wake"-study of ammonia should include.

Life Cycle Inventory: Data collection and validation

- Chemical and physical properties of ammonia (NH<sub>3</sub>)
- Chosen pathway(s) of ammonia
- Energy consumption (of specific marine vessel)
- Emission factors in all areas (Well to Wake)

Figure 3.6: Life Cycle Inventory in "Well to Wake" for ammonia.

## **3.5 Impact assessment**

For the impact assessment, the following must and should be done:

- Classification and characterization (must)
- Normalization (optional)
- Grouping and weighting (optional)

If the data is not intended to be used for comparisons or other valid reasons can be given, normalization, grouping, and weighting can be skipped [121].

According to the ILCD handbook, a complete LCA must consider several impact categories. The following impact categories should thus be examined in accordance with the ILCD handbook:

#### Impact Assessment

- Global Warming Potential (GWP)
- Acidification Potential (AP)
- Eutrophication Potential (EP)
- Photochemical Ozone Creation Potential (POCP)
- Primary Energy Demand (PED), renewable
- Primary Energy Demand (PED), non-renewable.

Figure 3.7: Impact categories in accordance with the ILCD handbook [120]

### **3.5. Interpretation and evaluation**

This phase includes the following:

- Identification of significant issues in the Life Cycle Inventory Analysis results
- Evaluation of results
  - Completeness check
  - Sensitivity check
  - Consistency check
  - Uncertainty check
- Conclusions, limitations, and recommendations

Any issues with the study should be listed and fixed if possible. If the completeness level of the study does not satisfy the scope or goal, either data of higher quality must be used, or the goal and scope must be adjusted.

It is important to identify the processes that are major contributors to the impact assessment. This helps identify which parts can be improved or changes can be used to reduce impacts.

## 3.6. Reporting and critical review

This phase consists of the following:

- Reporting (must)
- Confidential report (can)
- Critical review from independent, experienced reviewer (not required for internal studies)

Finally, the findings of the study must be presented in a technical report that includes unbiased results and procedures that can be replicated. It must be considered that the report can be understandable for a non-technical audience, if they were to use it to make decisions. A confidential report might be included if necessary.

The reviewer must be impartial, knowledgeable about LCA technique, and have competence in verification and auditing of such analysis. In addition, the reviewer should have a technical understanding of the system under consideration.

In the case of "Well to Wake" of ammonia in *Figure 3.8*.

Reporting and critical review of the LCA of ammonia

- A report that includes methods, findings, and conclusions
- Confidential report (could)
- Review by an independent EPD-verifier

Figure 3.8: Reporting and critical review of LCA of ammonia

As stated, the LCA on ammonia must be verified by an independent EPD verifier. A full evaluation of GWP, AP, and EP will generally be adequate for a product to be EPD-approved, but it should be investigated thoroughly if further impact categories will need to be addressed [122].

# 4. Estimation tool for emissions 4.1. Developing the Excel model

The first step was looking at the value chain of hydrogen and dividing the model into sections. From an LCA perspective, the sections A1, A3, A4 and B4 had to be included. These are marked red in *Figure 4.1*, and the sections in the model are named accordingly as shown in *Table 4.1*. A2 was also considered but was only included as an optional extra input for special cases. Equations used in the model is included in Appendix.

Product stage		Construction stage		Use stage				
Raw Materials	Transport	Manufacturing	Transport	Construction	Maintenance	Repair	Replacement	Operational energy use
A1	A2	A3	A4	A5	B1	B2	B3	B4

Figure 4.1: Sections chosen from an LCA perspective marked in red [123].

Section	Process	Comment
A1: Raw materials	Production of hydrogen	<ul> <li>Production from NG with CCS</li> <li>- CCS rate</li> </ul>
		<ul> <li>Production from Electrolysis</li> <li>Electricity source</li> <li>Efficiency</li> </ul>
A2: Transport	• Transport of hydrogen to ammonia synthesis plant	Only added as extra input. Pipeline viewed as only viable option
A3: Manufacturing	<ul><li>Ammonia synthesis</li><li>Nitrogen generation</li></ul>	Nitrogen generation assumed part of ammonia plant
A4: Transport	• Ammonia transport and bunkering	<ul> <li>Transport via rail</li> <li>Transport via truck</li> <li>Transport via ship</li> <li>Transport via pipeline</li> <li>Bunkering</li> </ul>
B4: Operational energy use	• Consumption of ammonia	<ul> <li>Use in high temperature fuel cell (without cracking)</li> <li>Use in low temperature fuel cell (with cracking)</li> <li>Use in combustion engine</li> </ul>

Table 4.1: Sections chosen from an LCA perspective

#### 4.1.1. A1: Primary energy production

The feedstock phase usually considers raw material extraction or generation. In this case, it considers the production of hydrogen from two paths. From an LCA perspective this would be called "Well to gate". Pathway A is by natural gas with CCS and pathway B is electrolysis [Figure 4.2].





Figure 4.2: Section A1: Pathway A and Pathway B. Illustration by author

Emission estimates are calculated per kilogram hydrogen and given both as the unit [g  $CO_2$ -eq /kg H] and [g  $CO_2$ -eq /kg kWh], of which the latter is calculated using the lower heating value of hydrogen. The carbon capture rate is applied directly to the SMR-process. Inputs to the section shown in *Table 4.2*.

