



DEGREE PROJECT IN CHEMICAL SCIENCE AND ENGINEERING,  
SECOND CYCLE, 30 CREDITS  
*STOCKHOLM, SWEDEN 2019*

# **Environmental Assessment of Electrolyzers for Hydrogen Gas Production**

Comparative LCA of Electrolyzers

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# Abstract

Hydrogen has the potential to become an important energy carrier in the future with many areas of applications, as a clean fuel for transportation, heating, power generation in places where electricity use is not fit, etc. Already today hydrogen plays a key role in numerous industries such as petroleum refineries and chemical industries. There are different production methods for hydrogen. Today, natural gas reforming is the most commonly used. With the growing importance of green production paths, hydrogen production by electrolysis is expected to grow.

Two main electrolyzer technologies are used today; alkaline and polymer electrolyte membrane electrolyzer. High-temperature electrolyzers are also interesting techniques, where solid oxide is under development and molten carbonate electrolyzers is researched. In this thesis, a comparative life cycle analysis was performed on the alkaline and molten carbonate electrolyzer. Due to inaccurate inventory data for the molten carbonate electrolyzer, those results are excluded from the published thesis. The environmental performance of the alkaline electrolyzer technology was compared to that of the solid oxide and the polymer electrolyte membrane electrolyzers. The system boundaries were set as cradle to gate. Thereby, the life cycle steps included in the study are raw material extraction, electrolyzer manufacturing, hydrogen production, and transports in between these steps. The functional unit was chosen as 100 kg produced hydrogen gas.

The results show that the polymer electrolyte membrane electrolyzer has the lowest environmental impact out of the compared technologies. It is also determined that the lifetime and the current density of the electrolyzers have significant impact on their environmental performance. Moreover, it is established that electricity for hydrogen production has the highest environmental impact out of the electrolyzers life cycle steps. Therefore, it is important to make sure that the electricity used for hydrogen production derives from renewable sources.

# Sammanfattning

Vätgas har potential att spela en viktig roll som energibärare i framtiden med många användningsområden, såsom ett rent bränsle för transporter, uppvärmning, kraftförsörjning där elproduktion inte är lämpligt, med mera. Redan idag är vätgas ett viktigt inslag i flera industrier, där ibland raffinaderier och kemiska industrier. Det finns flera metoder för att producera vätgas, där reformering av naturgas är den största produktionsmetoden idag. I framtiden spås vätgasproduktion med elektrolys bli allt viktigare, då hållbara produktionsprocesser prioriteras allt mer.

Idag används främst två elektrolysertekniker, alkalisk och polymerelektrolyt. Utöver dessa är högttemperaturelektrolysörer också intressanta tekniker, där fastoxidelektrolysören är under utveckling och smältkarbonatelektrolysören är på forskningsstadium. I det här examensarbetet har en jämförande livscykelanalys utförts på alkalisk- och smältkarbonatelektrolysören. På grund av felaktiga indata för smältkarbonatelektrolysören har dessa resultat uteslutits från den publika rapporten. Miljöpåverkan från den alkaliska elektrolysören har sedan jämförts med miljöpåverkan från fastoxid- och polymerelektrolytelektrolysörerna. Systemgränserna sattes till vagga till grind. De livscykelsteg som inkluderats i studien är därmed råmaterialutvinning, elektrolysertillverkning, vätgasproduktion och transporter mellan dessa steg. Den funktionella enheten valdes till 100 kg producerad vätgas.

Resultaten visar att polymerelektrolytteknologin har den lägsta miljöpåverkan utav de tekniker som jämförts. Resultaten påvisar också att livstiden och strömtätheten för de olika teknikerna har signifikant påverkan på teknikernas miljöpåverkan. Dessutom fastslås att elektriciteten för vätgasproduktion har högst miljöpåverkan utav de studerade livscykelstegen. Därför är det viktigt att elektriciteten som används för vätgasproduktionen kommer ifrån förnybara källor.

# Acknowledgments

This master thesis was conducted at IVL Swedish Environmental Research Institute. I want to thank my supervisor Cecilia Johannesson at IVL, all your thoughtful advice and valuable knowledge regarding LCA was vital for the completion of this thesis. I also want to thank my second supervisor Tomas Rydberg at IVL for making this project possible, and for appreciated advice during the course of my thesis. Further, I want to thank Sofia Klugman and all colleagues in the LCA group for your support and nice company during my work.

At KTH Royal Institute of Technology, I want to thank my supervisor and examiner Ann Cornell and her colleague Andries Krüger. Your guidance and input on electrolyzer technologies have been very valuable and much appreciated.

Susanne Lundberg, thank you for making this spring as fun as it has been, our walks and fikas were much appreciated breaks in the work. Lastly, a big thanks to all thesis workers at IVL during this spring. I am very happy that this thesis also resulted in so many new friends.