Process	Data	Unit	Source
Natural gas extraction	53	[g CO <sub>2</sub> -eq /kg H]	[32]
and transport			
SMR process	10500	[g CO <sub>2</sub> -eq /kg H]	[41]
Carbon capture rate	50-95	[%]	
	(User input)		
Electrolyzer unit	43	[g CO <sub>2</sub> -eq/kg H]	[60]
Electricity carbon	10-60	[g CO <sub>2</sub> -eq/kWh]	
intensity	(User input)		
Electrolyzer efficiency	40-60	[%]	
	(User input)		

Table 4.2: Inputs in section A1: Primary energy production

Emissions from use of water, including pumps, desalination and other water treatment processes has not been considered. This is due to lack of data, and as both pathways consume about the same amount of water. It is also considered to be quite low, if not completely negligible. As both SMR and electrolysis requires a significant amount of water, but no data was available for specific emissions it is thus not considered. Water pumping and treatment is expected to be negligible in comparison to the energy requirements of electrolysis.

Facility construction has not been considered due to lack of data. SMR had data available, but since electrolysis had no data, a comparison could not be made.

#### 4.1.2. A2: Transport of hydrogen

As mentioned, it is assumed that one facility handles both the hydrogen and ammonia production. This is due to high energy demands for compressing, storing, and transporting hydrogen. This section was added as an extra input to make it possible to take either distribution of hydrogen, or other factors into consideration if it should be necessary [Figure 4.3].

Primary energy production total	
Compression, storage and transport of hydrogen	
Special input [g CO2 /kg H]	0

Figure 4.3: Special input for primary energy production section. Cut-out from Excel model

#### 4.1.3. A3: Ammonia synthesis

The ammonia synthesis process is considered in section A3 of the spreadsheet estimation. The inputs are hydrogen and electricity, and the output is ammonia, where the electricity is used for generating nitrogen and for ammonia synthesis via the Haber Bosch-process [Figure 4.4]. The local storage of ammonia has not been considered, as from the data found, the values were negligible. From this process and onward alle emissions are given as [g CO<sub>2</sub>-eq /kg NH<sub>3</sub>] and from the lower heating value of ammonia the unit [g CO<sub>2</sub>-eq /kg kWh] is also derived. All inputs shown in *Table 4.3*.



Figure 4.4: Section A3: Ammonia synthesis

Table 4.3: Inputs section A3: Ammonia synthesis.

Nitrogen generation0.20[g CO2-eq /kg NH3][32]Electricity carbon10-60[g CO2-eq/kWh]	Process	Data	Unit	Source
<i>Electricity carbon</i> 10-60 [g CO <sub>2</sub> -eq/kWh]	Nitrogen generation	0.20	[g CO <sub>2</sub> -eq /kg NH <sub>3</sub> ]	[32]
	Electricity carbon	10-60	[g CO <sub>2</sub> -eq/kWh]	
intensity (User input)	intensity	(User input)		
<i>Energy demand for</i> 1.00 [kWh / kg NH3] [32]	Energy demand for	1.00	[kWh / kg NH3]	[32]
$NH_3$ synthesis	NH <sub>3</sub> synthesis			
Part Hydrogen (From17.7 %Mass balance	Part Hydrogen (From	17.7 %		Mass balance
A1)	A1)			
Part Nitrogen82.4 %Mass balance	Part Nitrogen	82.4 %		Mass balance

#### 4.1.4. A4: Distribution, storage, and bunkering

Distribution of ammonia covers transport, storage, and bunkering. To give a better overview of the processes, section A4 of the spreadsheet was divided into two sub-sections. [Figure 4.5].



Figure 4.5: Section A4: Distribution, storage, and bunkering

#### Distribution

Ammonia is used as both an input and an output in the distribution section. The emissions are almost entirely due to the use of fuel for transportation, in addition to a small amount of energy used for pumps and reliquification. The emissions are determined by the means of transport and the distance travelled, with rail, truck, ship, or pipeline being the considered options, or a combination of these. As the data is based on averages, an input field for other emission values have been added as an option in the model. This means that electric trains, hydrogen-fuelled trucks, and ships that use boil-off gas can all be factored into the calculation. Inputs for this section are shown in *Table 4.4*.

-

Table 4.4: Inputs section A4: Distribution

Process	Data	Unit	Source
Transportation by	Km user input	[g CO <sub>2</sub> /kg NH <sub>3</sub> ]	[79]
ship [km]	(8.4/km)		
Transporation by rail	Km user input	[g CO <sub>2</sub> /kg NH <sub>3</sub> ]	[79]
[km]	(22.0/km)		
Transportation by	Km user input	[g CO <sub>2</sub> /kg NH <sub>3</sub> ]	[79]
truck [km]	(62.0/km)		
Transportation by	Km user input	[g CO <sub>2</sub> /kg NH <sub>3</sub> ]	[79]
pipeline [km]	(5.0/km)		
Unloading/loading	0.08	[kWh/kg NH <sub>3</sub> ]	[32]
pump energy			
Electricity carbon	10-60	[g CO <sub>2</sub> -eq/kWh]	
intensity	(User input)		
Receiving side	17	[g CO <sub>2</sub> -eq/kWh]	[124]
(Norway)			

#### Storage and bunkering

As stated in *A3: Ammonia synthesis*, storage emissions are assumed to be minimal. Because there isn't enough data regarding NH<sub>3</sub> bunkering, it hasn't been considered. Only required pump power for loading/unloading and reliquification has been considered. Inputs shown in *Table 4.5*.

Table 4.5: Inputs section A4: Storage and bunkering

Process	Data	Unit	Source
Unloading/loading	0.08	[kWh/kg NH <sub>3</sub> ]	[32]
pump energy			
Electricity carbon	10-60	[g CO <sub>2</sub> -eq/kWh]	
intensity	(User input)		

#### 4.1.5. B4: Utilization as fuel



Figure 4.6: Section B4: Ammonia used as fuel

The final section is the use phase where ammonia is consumed in a fuel cell or burned in a combustion engine. Ammonia is the input, and the output is energy (kWh) [Figure 4.6]. It is assumed that a high temperature fuel cell will be the choice of use, but options for low temperature fuel cell either with on-board cracking, or cracking using land electricity grid and an internal combustion engine was added for comparison. As mentioned earlier there are no direct emissions in this phase apart from NO<sub>x</sub> when ammonia is burned. The efficiency factor determines how much ammonia is needed per unit of energy.