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# Nomenclature

ADP – Abiotic Depletion Potential

AEL – Alkaline Electrolyzer

AP – Acidification Potential

BOP – Balance of Plant

CO<sub>2</sub> – Carbon Dioxide

EP – Eutrophication Potential

GHG – Green House Gases

GWP – Global Warming Potential

HHV – Higher Heating Value

HTP – Human Toxicity Potential

Hybrit - Hydrogen Breakthrough Ironmaking Technology

KOH – Potassium Hydroxide

LCA – Life Cycle Analysis

LHV – Lower Heating Value

MCEC – Molten Carbonate Electrolyzer Cell

MCFC – Molten Carbonate Fuel Cell

NaOH – Sodium Hydroxide

NMP - N-methyl-2-pyrrolidone

NO<sub>x</sub> – Nitrous oxides

ODP – Ozone Depletion Potential

PEMEC - Polymer Electrolyte Membrane Electrolyzer Cell

PGM – Platinum Group Metals

POCP – Photochemical Ozone Creation Potential

PTFE - Polytetrafluoroethylene

PV - Photovoltaic

PVC – Polyvinyl chloride

RES – Renewable Energy Source

Ryton - Polyphenylene Sulfide

SO<sub>2</sub> – Sulphur Dioxide

SOEC – Solid Oxide Electrolyzer Cell

SO<sub>x</sub> – Sulphur Oxides

STP – Standard Temperature Pressure

Zirfon - Polysulfone Bonded Zirconium Oxide



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# Chapter 1. Introduction

Hydrogen has the potential to become an important energy carrier in the future with many areas of applications, e.g. as a clean fuel for transportation, heating, power generation in places where electricity use is not suitable. Already today hydrogen plays a key role in numerous industries such as petroleum refineries, chemical industries, electronics production, and many more. The importance of hydrogen is expected to grow in the following years, as greener hydrogen production paths become further developed, making hydrogen a clean energy carrier. [1]

An interesting application that is topical in Sweden today is the use of hydrogen in steel production which is one of the largest sources of carbon dioxide ( $\text{CO}_2$ ) emissions in Sweden, emitting over 790 000 ton  $\text{CO}_2$  equivalents in 2017 [2], [3]. One step in the steel production process is the reduction of iron ore, which is performed with the addition of coke. This step is connected with emissions of  $\text{CO}_2$  into the atmosphere. [4] The aim for future steel production is to replace the reducing agent coke with hydrogen gas and thereby eventually reach a fossil free steel production. By using hydrogen gas as the reducing agent, water vapor is produced instead of  $\text{CO}_2$ . [5]

The hydrogen gas could be produced through water electrolysis, a process where water is cleaved into hydrogen and oxygen gas using electric energy. To reach a fossil free production of hydrogen gas, an important aspect is that the electric energy used for electrolysis should be produced from renewable sources. [5]

There are several different electrolyzer technologies available for electrolysis. Two main technologies are commercially used today, AEL (Alkaline Electrolyzer) and PEM (Polymer Electrolyte Membrane) [6]. High-temperature electrolyzers are also interesting techniques, where SOEC (Solid Oxide Electrolyzer Cell) and MCEC (Molten Carbonate Electrolyzer Cell) are under development.

In this thesis, two life cycle analyses (LCA) have been performed, on AEL and MCEC. The LCA's have been performed in the software GaBi [7]. In a concurrent

thesis, conducted by Lundberg [8], LCA's of PEMEC and SOEC was performed. The results from all LCA's have been compared in this thesis.

## 1.1 Project Execution

In this section, the aim and objective of this thesis will be introduced. A more thorough description of the goal and scope is given in Chapter 3.

### 1.1.1 Aim

The aim of this thesis is to investigate the environmental impact of electrolyzers by life cycle analysis from a cradle to gate perspective.

### 1.1.2 Objective

The project is divided into the following objectives to meet the aim

- Compare the electrolyzers and evaluate which technology is more environmentally sustainable in the chosen environmental impact categories
- Find environmental hotspots in the electrolyzers life cycle
- Perform sensitivity analysis on aspects identified as relevant

### 1.1.3 Delimitation

The project is limited to investigating the environmental impact of the electrolyzers. In this project, social and economic factors are not investigated, only environmental aspects are considered.

## Chapter 2. Background

In this chapter, some background for this project is given. Moreover, a description of the LCA method will be provided.

### 2.1 Hydrogen

Hydrogen is abundantly present everywhere in our environment. 90 vol% of all matter constitutes of hydrogen. [6] Hydrogen is not present as an individual element. Rather, it is found as a compound together with other elements. The most common form of hydrogen in nature is in water. [9] Hydrogen is the simplest element, consisting of one proton and one electron. [10] In standard temperature and pressure (STP), 0°C and 1 bar [11], hydrogen is present as a gas consisting of two hydrogen atoms. Hydrogen is not a primary energy source, meaning it must be produced from other energy sources such as fossil or renewable fuels. Instead, it is an energy carrier, meaning it can be used to store and provide energy. [6]

Hydrogen has a high energy-to-weight ratio, 33.3 kWh/kg is the lower heating value (LHV). LHV is the heat released when combusting hydrogen and the product water is condensed back into its liquid state. The energy-to-weight ratio of hydrogen is about three times as high as that of gasoline or diesel. However, the flammability of hydrogen is higher than that of gasoline or diesel, and it has a wider flammability range. This means that safety precautions are necessary. Moreover, concern might arise in the public if hydrogen is to be stored for example close to residential areas. However, if hydrogen is kept in a well-ventilated space, there is no explosion risk. [6]

#### 2.1.1 Production Methods

There are several ways to produce hydrogen gas. The main production methods are

through natural gas, oil, coal, and electrolysis. It is estimated that about 48% of the world's hydrogen production is from natural gas, 30% from oil, while coal stands for 18% of the production and electrolysis only 4%. [6]

Gas reforming is a production method when the feedstock is natural gas. This is the cheapest and most established method to produce hydrogen, and it is used mainly within petrochemical industries. When coal is the feedstock, gasification is the main hydrogen production method. With gasification of coal, syngas (mix of H<sub>2</sub> and carbon monoxide, CO) is produced, that can be further processed into pure hydrogen. Using oil, hydrogen is produced in a reforming technique called partial oxidation. In electrolysis, water and electricity is the feedstock to produce hydrogen. In order to reach a sustainable hydrogen production, it is important that the electricity used for the electrolysis is produced in a sustainable matter. [6], [9] The process of electrolysis will be described in more detail in section 2.2.