The different methods of consumption have each been given an indicator 0 = no, 1 = yes. Cracking loss is set at 12,4% and the use of electricity for cracking is user input. This assumes renewable electricity can be used for cracking. NO<sub>x</sub>-emission must be entered manually. Inputs shown in *Table 4.6*.

Process	Data	Unit	Source
High temperature	40-70%	[%]	
fuel cell system	(user input)		
efficiency			
Low temperature	40-70%	[%]	
fuel cell system	(user input)		
efficiency			
Cracking total loss	30%		[32]
(on-board, including			
electricity use)			
Cracking loss	12%		[32]
(process)			
Cracking electricity	0.4	[kWh/kgNH <sub>3</sub> ]	[32]
use			
Combustion engine	10-50%	[%]	
system efficiency	(user input)		
NO <sub>x</sub> -emissions	Unknown	[g CO <sub>2</sub> -eq/kWh]	
	(user input)		

Table 4.6: Inputs section B4.

## 4.2. Using the Excel tool

The first thing that should be noted is the colour codes of the data inputs as displayed *in Figure* 4.7. The "enter data" colour code is the only intended use. The user must choose either blue ammonia (SMR with CCUS) or green ammonia (electrolysis) by typing "yes" into the field of choice. Emission goal should also be filled if a specific goal is in mind. Cut-out from the model shown in Figure 4.8.

For electrolysis the carbon intensity of electricity used must be filled. Common values for different production methods are shown on the sheet, and in *Table 2.6* on page 15. If known, the efficiency of the electrolyzer should also be given.

Colour code
Enter data
Automatic data from input
Calculated data
Automatic data

Figure 4.7: Colour codes for the Excel tool.

If SMR is chosen, carbon capture rate should be given. The carbon intensity of electricity is also used for ammonia synthesis

and should be filled if know. If unknown, it should be determined by grid carbon intensity of country of choice.

User input		
Emission goal	130	[gCO2-eq/kWh]
"Yes" for blue ammonia (Steam reforming and CCUS)		
"Yes" for green ammonia (Electrolysis)	Yes	
Electrolysis		
Efficiency of electrolyzer (Usually 50-80%)	65 %	
Carbon intensity of electricity used	15,00	[gCO2-eq/kWh]
Steam reforming		
Carbon capture rate of SMR (usually 70-95%)	70 %	

*Figure 4.8: User input for Excel model (1/2)* 

Transportation		
Transportation by ship [km]	1369	[kilometers]
Transporation by rail [km]	0	[kilometers]
Transportation by truck [km]	40	[kilometers]
Transportation by pipeline [km]	5	[kilometers]
Propulsion system	"Yes" for choice	Efficiency of system for propulsion
Propulsion system High temperature fuel cell	"Yes" for choice yes	Efficiency of system for propulsion 60 %
Propulsion system High temperature fuel cell Low temperature fuel cell (on-board cracking)	"Yes" for choice yes	Efficiency of system for propulsion 60 % 60 %
Propulsion system High temperature fuel cell Low temperature fuel cell (on-board cracking) Low temperature fuel cell (cracking by land-electricity)	"Yes" for choice yes	Efficiency of system for propulsion 60 % 60 %

*Figure 4.9: User input for Excel model (2/2)* 

Kilometres per means of transport (multiple choices possible) and choice of propulsion system must also be given. "Yes" in the field indicates choice [Figure 4.9]. If multiple choices or no choice is given, an error message will occur.

To give a brief introduction, a hypothetical case could be:

"Ammonia would be produced in Le Havre, France. Electrolysis would be used to produced the hydrogen, with the supplied electricity coming directly from a nuclear power station. Electrolysis (60% efficient) and ammonia synthesis is handled at one facility and is directly linked to the harbour by a 5 km pipeline. The fuel will be transported to Bergen, Norway and used as fuel for a ship docked 40 km (by truck) from Bergen. For propulsion the ship is utilizing a high temperature fuel cell-system at 60% efficiency."

The carbon intensity of nuclear electricity is estimated to be around 15 g  $CO_2$ -eq/kWh. The shipping distance is estimated by a online shipping calculator to be 1369 kilometres.

User input		
Emission goal (if any)	100	[g CO2-eq/kWh]
"Yes" for blue ammonia (Steam reforming and CCUS)		
"Yes" for green ammonia (Electrolysis)	yes	
Electrolysis		
Efficiency of electrolyzer (Usually 50-80%)	60 %	
Carbon intensity of electricity used	15,00	[g CO2-eq/kWh]
Disregard as green ammonia is chosen		
Steam reforming	0.%	
Carbon capture rate or OMR (usually 70-35%)	0 70	
Transportation		
Transportation by ship [km]	1369	[kilometers]
Transporation by rail [km]	0	[kilometers]
Transportation by truck [km]	40	[kilometers]
Transportation by pipeline [km]	5	[kilometers]
Description metam	"Vee" fee sheire	Efficiency of system for
Propulsion system	Tes for choice	propulsion
High temperature fuel cell	yes	60 %
Low temperature fuel cell (on-board cracking)		60 %
Low temperature fuel cell (cracking by land-electricity)		60 %
Combustion engine		30 %

Figure 4.10: User input from specific scenario. Cut-out from Excel.

The parameters filled are thus [Figure 4.10]:

- "Yes" for green ammonia: Yes
- Efficiency of electrolyzer: 60%
- Carbon intensity of electricity used: 15,00
- Transportation by ship [km]: 1369
- Transportation by truck [km]: 40
- Transportation by pipeline [km]: 5
- (Emission goal: 100) is also filled, although this is not given.

*Figure 4.11* shows that the illustrated scenario would result in a low-emission fuel for marine vessel. The primary energy production is the main contributor, with propulsion being a close second.

Results		
A1 Primary energy production	34,8	[g CO2-eq/kWh]
A3 Ammonia synthesis	3,4	[g CO2-eq/kWh]
A4 Transport and distribution	5,2	[g CO2-eq/kWh]
A4 Storage and bunkering	0,26	[g CO2-eq/kWh]
B4 Propulsion "contribution"	29,1	[g CO2-eq/kWh]
Total GWP "Well to Wake" estimate	72,8	[g CO2-eq/kWh]
Goal	100	[g CO2-eq/kWh]



Figure 4.11: Results from simulation. Cut-out from Excel model.

The "Calculations" tab, shown in Figure 4.12, would have to be examined to understand how the results are calculated in each section. The hydrogen is produced from a 60% efficient electrolyzer, with the input of 15.0 g CO<sub>2</sub>/kWh. Eventually, pure hydrogen with a carbon intensity of 1028.0 g CO<sub>2</sub>/kg H2, or 30.8 g CO<sub>2</sub>/kWh, is achieved.

Calculations	1							
A1							_	
Primary energy production (Hydrogen)	Input	-20 %	-10 %	Baseline	10%	20%	CO2 emission	per mass of product
		-	-	[gCO2-eq/kWh]	+	+		
Steam methane reforming (SMR)	0 %							
Electrolysis (El)	100 %							
Electrolysis								
Electricity emission [gCO2-eq/kWh]	15,00	23,6	26,6	29,6	32,5	35,5	985	[g CO2-eq /kg H]
Efficiency	60 %							
Electrolyzer unit [g CO2-eq / kg H]	43,0			1,3			43	[gCO2-eq/kgH]
Electrolysis total							1028	[gCO2-eq <i>l</i> kgH]
Hydrogen mix								
SMR contribution		0,0	0,0	0,0	0,0	0,0	0,0	[gCO2-eq <i>l</i> kgH]
Electrolysis contribution		24,7	27,8	30,8	33,9	37,0	1028,0	[gCO2-eq/kgH]
Total		24,7	27,8	30,8	33,9	37,0	1028,0	[gCO2-eq <i>l</i> kgH]
Primary energy production total		24,7	27,8	30,8	33,9	37,0	1028,0	[gCO2-eq/kgH]

Figure 4.12: Calculations A1. Cut-out from Excel model. SMR-part has been cut to reduce clutter

Following the flow to section *A3: Ammonia synthesis*, the hydrogen part from A1 has been converted to ammonia using the same source of electricity. As shown in *Figure*, the ammonia has a carbon intensity of 199.4 g  $CO_2/kg$  NH<sub>3</sub> or 38.2 g  $CO_2/kWh$ . In addition to the contribution of 3.4 g  $CO_2/kWh$  ammonia and hydrogen has different energy contents which leads to slightly different emission per kWh.

A3							
Ammonia synthesis	Input	-20 %	-10 %	Baseline	10 %	20%	CO2 emission per mass of product
		-	-	[gCO2-eq/kWh]	+	+	
Nitrogen generation [kWh/kg NH3]	0,2						
Electricity carbon intensity [gCO2-eq/kWh]	15,00			0,6			3 [gCO2-eq/kgNH3]
Part Hydrogen (From A1)	17,7 %			34,8			181,4 [gCO2-eq/kgNH3]
Part Nitrogen	82,4 %			0,6			3,0 [gCO2-eq/kgNH3]
Energy demand [kWh / kg NH3]	1,00						
Ammonia synthesis							
Part electric powered	100 %						
Part thermal powered	0%						
Electricity source	15,00			2,9			15,0 [gCO2-eq/kgNH3]
Thermal power source	180			0,0			0,0 [gCO2-eq/kgNH3]
Syntheis total contribution				3,4			18,0 [gCO2-eq/kgNH3]
Ammonia accumulated		30,6	34,4	38,2	42,0	45,8	<b>199,4</b> [g CO2-eq / kg NH3]

Figure 4.13: Calculations A3. Cut-out from Excel model

A4				•					
Distribution	Input	-20%	-10 %	Baseline	10 %	20%	CO2 emission	per mass of	product
		-	-	[gCO2-eq/kWh]	+	+			
Transportation by ship [km]	1369	3,4	3,8	4,2	4,6	5,0	21,9	[gCO2-eq	/kg NH3]
Transporation by rail [km]	0	0,0	0,0	0,00	0,0	0,0	0,0	[gCO2-eq	/kg NH3]
Transportation by truck [km]	40	0,4	0,4	0,5	0,5	0,6	2,5	[gCO2-eq	/kgNH3]
Transportation by pipeline [km]	5	0,0	0,0	0,0	0,0	0,0	0,2	[gCO2-eq	/kgNH3]
Transportation special input [km]	0								
Transportation special input [gCO2-eq/km]	0	0,0	0,0	0	0,0	0,0	0,0	[gCO2-eq	/kgNH3]
Loading electricity source [g CO2-eg/kWh]	15,00			0,2			1.2	[aCO2-ea	/ka NH3]
Unloading electricity source (g CO2-eg/kWh)	17.00		_	0.3		_	1.4	la CO2-ea	/ka NH31
Pump energy requirement (from data) [kWh/kg NH3]	0.08		_			-			
Reliquification included									
Transportation total contribution		4.2	4.7	5.2	5.7	6.2	27.1	la CO2-ea	/ka NH31
Ammonia accumulated		34.7	39.1	43.4	47.7	52.1	226.6	Ia CO2-ea	/ka NH31
		0.00	00,1	דוכד	1121	02,1	220,0	igeor eq	rikgranoj
<b>A</b> 4	1								
Storage and hunkering	Input	-2012	-10 12	Basalina	10 2	20.2			
Storage and bunkering	in poix		-	In CO2-en/Whi	+	+			
Storage				Geor educing					
Assumed pegligible									
Bunkering									
Pump electricity courses [a CO2-call/2/b]	47								
Pump electricity source [g CO2=eqrk wh]	1/			0.00				1.000	U. NU.01
Pump energy requirement (from data) (kWh/kg NH3) Delian/Res/Sectorelated	0,08			0,26			1,4	ig COZ-eq	r kg INH3]
Reliquification included									
Share and have been a state of a state of the state		1		0.00			4.4	1-002 -	LL - NUST
Storage and bunkering total contribution				0,26		_	1,4	ig COZ-eq	rikg (VEI 3]
Ammonia accumulated		34.9	39.3	43.7	48.0	52.4	227.9	la CO2-ea	/ ka NH31