### 2.1.2 Areas of Use

Today, 55% of the world's hydrogen use is for ammonia production. Almost all ammonia produced is used as fertilizers. 25% of the hydrogen is used in refineries, where one application is the reduction of sulfur content in fossil-based fuels. 10% goes to methanol production, which is then used as a fuel. All other uses of hydrogen share the remaining 10% of the world's hydrogen use. These other applications include industrial use in for example metal alloying, as a reductant within the steel industry, fuel in fuel cell driven vehicles, etc. [12]

## 2.2 Electrolysis

An electrochemical cell typically has two electrodes, an electrolyte, and a separator dividing the cell into two chambers called half-cells. It also contains a power source that adds the energy needed to make the reactions move forward. [6], [9] By

electrolysis, electrical energy is converted to chemical energy [13]. In the power source and electrode part of the electrolyzer, electrons are the charge carriers. In the electrolyte, it is the mobile ions that carry the charge. [6], [9] A schematic overview of an electrolyzer can be found in Figure 1. Often, an electrolyzer consists of several of these cells connected in series or parallel. The series of cells is referred to as an electrolyzer stack.

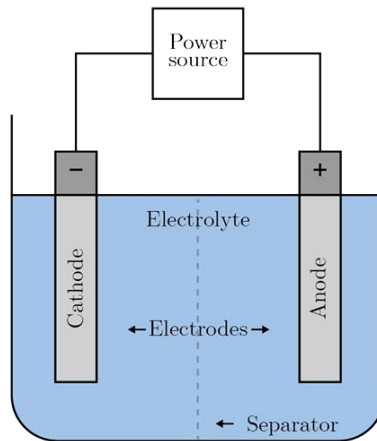
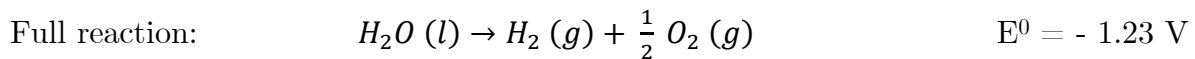
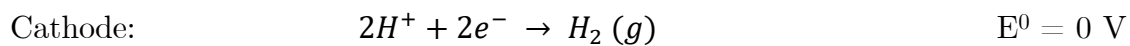
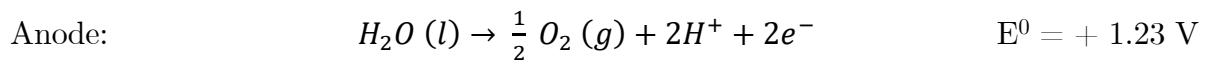


Figure 1. Schematic illustration of an electrolyzer. Inspired by [14].

At the anode an oxidation reaction takes place and at the cathode a reduction reaction takes place. The electrons move from the anode where electrons are emitted to the cathode where the electrons react. In acidic low-temperature water electrolysis, the reactions take place as described in reactions below.



As is readily seen from the above reactions, one mole of water results in one mole of hydrogen produced. At STP, liquid water dissociates into hydrogen and oxygen gas. The reaction is endothermic, meaning it is not spontaneous, but rather needs the addition of energy to occur. Usually, the energy added in electrolysis is electrical energy, but to some extent, it can also be thermal energy in the form of heat. At

STP, heat makes up only 15% of the total energy need for electrolysis to occur, meaning that the other 85% of the supplied energy must come from electricity. If the temperature is raised to 1 000°C, the electric energy needed is reduced to about 65% of the energy demand. This is illustrated in Figure 2 where a clear decrease in  $\Delta H$  and  $\Delta G$  occur at approximately 360 K or about 90°C (0°C = 273.15 K). [6], [9], [15]

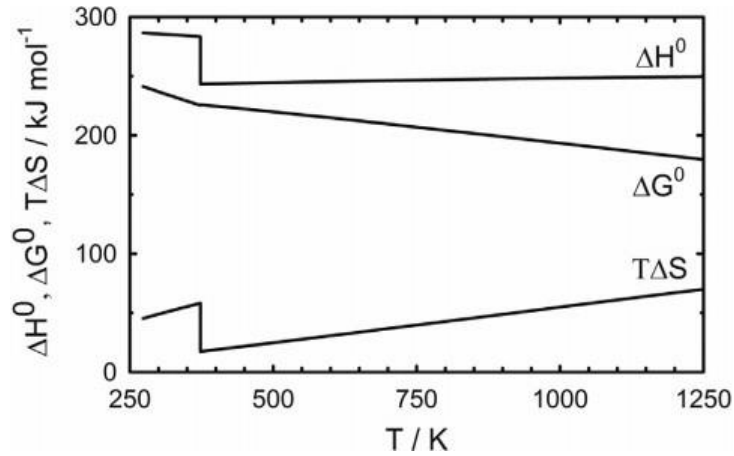


Figure 2. Thermodynamics involved in water electrolysis versus temperature. [14]

Since electric energy is more expensive than heat, high-temperature electrolyzers are interesting technologies with lower operational expenses than conventional electrolyzers. [6], [9], [15]

## 2.3 Life Cycle Analysis

In this thesis, a life cycle analysis has been performed on the alkaline and molten carbonate electrolyzer cells. The method for performing an LCA is well established, it is even standardized by ISO, in the ISO 14040 series [16]. How and when an LCA is used will be described in this section.