Figure 4.14: Calculations A4: Distribution, storage and bunkering. Cut-out from Excel model

As shown above, in *Figure 4.14*, in the distribution part of the calculation the inputs are 1369 km ship transportation, 40 km for truck and 5 km for pipeline. In this scenario the transportation has a low contribution to emissions where ship transportation is the main contributor. Bunkering is almost negligible. The output flow to B4 has a carbon intensity of 227.9 g CO<sub>2</sub>/kg NH<sub>3</sub>.

	_						
B4							
Operational energy use	Input	-20% -10%	Baseline	10 % 20 %			
			[gCO2-eq/kWh]	+ +			
High temperature fuel cell (1= true)	1						
Efficiency of system [%]	60 %		29,1				
Low temperature fuel cell (on board cracking)	0						
Cracking loss (energy use of cracker included) [%]	30%						
Efficiency of system [%]	60 %		0,0				
Low temperature fuel cell (land electricity cracking)	0						
Cracking electricity source [g CO2-eq/kWh]	17						
Cracking loss [%]	12%						
Cracking energy requirement [kWh/kg NH3]	0,4		0,0				
Efficiency of system [%]	60 %		0,0				
Combustion engine	0						
NOX-emissions [g CO2-eq/kWh]	0						
Efficiency of system [%]	30 %		0,0				
Propulsion total "contribution"		23,3 26,2	29,1	32,0 <mark>34,9</mark>			
Final GWP-value Well to Wake		58,2 65,5	72,8	80,1 87,3			

Figure 4.15: Calculations B4: Operational energy use. Cut-out from Excel model

The final step is the utilization in a vessel, shown above in *Figure 4.15*. For this case, a high temperature fuel cell with a system efficiency of 60% has been chosen. This results in a final well-to-wake impact of 72.8 g CO<sub>2</sub>-eq/kWh which is also shown in the results tab discussed earlier. Propulsion will always have a significant "contribution" as fuel efficiencies above 60% are not common.

# 5. Discussion

## 5.1. Value chain

#### Steam methane reforming

For the two pathways, SMR with CCUS will most likely play a larger role in the coming years. SMR is already a mature technology, and as the technology of carbon capture evolves and improves, implementing CCUS to existing SMR plants seems to be a feasible approach to drastically reduce emissions. There is some data suggesting that SMR plants have a high emission from facility construction and decommissioning, but the data is insufficient to draw a conclusion.

#### Electrolysis

Similarly for electrolysis plants, more data on facility construction and decommissioning is needed. Only production of electrolyser data was found, which was almost negligible compared to the electrolysis process itself.

Electrolysis has the disadvantage of using a significant amount of electricity, which must be sourced almost completely from renewable sources to be a viable option for hydrogen generation. One can argue that it is pointless to allocate electricity for renewable hydrogen generation if other grid consumers must compensate by using more carbon-intensive electricity.

While it may be desirable to use grid electricity for electrolysis, this complicates fulfilling final product emission goals, as this electricity is usually quite high in carbon intensity. Surplus energy from intermittent sources, such as wind during peak power generation phases, should be used. Alternatively, energy from continuous sources, such as hydropower or nuclear, which typically see lower demand or surplus during the night, should then be used instead, at the time of lowest demand.

Because Europe is planning a significant increase in electrolysis capacity, this surplus energy may be reduced in the coming years, increasing the demand for renewable energy alternatives. Offshore wind, remote nuclear plants, and other forms of location restricted energy from countries such as Iceland could therefore prove to be a valuable producer of ammonia by utilizing surplus energy that cannot be used elsewhere.

#### Ammonia transportation

Factories that receive hydrogen and deliver ammonia are unlikely to become more prevalent in the future. Transporting and storing hydrogen is already an energy-intensive process, so delivering hydrogen to a factory, synthesizing ammonia, and then delivering it as ammonia makes little sense. These processes necessitate a significant amount of energy. Pipeline transport may be an option because it has low emissions and essentially connects one facility to another.

Ammonia storage is well known due to the chemical's use as a fertilizer and appears to have a low carbon footprint. If ammonia is stored in a refrigerated state, boil off gas must be recycled

back to the system. As temperatures aren't significantly low, the energy use to maintain these temperatures are minimal. The process of pumping ammonia also consumes a low amount of energy. While these processes are low, having multiple transport sections such as ship, then rail, then truck means the processes must be done several times with different energy sources. This could accumulate more emissions than expected depending on electricity source used for these processes.

Carbon emissions from ammonia transportation are essentially negligible across distances of less than 1000 km, but as distances increase the emissions become more significant. Alternative modes of transport should be considered for long hauls. Trucks powered by hydrogen and ships powered by ammonia boil off will likely be the best options to be uncovered in later research. Instead of having a fixed emission value per kilometre travelled, a BOG-powered NH<sub>3</sub> ship would consume a small amount of cargo every day, resulting in a nearly negligible distribution emission factor.