An LCA is a holistic take on the environmental impact of a product. That is, the environmental impact of the whole life cycle of a product is compiled and investigated. From raw material extraction to production and assembly, to the whole using phase, and how the product is handled at its end of life. Moreover, transportations in between



these different steps could be included. The steps in a products life cycle are illustrated below in Figure 3. The product can be e.g. a physical object, a process, or a service. [16]

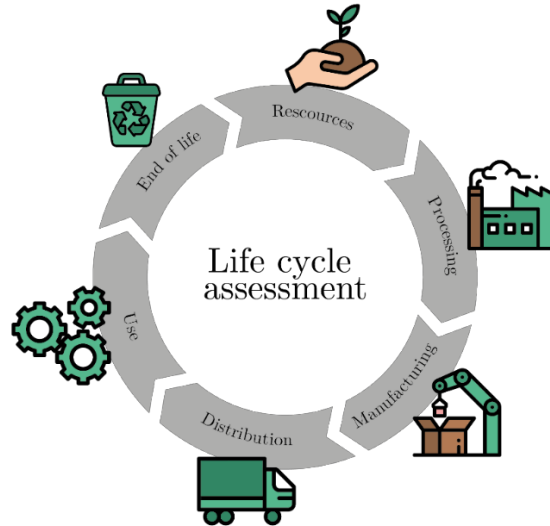


Figure 3. Illustration of a products life cycle. Figure inspired by [17].

In the beginning, the purpose of LCA was to avoid the common problem of environmental impact transfer. [18] One common example of such a transfer is in flue gas treatment. Many methods for cleaning flue gas from emissions results in the same emissions ending up in a water stream instead. Thus, the original problem is solved, but a new problem arises, not necessarily smaller than the original problem. Using LCA is one way to identify the risk of environmental impact transfer and finding ways to avoid it [18]. Other uses of LCA is to choose the environmentally better one out of comparable products, analyze environmental problems that are associated with a product and where that problem originates, or when designing new products. [16]

Some limitations are defined with the LCA method. One is that LCA solely considers environmental sustainability. [16] Economic and social sustainability are not accounted for in conventional environmental LCA, although social LCA and life cycle cost account for these aspects. Another is that the results depend on the decided functional unit and system boundaries, meaning that if several LCA's are conducted on the same product, they can give very different results [16]. Moreover, an important limitation lies in the availability of data. The data collection is a very important part

of the LCA, and it is not uncommon to find that the data is incomplete or incomparable. [16] This means that an LCA often contains simplifications and assumptions. Therefore, it is very important that LCA reports are very transparent, all decisions that might influence the result should be openly stated. [18]

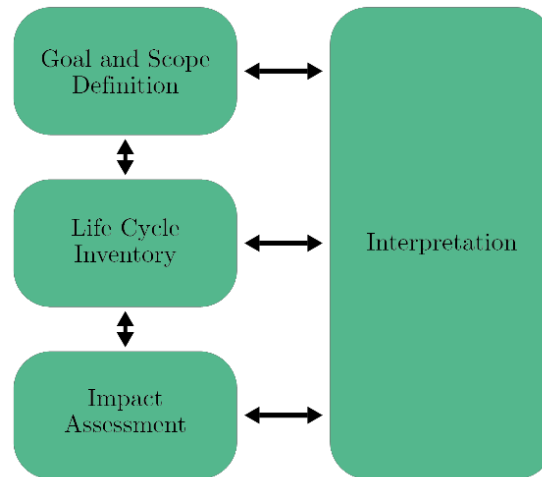


Figure 4. Steps in the LCA method. Figure inspired by [19].

The method of LCA mainly follows four steps, as stated in the ISO 14044; goal and scope definition, inventory analysis, impact assessment, and interpretation, as illustrated in Figure 4 above. [16] What these steps contain will be described below.

### 2.3.1 Goal and scope definition

LCA is an iterative method, meaning that the four steps are not always conducted such that step two follows directly on step one, and only when step two is finished, step three begins, etc. Rather, the process is iterative. However, the goal and scope definition is always the first steps. The goal should be clearly stated early in the project, to help define the scope and limitations. However, it is still common that the goal and scope are revisited and altered along the way of the project. [18]

In the goal and scope definition, the purpose of the study should be stated clearly. Why should the study be conducted? Who should take part in the results? [20] Some aspects that will be important for LCA modeling should also be defined during the

goal and scope definition. Namely the functional unit, system boundaries, how the results should be measured (i.e. which environmental impacts are in focus?), and what data will be needed. [18] The functional unit should represent what the function of the product is and serves as a basis to which material and energy balances are related. If the LCA is conducted to compare two or more products, as is the case in this thesis, it is important that the functional units are the same and that they give a fair comparison of the technologies. [18]

### 2.3.2 Inventory analysis

The inventory analysis is a mass and energy balance to and from the chosen product. It functions as the basis of the environmental impact assessment, and it is therefore important that the inventory is complete and performed in a sound manner. [18], [20] The inventory analysis begins by building a detailed flow chart of the products life cycle. The flow chart should contain all unit processes throughout the production, use, and end of life of the chosen product. In the flow chart, the unit processes are treated as black boxes, having inlet and outlet streams of mass and energy. The inventory analysis then goes on by collecting all the data for the steps in the flow chart. Materials, energy, water, waste, emissions, etc., and their respective amounts should be identified. [18]

A problem that one can encounter while performing an inventory analysis is that different products life cycles are connected. For example, a production process can lead to more products than the one being studied. How should the environmental impact of the production process be divided between the products? This situation is an allocation problem, i.e. how to decide which environmental burdens are associated with the intended product of the study [21]. Allocation means to partition material and energy flows of a process to the studied product. Allocation can, for example, be made by mass or economy. That is, if one product weighs 90 kg and the other product weighs 10 kg, 90% of the environmental burden is allocated to the first product. How

the environmental burden is partitioned can have a significant impact on the results. If allocation is performed, the method should be clearly stated, and sensitivity analysis of the result could be performed. [22]

An important part of the LCA is, as mentioned earlier, to reflect on what consequences the assumptions, simplifications, and choices made throughout the process might have. One way to analyze the consequences is by performing a sensitivity analysis. As the work goes on with the impact assessment and interpretation, something might come up that seems reasonable to make a sensitivity analysis on. The iterative nature of the LCA process is then made use of again, going back to collect more data to be able to perform the sensitivity analysis. [18]

### 2.3.3 Impact assessment

The part of an LCA called impact assessment consists of two steps; classification and characterization. The aim of these steps is to transform the inventory data into information on what impacts the resource use and emissions have on the environment. [21]

The first step, classification, aims to sort the inventory data into categories depending on what environmental impact they cause. Such categories are for example climate change, eutrophication, acidification, etc. In the following step, characterization, the relative impact each emission or resource use contributes to is calculated. For example, in the first step all greenhouse gases (GHG) are classified as contributing to the impact category climate change. The impact that all different GHG contribute to in the category climate change is then summarized by using a certain index, depending on the GHG ability to absorb heat. [21]

### 2.3.4 Interpretation

In the interpretation phase, the results from the impact assessment are summarized and analyzed in relation to the formulated goal and scope of the study. [18] Some conclusions and recommendations should also be set forth based on the study. Any identified limitations with the study should be brought up under the interpretation. The formulation of the conclusions and recommendations are important. A conclusion from an LCA can never be that a product is environmentally friendly or sustainable. The conclusion can only be that, for example, product A is more sustainable than product B. [18]

## Chapter 3. Goal and Scope

In this chapter, the goal and scope of the study are defined. Moreover, the purpose that the study serves is discussed, and some more detail on how the study was performed is presented.

### 3.1 Goal of the Study

The LCA performed in this thesis serves the purpose of filling the gap regarding knowledge of environmental impacts from electrolyzers. No previously published LCA's that compare the AEL, PEMEC, MCEC, and SOEC technologies to each other have been found in the literature study performed within this thesis. By investigating the environmental impact from a cradle to gate perspective, hot spots in the electrolyzer lifecycle can be identified. These hotspots can then be considered when deciding where further research on the electrolyzer technologies should be directed. Additionally, the electricity used to run the electrolyzers has been proven in earlier LCA's to have a significant effect on the results. Therefore, a sensitivity analysis will be performed for different electricity mixes. The goals of this study are summarized in the research questions below.

- Out of the electrolyzers, which technology is the most environmentally sustainable?
- What steps in the electrolyzer lifecycles have the most significant environmental impact?
- How does the electricity used for hydrogen production by electrolyzers impact the results from the LCA?

Since hydrogen is predicted to be an important energy carrier and component in industrial processes in the future, the results of this study might be used to identify which electrolyzer technology is the most suitable to produce hydrogen in the future.

## 3.2 Type of LCA

This study is a comparative, attributional LCA. Comparative LCA compares two or more products with similar applications. An attributional LCA describes the system the way it is and aims to investigate the environmental impact of that system. [23] Input and output flows are allocated to the functional unit and the environmental impact is investigated. [24]

## 3.3 Functional Unit

The functional unit should describe the function of the studied system. Moreover, the functional unit serves as basis for calculations, i.e. all inputs and outputs to the model are related to the functional unit. In a comparative LCA, which has been performed in this study, it is important that the functional unit gives a fair comparison between the technologies. In this study, the functional unit was set as 100 kg produced hydrogen gas. As a result, the expected lifetime and the efficiency of the respective electrolyzers are considered in the functional unit. See further description in Appendix 4.

The functional unit in this study is set to 100 kg produced hydrogen gas.

## 3.4 Data Collection

The data used for the LCA is collected from the literature. A comprehensive literature study has been performed, and the sources with the most detailed and clear inventory data chosen. Some authors of studies who did not entail their LCI were contacted, hoping to achieve more detailed data. For MCEC, certain data were attained in this manner. For further information and collected data, see Chapter 5. Moreover, contact with professor Ann Cornell and postdoc Andries Krüger at KTH Royal Institute of Technology was significant to reach a deeper understanding of the technologies.

### 3.5 System Boundaries

This study focuses on the cradle to gate of the electrolyzers life cycle. In this case, raw material extraction is considered the cradle. The gate is considered as the step where the hydrogen gas is produced. Accordingly, the use of the produced hydrogen and the end of life of the electrolyzers is excluded from this study. End of life is excluded since the knowledge on recycling of materials within the electrolyzers is limited. Additionally, the balance of plant (BOP) is excluded from this study. The system boundary for the LCA is visualized in Figure 5.

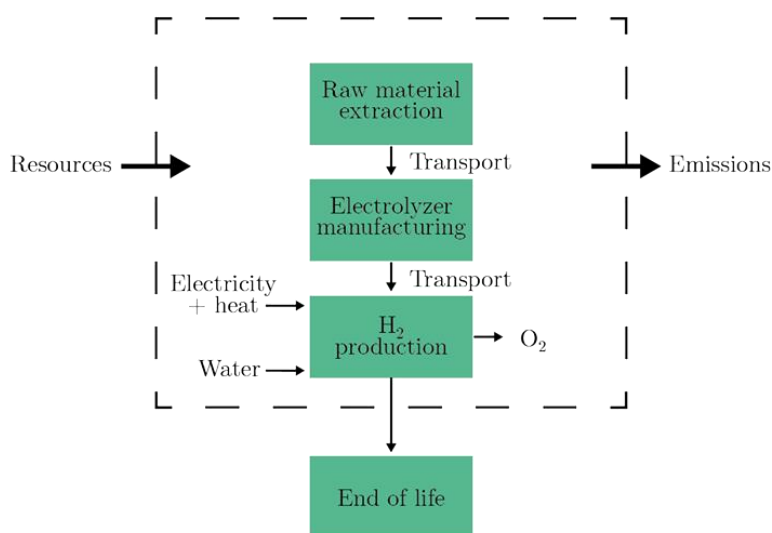


Figure 5. System boundaries for LCA of electrolyzers. Dotted line depicts the system boundary.