Empty run trips have been assumed to contribute around 25% of the total voyage's carbon footprint. When performing a complete LCA, this should be investigated and considered further. It would be preferable if the truck or ship returned with a new cargo, but it would necessitate cleaning of the tanks in between transports, which might affect emissions, depending on the chemicals used and the amount of energy consumed, and therefore should be included in an LCA.

### Ammonia bunkering

Ammonia bunkering lacks infrastructure and is one of the challenges to be addressed before ammonia can be used as fuel. The infrastructure is expected to be in place in the coming years as the demand for ammonia is increasing. This also means more data for the process should be available in the future for performing LCAs. When comparing ammonia bunkering to LNG, the former requires less energy as less refrigeration is needed, but a different approach to leaks and spillage should be considered because of the hazardous properties of ammonia. In the report only the pump energy and reliquification is considered which is a small contributor to the overall picture.

There are three relevant options for propulsion - the use of a high temperature fuel cell is the system of choice, followed by a low temperature fuel cell with cracking. An ammonia-fed combustion engine is being regarded as the least favoured. They all have their own advantages and disadvantages:

- A high temperature fuel cell has a high efficiency, but the entire system should be considered for a complete well-to-wake assessment. As a result, the total efficiency may be lower than anticipated, necessitating the use of additional ammonia for propulsion energy.
- The cracking process required for hydrogen to be used in a low temperature fuel cell results in a significant loss of energy. There is also the aspect of strict regulations for

hydrogen storage if the cracking is powered by grid electricity rather than on-board generated power. This method essentially converts ammonia into a hydrogen carrier, and other less energy-intensive forms of transporting hydrogen should be considered.

• Internal combustion engine efficiencies are generally low, which means that a large amount of ammonia is required to produce the same amount of energy as the alternatives. Furthermore, NOx-emissions must also be considered, due to the nitrogen content of ammonia.

## 5.2. Life Cycle Assessment

The life cycle assessment methodology is a powerful tool for calculating all the greenhouse gas emissions to air, water, and soil. However, it requires a large database of available and updated data. It is also unclear what must be done in order to obtain an official and certified approval.

#### Lack of clarity in use of data in previous LCAs:

This report only considers the GWP generated during the ammonia life cycle, and that data alone is not enough for approval by an independent EPD verifier. If GWP is the only impact category of interest, a different type of verification could be considered. Instead of EPD verification, an independent carbon footprint verification (CFV) could be used to confirm the accuracy of the analysis data and estimated carbon footprint. This would be done in the same way as for EPD, but unlike for an LCA with EPD verification, approval of carbon emissions by CFV is done according to ISO 14064 [125] [126]. This would have to be discussed with the Norwegian Public Roads Administration.

Many LCA studies that have been done previously consider hydrogen production and utilisation, but almost none of them take ammonia as a marine transport fuel into account, as there is simply insufficient data. Particularly for renewable-based ammonia, there appears to be a gap in impact categories other than GWP. Another factor for different studies is that there does not seem to be a common ground for which impact categories are being assessed, leading to results not being comparable.

Not all analyses consider facility construction and decommissioning which suggests it may not be required, but more research is required to confirm whether it could have a significant impact. As more ammonia producing plants utilising either CCUS technology or electrolysis are being built, better data and a better understanding of emissions will be emerging.

Another issue with obtaining data on ammonia production and current LCAs is that the whole process of converting natural gas to ammonia takes place at a single plant. This makes sense, as storing and transporting hydrogen is a difficult process, which ultimately means the final product is less expensive if it is avoided. The cost of production and distribution is critical in determining whether an alternative solution should be developed and implemented.

### Insufficient reliable data in the LCA software

Because LCA software is intended to provide a comprehensive analysis of as many impact categories as possible, MS Excel is difficult to use. There is essentially too much data required, and most of it is not easily accessible. LCA software is also advantageous since it already includes comprehensive databases that cover all necessary flows and impact categories. Databases can also be purchased or imported for free. It is not a given that these databases contain all information needed, and the user should have a general idea of the emissions associated with every step of the chain.

It would have been very helpful if reliable and extensive data for GHG emissions from various processes was easily accessible in LCA software and databases to use in the analysis. It is important to find relevant data through existing life cycle analyses if you don't have access to LCA software. The thesis and Excel spreadsheet are primarily based on input and output values from various assessments, such as analyses of ammonia as a marine transportation fuel and its comparison to other marine fuels, as well as comparative life cycle assessments, which compare different reports and their findings. The life cycle assessments of E. Cetinkaya et al. and A. Rödl et al., in addition to the value chain analysis of Y. Ishimoto et al. and the comparative life cycle assessment of A. J. Boero et al., have all been particularly useful in gathering data.

## Use of excel tool:

The excel tool is very useful in providing a good estimate for emissions in different scenarios and can be used as an early-stage assessment for choosing a distributor. Emissions regarding facility construction and energy usage for water treatment and utilization through hydrogen production have not been included. This will have an effect, albeit small, on the actual emission factor particularly in terms of emissions from building materials, machineries, and maintenance.

## 6. Conclusion and further work

## 6.1. Conclusion

The LCA methodology is a powerful tool for estimating environmental impacts in all areas, but LCA databases have too much data and are not feasible to import to Excel for modelling purposes.

For hydrogen production from the SMR CCUS route, a high amount of carbon capture must be documented to be viable. An increased CCUS-rate requires a higher energy input meaning other emission factors than GWP will be increased and must thus be addressed in an LCA-study.

For hydrogen production via electrolysis, few countries have grid electricity with low enough carbon emissions to be a feasible option. This means dedicated renewable electricity must be connected to the electrolysis plant, and ideally surplus energy should be used.

Unless hydrogen is supplied over a short distance by pipeline, transporting hydrogen to an ammonia manufacturing facility is found to be too energy intensive. As a result, hydrogen and ammonia production should be merged in a single plant.

Ammonia synthesis and nitrogen generation has a low impact on the carbon footprint of the final product. Using grid electricity for this step makes little difference to the total carbon footprint.

Long distance transportation, especially by truck, has a moderate impact on the total emissions generated and alternative fuels should be considered. Sufficient data for ammonia bunkering is lacking and is also not available in LCA-databases, which ultimately makes it difficult to consider this aspect in an analysis.

When using ammonia as marine fuel, the efficiency of the energy system determines the carbon footprint of the whole value chain. A high fuel efficiency factor is crucial for a sustainable value chain.

As of today, an EPD-approval for an LCA of ammonia will not be possible without considering other LCA impact categories in addition to GWP. This may change in the future if the Norwegian Roads Administration changes the requirement to another form of GWP-verification.

The excel tool provides a reasonable estimate of the final product, however there are some unknowns in the facility construction and decommissioning phases. It can't replace a complete LCA, but it can assist to determine whether a potential ammonia source is worth investigating
## 6.2. Further work

Hydrogen distribution and storage can be included in the excel model.

The excel model can be improved to be more accurate if better data for facility construction and propulsion systems can be acquired. Other impact categories can also be imported if data is acquired. NG leakage should be addressed for GWP.

Possibility of considering heat generated in addition to mechanical energy to propeller in propulsion systems should be researched.

GWP from NO $_{x}$  formation in combustion engines and thermal NO $_{x}$  should also be researched further.

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# Appendix

## A.1. Recommended read - Environmental Life Cycle Assessment of Ammonia

The following tables and figures are from an article in "Energies" from 2021. They show LCAdata of different scenarios of ammonia production [127]. *Table A1* shows the different scenarios and their related "tag". *Figure A1* shows the system boundaries for natural gas pathway and electrolysis pathway. *Table* shows the impact categories addressed. *Table A3* shows findings. *Table* shows findings in the impact categories.

Table A1: Abbreviations and descriptions of different scenarios considered [127].

Abbreviation Description

SMR-S-UK	Methane to ammonia via steam methane reforming process, small capacity
	(20,000 t of NH3 per annum) in the UK.
SMR-M-UK	Methane to ammonia via steam methane reforming process, mid-capacity
	(100,000 t of NH3 per annum) in the UK.
SMR-CCS-M-	Methane to ammonia via steam methane reforming process, with carbon
UK	capture and storage, mid-capacity (100,000 t of NH3 per annum) in the UK.
E-W-S-UK	Power to ammonia via electrolysis process, electricity from wind, small
	capacity (20,000 t of NH3 per annum) in the UK.
E-W-M-UK	Power to ammonia via electrolysis process, electricity from wind, midcapacity
	(100,000 t of NH3 per annum) in the UK
E-W-M-MA	Power to ammonia via electrolysis process, electricity from wind, midcapacity
	(100,000 t of NH3 per annum) in Morocco.
E-W-M-AU	Power to ammonia via electrolysis process, electricity from wind, midcapacity
	(100,000 t of NH3 per annum) in Australia
E-PV-M-CL	Power to ammonia via electrolysis process, electricity from photovoltaics,
	mid-capacity (100,000 t of NH3 per annum) in Chile.
E-H-M-BR	Power to ammonia via electrolysis process, electricity from hydropower,
	mid-capacity (100,000 t of NH3 per annum) in Brazil.
E-GT-M-IS	Power to ammonia via electrolysis process, electricity from geothermal,
	mid-capacity (100,000 t of NH3 per annum) in Iceland.
E-N-M-AE	Power to ammonia via electrolysis process, electricity from nuclear, midcapacity
	(100,000 t of NH3 per annum) in the United Arab Emirates.



*Figure A1: System boundary of the ammonia production system. (a) based on natural gas and SMR, (b) based on electrolysis [127].* 

Characterisation Factor	Impact Category	Indicator	Unit
GWP100 - Global	Climate change	Infra-red radiative	kg CO <sub>2</sub> -eq.
warming potential		forcing increase	
FDP- Fossil depletion	Fossil resource scarcity	Upper heating value	kg oil-eq.
potential			
FEP – Freshwater	Freshwater	Phosphorus increase	kg P-eq.
eutrophication potential	eutrophication	in freshwater	
ODP – Ozone depletion	Ozone depletion	Stratospheric ozone	kg CFC-11-eq.
potential		decrease	
POFP – Photochemical	Photochemical oxidant	Tropospheric ozone	kg NMVOC-
oxidant formation	formation	increase	eq.
potential			
TAP100 – Terrestrial	Terrestrial acidification	Proton increase in	kg SO <sub>2</sub> -eq.
acidification potential		natural soils	
IRP – Ionizing radiation	Ionizing radiation	Absorbed dose	kg U235-eq.
potential		increase CLM	

#### Table A2: Impact categories considered [127].

Table A3: Data for impact categories [127].

Scenario Abbreviation	GWP100 [t CO2- eq /t NH3]	FDP [kg oil- eq / t NH3]	FEP [kg P- eq / tNH3]	ODP [ g CFC-11- eq / t NH3]	POFP [kg NMVOC -eq / t NH3]	TAP100 [kg SO2- eq / t NH3]	IRP [kg U235-eq / t NH3]
SMR-S-UK	2.60	1220	0.068	0.167	2.31	1.86	286.42
SMR-M-UK	2.75	1285	0.013	0.172	1.80	1.24	69.51
SMR-CCS-M-	1.12	1359	0.020	0.180	1.89	1.35	102.15
UK							
E-W-S-UK	0.28	68	0.254	0.017	1.20	1.51	7.93
E-W-M-UK	0.24	58	0.220	0.015	1.04	1.30	6.37
E-W-M-MA	0.54	133	0.492	0.034	2.36	2.71	19.89
E-W-M-AU	0.26	58	0.219	0.015	1.04	1.30	6.18
E-PV-M-CL	0.70	214	0.371	0.082	2.84	3.38	18.15
E-H-M-BR	0.66	4	0.020	0.001	0.21	0.27	0.12
E-GT-M-IS	0.27	47	0.116	0.006	0.77	0.85	22.51
E-N-M-AE	0.09	17	0.048	0.005	0.36	0.53	7043.07

### A.2. Equations used in Excel model

Equation A.1: Baseline of emission in Excel model.