Geographically it is assumed that the production of the electrolyzers is set in Germany. Therefore, German grid mix was assumed to be the electricity used for electrolyzer manufacturing. As far as it is possible, average European data will be used in the modeling of the raw material extraction. Moreover, the hydrogen production is assumed to be set in Sweden, using Swedish grid mix as electricity for the electrolysis.



## 3.6 Environmental Impact Categories

In ISO 14044 it is stated that the choice of environmental impact categories to study should reflect the goal and scope of the LCA. The impact categories must, of course, be related to the environmental impacts of the studied system. Other than that, not much guidance on how to choose impact categories is provided in the standard. [25] A report from the Danish Ministry of the Environment states that the recommendation is to consider all impact categories that have reached an international consensus. Impact categories should only be excluded if there are specific reasons in the intended study. [26]

When conducting the impact assessment part of an LCA, there are several different methods available. The methods are developed to relate the results from the inventory analysis to the environmental impact categories in question. Examples of these methods include CML, Recipe, and TRACI. [27] In this study, selected impact categories from the CML method will be used. The CML method includes the following environmental impact categories; abiotic depletion, acidification, eutrophication, freshwater aquatic ecotoxicity, global warming, human toxicity, marine aquatic ecotoxicity, ozone layer depletion, photochemical ozone creation, and terrestrial ecotoxicity [27].

In a book written by Tillman and Baumann describing the LCA method [21], some requirements when choosing impact categories are given, e.g. completeness, practicality, and independence. With completeness, they mean that all relevant environmental impacts of the studied system should be represented by the categories. Moreover, practicality means that the categories should be relatively easy to get an overview of, there should not be too many categories considered. Lastly, independence means that double-counting should be avoided, i.e., the categories should be independent of each other. [21]

FC HyGuide is a report intended to provide guidance when performing an LCA on hydrogen production systems, based on the ISO 14040 series. In FC HyGuide some

environmental impact categories are mentioned that should be used, namely GWP, AP, EP, and Photochemical Ozone Creation Potential (POCP), as well as renewable and non-renewable primary energy demand. Additionally, some impact categories are recommended; ODP, HTP, respiratory inorganics, ionizing radiation, eco-toxicity (freshwater, marine, terrestrial) potential, land use, resource depletion, and water footprint. [28]

In summary, there are recommendations on how to choose impact categories and even which categories are relevant for hydrogen production systems. However, there are no rules stated by the ISO 14040 or 14044 which categories must be used. Therefore, it is ultimately up to the conductor of the study to decide on the impact categories.

In this study, six environmental impact categories are chosen to be included; abiotic depletion (ADP) (elements and fossil), acidification potential (AP), eutrophication potential (EP), global warming potential (GWP) (excluding biogenic carbon), and photochemical ozone creation potential (POCP). These categories are commonly included in LCA studies and corresponds to the recommendation in the FC HyGuide. The environmental impact categories are presented in Table 1, and a short description of the impact categories is provided below.

*Table 1. Environmental impact categories included in this study.*

Environmental Impact Category	Unit	Method
Abiotic Depletion Elements	kg Sb eq	CML 2001
Abiotic Depletion Fossil	MJ	CML 2001
Acidification Potential	kg SO <sub>2</sub> eq	CML 2001
Eutrophication Potential	kg PO <sub>4</sub> <sup>3-</sup> eq	CML 2001
Global Warming Potential	kg CO <sub>2</sub> eq	CML 2001
Photochemical Ozone Creation Potential	kg C <sub>2</sub> H <sub>4</sub> eq	CML 2001

## Abiotic Depletion

Two types of abiotic depletion are included; elements and fossil. Abiotic depletion refers to resource depletion, i.e. reduced stocks of non-living materials such as fossil

fuels, minerals, metals, etc., causing shortages. [29] Abiotic depletion of elements is reported in kg antimony equivalents [kg Sb eq], while abiotic depletion of fossil resources is reported in MJ.

### Acidification Potential

Acidification is caused by acid substances, mostly containing sulphur and nitrogen, being released into nature and disturbing the pH-balance. These emissions mainly derive from burning of fossil fuels. [30] Acidification affects, among other things, water bodies and forests. [29] Acidification potential is reported in kg sulphur dioxide equivalents [kg SO<sub>2</sub> eq].

### Eutrophication Potential

Eutrophication occurs due to excessive amounts of nutrients (phosphorous and nitrogen) being released into nature. The sources of emissions include agriculture and waste water treatment plants. [31] The excess of nutrients causes algae blooming, which in its turn can lead to oxygen depletion in the affected water bodies. [29], [31] Eutrophication is reported in kg phosphate equivalents [kg PO<sub>4</sub><sup>3-</sup> eq].

### Global Warming Potential

Global warming, or more correctly climate change, is the consequence from emissions of GHG, i.e. gases that absorb and emit radiant energy within the infrared spectra. [32] Large contributors to the emissions of GHG is burning of fossil fuels and agricultural production. [29] In this study, a time horizon of 100 years is used for the characterization factors. Biogenic carbon is excluded. Climate change is reported in kg carbon dioxide equivalents [kg CO<sub>2</sub> eq].

### Photochemical Ozone Creation

Ozone is an important part of the Earths stratosphere at about 15-30 kilometers above ground. However, ground-level ozone is an air pollutant which can be harmful for humans, disrupt agricultural production, as well as contribute to climate change

as a GHG. [33] Ground-level ozone is created through photochemical reactions between other air pollutants, such as hydrocarbons and nitrous oxides, and sunlight. [34] Photochemical ozone creation is reported in kg ethene equivalents [kg C<sub>2</sub>H<sub>4</sub> eq].