Baseline values of the unit 
$$\left[\frac{g CO_2 eq}{kWh}\right]$$
 is derived from  $\frac{\left[\frac{g CO_2 eq}{kg (H_2 \text{ or } NH_3)}\right]}{LHV (H_2 \text{ or } NH_3)}$ 

### A.2.1 Hydrogen production

Steam reforming

Equation A.2: Steam reforming in Excel model

Emission (H<sub>2</sub>) 
$$\left[\frac{g CO_2 eq}{kg H_2}\right] =$$

NG production and transport emission + SMR process emission \*(1 - CCUS rate)

*Electrolysis Equation A.3: Electrolysis in Excel model* 

$$Emission (H_2) \left[ \frac{g CO_2 eq}{kg H_2} \right] =$$

$$Electrolyser unit emission + \frac{Electricity \left[ \frac{g CO_2}{kWh} \right] * HHV hydrogen}{\eta_{electrolyser}}$$

### A.2.2 Ammonia synthesis

Nitrogen generation Equation A.4: Nitrogen generation in Excel model

$$Emission (NH_3) \left[ \frac{g CO_2 eq}{kg NH_3} \right] =$$

$$Nitrogen \ generation \ electricity \ requirement Electricity \ \left[ \frac{g CO_2}{kWh} \right]$$

Ammonia synthesis

Equation A.5: Ammonia synthesis in Excel model

$$Emission (NH_3) \left[ \frac{g \ CO_2 eq}{kg \ NH_3} \right] =$$

$$17,7\% \ H_2 \ emission + Nitrogen \ generation \ emission \ \left[ \frac{g \ CO_2 eq}{kg} NH_3 \right]$$

$$+ \ Energy \ demand \ synthesis \ \left[ \frac{kWh}{kg \ NH_3} \right] * \ Electricity \ \left[ \frac{g \ CO_2}{kWh} \right]$$

$$+ (optional) \ \% \ NG \ thermal \ powered \ * \ thermal \ carbon \ intensity$$

### A.2.3 Distribution and bunkering

*Transportation (mode of transport) Equation A.6: Transportation in Excel model* 

$$Emission (NH_3) \left[ \frac{g CO_2 eq}{kg NH_3} \right]$$
  
= kilometres of transportation method \*  $\frac{g CO_2}{1000 * km * kg NH_3}$ 

*Transportation pump and reliquification Equation A.7: Pump energy and reliquification in Excel model* 

$$Emission (NH_3) \left[ \frac{g CO_2 eq}{kg NH_3} \right]$$
  
= Pump energy requirement \* Electricity production side  $\left[ \frac{g CO_2}{kWh} \right]$   
+ Pump energy requirement \* Electricity recieving side  $\left[ \frac{g CO_2}{kWh} \right]$ 

Bunkering Equation A.8: Bunkering in Excel model

$$Emission (NH_3) \left[ \frac{g CO_2 eq}{kg NH_3} \right]$$
$$= Pump \ energy \ requirement \ * \ Electricity \ recieving \ side \left[ \frac{g CO_2}{kWh} \right]$$

### A.2.4 Operational energy use

This section uses fuel efficiency to determine emissions per kWh.

*High temperature fuel cell Equation A.9: High temperature fuel cell in Excel model* 

$$Emission (kWh) \left[ \frac{g \ CO_2 eq}{kWh} \right]$$
$$= \frac{Ammonia \ accumulated \ \left[ \frac{g \ CO_2}{kWh} \right]}{\eta_{system}} - Ammonia \ accumulated \ \left[ \frac{g \ CO_2}{kWh} \right]$$

*Low temperature fuel cell (on board cracking)* 

Equation A.10: Low temperature fuel cell (on board cracking) in Excel model

$$Emission (kWh) \left[ \frac{g CO_2 eq}{kWh} \right]$$
$$= \frac{Ammonia \ accumulated \ \left[ \frac{g CO_2}{kWh} \right]}{(1 - total \ cracker \ loss \ \%) \ * \ \eta_{system}}$$
$$- \ Ammonia \ accumulated \ \left[ \frac{g CO_2}{kWh} \right]$$

Low temperature fuel cell (land electricity for cracking)

Equation A.11: Low temperature fuel cell (land electricity for cracking) in Excel model

$$\begin{split} & Emission \ (kWh) \left[ \frac{g \ CO_2 eq}{kWh} \right] \\ &= \frac{Cracking \ energy \ requirement \ \left[ \frac{kWh}{kg \ NH_3} \right] * \ Electricity \ recieving \ side \ \left[ \frac{g \ CO_2}{kWh} \right]}{\eta_{system}} \\ &+ \frac{Ammonia \ accumulated \ \left[ \frac{g \ CO_2}{kWh} \right]}{(1 - cracker \ loss \ \%) * \ \eta_{system}} - \ Ammonia \ accumulated \ \left[ \frac{g \ CO_2}{kWh} \right] \end{split}$$

Combustion engine

Equation A.12: Combustion engine in Excel model

Emission (kWh) 
$$\left[\frac{g CO_2 eq}{kWh}\right]$$
  
=  $\frac{Ammonia accumulated \left[\frac{g CO_2}{kWh}\right]}{\eta_{system}}$  - Ammonia accumulated  $\left[\frac{g CO_2}{kWh}\right]$   
+ NO<sub>x</sub> emissions  $\left[\frac{g CO_2}{kWh}\right]$ 