### 3.7 Simplifications and Assumptions

No primary data were collected for this study. Therefore, the data collection relies on secondary data found in the literature and data gathered through contact with writers of earlier LCA reports. Due to this, this thesis is based on some key assumptions, stated below.

- The aim was to find current data on the technologies; ideally not older than from 2014. However, this was not accessible for the MCEC. Therefore, the sources of data range from 2012-2017. It is assumed that this does not influence the comparability of the technologies.
- For MCEC, it is assumed that the fuel cell counterpart has identical materials and amounts of those materials as the electrolyzer.
- The specific MCFC that the inventory data was retrieved for had a capacity of 135 kW. That is assumed to be converted to 165 kW for the electrolyzer counterpart. How the conversion was made is stated in Appendix 4.
- It is assumed that amounts of materials change linearly with stack size. That is, data for e.g. a 6 MW electrolyzer can be linearly scaled down to 2 MW.
- Data from the different sources are assumed to be comparable, even though the level of detail might differ.
- Production of BOP for the electrolyzers is assumed to have only minor impact compared to stack production, based on the results of [35] and [36]. Moreover, the BOP is assumed to be similar for the four electrolyzer technologies. The BOP is therefore not considered in this study.
- There was no operational data available for MCEC, since the technology is so new. Therefore, operational data for MCEC is assumed to be the same as

for SOEC.

- Some materials in the inventory of the technologies are not available in the program used to build the models; GaBi. Therefore, some simplifications and assumptions had to be made for some of the materials. These assumptions are stated in Appendix 3.
- It is assumed that no parts of the electrolyzers will need replacement during the technical lifetime set in this study. This is further discussed in section 4.6.

## Chapter 4. Electrolyzers

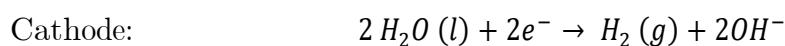
In this chapter, the four electrolyzer technologies investigated in this project are described. Alkaline and molten carbonate electrolyzers are described in depth since these are the technologies that are studied in this thesis. Polymer electrolyte membrane and solid oxide electrolyzers are further described in the concurrent thesis conducted by Lundberg [8]. Moreover, a literature study of earlier LCA's of electrolyzers is presented.

### 4.1 Alkaline Electrolyzer

The alkaline electrolyzer (AEL) is the oldest electrolyzer technology. Already in the early 1900s, the technology was used widely and is still today the electrolyzer mostly used for commercial purposes. [37]–[39] The AEL is still the simplest and most durable technology for water electrolysis. [38] The lifetime of the AEL is around 20-30 years or between 60 000-100 000 hours of operation. [37], [39], [40] Operating temperatures range from 40-90°C, most commonly around 60-90°C. [37]–[40]

#### Reactions

In the alkaline electrolyzer, water is oxidized at the anode and reduced at the cathode according to reactions as given below.



#### Materials

In this section, a brief introduction to the main materials used for the AEL will be given. A more thorough investigation of the materials will be performed in Chapter 5. The alkaline electrolyzer got its name from the alkaline media acting as the electrolyte. Typically, potassium hydroxide (KOH) or less commonly sodium

hydroxide (NaOH) is used as the electrolyte. [6]

The electrodes in the AEL must endure the corrosive environment that the electrolyte cause. It should also act as a suitable catalyst for the reactions taking place on its surface. Platinum is an example of a material that would be fit for the purpose, but due to its very high price, it is not used within the AEL. [37], [38] One main advantage of the AEL is that it is made from materials that are cheap and commonly occurring, compared to other technologies that require noble metals. [6] Nickel is another example of a metal that endures the corrosive environment as well as serves as a good catalyst. Therefore, nickel-based electrodes are commonly used. Common electrode materials used for both anode and cathode are Raney nickel, which is nickel activated by sulfur addition, or steel coated with nickel. A lot of research has gone into improving the electrodes during the last centuries. However, none of the new findings have yet made their way into commercial alkaline electrolyzers. [37], [38]

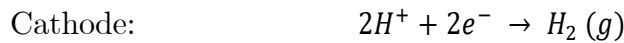
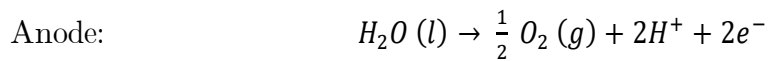
The membrane in the electrolyzer cells has historically been made from asbestos-containing materials. Since asbestos is considered a health hazard, newer electrolyzers use other materials. [15], [37], [38] The desired properties from the membrane are that it must be permeable for water and hydroxide ions, while not letting produced gases move through it. The membrane should be resistant to wear from the corrosive electrolyte, and lastly, it should not give rise to any significant ohmic resistance within the cell. [37] Materials that have shown good properties include composite materials such as polyphenylene sulfide (Ryton), polysulfone bonded zirconium oxide (Zirfon), and anion-selective polymers. [15], [37], [38] The materials that are used most commonly for the different components in the alkaline electrolyzer is summarized in Table 2.

Table 2. Materials in alkaline electrolyzer components. [35], [41]–[43]

Component	Material
Anode	Raney nickel
Cathode	Raney nickel
Mem brane	Zirfon
Electrolyte	25% KOH
Cell chamber	Nickel/Steel

## 4.2 Polymer Electrolyte Membrane Electrolyzer

The polymer electrolyte membrane electrolyzer (PEMEC) is another low-temperature electrolyzer, invented after the alkaline electrolyzer in the 1950s. PEMEC is also a low-temperature electrolyzer, operating at around 80°C. The lifetime of a PEMEC is between 10-20 years or 20 000 - 60 000 hours of operation [44]. The reactions taking place is as described in reactions below.



The electrolyte is typically a polymer, used for their good conducting properties. The electrodes consist of platinum or other noble metals. The membrane is typically Nafion, a fluorinated polymer. [45] The technology is not yet commercially available for large-scale hydrogen production. [41]

## 4.3 Molten Carbonate Electrolyzer

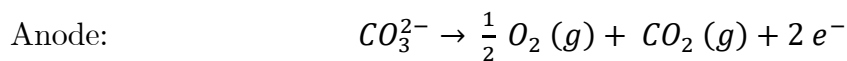
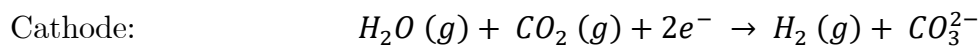
The molten carbonate electrolyzer (MCEC) is not a commercial technique, however, its fuel cell counterpart is. Due to the very restricted amount of literature on the MCEC, the information on this technique will be gathered from literature both on the electrolyzer and the molten carbonate fuel cell (MCFC). As of today, the MCEC and the MCFC technology are very similar. This might change in the future if MCEC



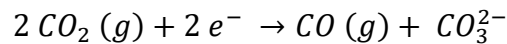
would be developed for commercial purposes. The MCEC is a high-temperature electrolyzer, typically operated at temperatures between 600-700°C. [46] For the MCFC, the lifetime is around 20 years or 40 000 operating hours. [47] The purity of outlet hydrogen gas from the electrolyzer is still unknown. However, it will not be as pure as the hydrogen outlet stream from AEL, PEMEC, and SOEC. [48]

## Reactions

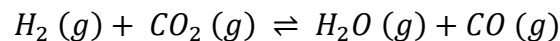
When the MCFC is run in reverse, as an electrolyzer, it can be used to produce hydrogen gas or syngas ( $H_2 + CO$ ). The inlet stream to the electrolyzer must contain both water and  $CO_2$ . The splitting of water then occurs at the cathode. Both electrochemical and chemical reactions take place in the MCEC. Reactions, as they occur in the electrolysis cell, are given below.



Since  $CO_2$  is present in the inlet gas, a side reaction that might take place is  $CO_2$  electrolysis, as below.



This reaction has proven to be much slower than the water electrolysis reaction in the MCEC. However, CO can also be produced from the water gas shift reaction, as stated in the reaction below.



At higher temperatures, such as 600-700°C where the MCEC is operated, this reaction quickly reaches equilibrium, and CO will be present in the outlet gas. [46]

## Materials

In this section, a brief introduction to the main materials used for the MCEC will be given. A more thorough investigation of the materials will be performed in Chapter 5.

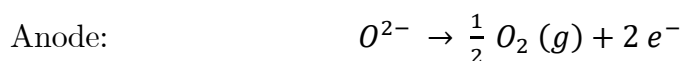
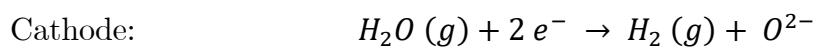
The electrolyte in the MCEC consists of either lithium and potassium carbonate or lithium and sodium carbonate. The electrolyte is a highly conducting liquid at the operating temperature. The electrolyte sits in a porous matrix made of lithium aluminate, that lets the carbonate ions move from cathode where it is produced to the anode where it is consumed. The matrix also helps to separate the inlet and outlet gases. [46], [47] The anode is made from a porous nickel electrode alloyed with either chromium or aluminum, while the cathode is a porous electrode made from a sintered nickel oxide that has been treated with lithium. [46] The materials that are used most commonly for the different components in the MCEC are summarized in Table 3.

Table 3. Materials in MCEC components. [46], [47]

Component	Material
Anode	Ni w Cr/Al
Cathode	Lithiated nickel oxide
Matrix	LiAlO <sub>2</sub>
Electrolyte	Li <sub>2</sub> CO <sub>3</sub> +K <sub>2</sub> CO <sub>3</sub>
Cell chamber	Stainless steel + aluminum

## 4.4 Solid Oxide Electrolyzer

The solid oxide electrolyzer (SOEC) is an electrolyzer still on demonstration scale. The SOEC is a high-temperature electrolyzer, typically running between 650-1000°C. The lifetime of a solid oxide electrolyzer is around 10 000 operating hours [49]. The reactions taking place in the cell are described below.



The electrolyte material in SOEC is ceramic, usually zirconia. The electrodes are also made from ceramic materials, usually porous cement electrodes doped with nickel or zirconia. [6]

## 4.5 Comparison of Technical Parameters

A comparison of some technical parameters for the electrolyzers is presented in this section. Data for the MCEC is not available to the same extent as for the more mature technologies. Therefore, parameters are only compared for AEL, PEMEC, and SOEC in Table 4.

Table 4. A selection of technical parameters on AEL, PEMEC, and SOEC. [6], [38], [44], [49], [50]

Parameter	Unit	AEL	PEM	SOEC
Temperature	°C	60-80	50-80	650–1 000
Pressure	bar	<30	<30	<25
Cell voltage	V	1.8-2.4	1.8-2.2	0.7–1.5
Current density	A/cm <sup>2</sup>	0.2-0.4	0.6-2.0	0.3-2.0
Voltage efficiency (HHV)	%	62-82	67-82	<110
Energy consumption stack	kWh/Nm <sup>3</sup>	4.2-5.9	4.2-5.5	>3.2
Lifetime	*1 000 h	60-100	20–60	<10
Technology maturity	-	Mature	Commercial	Demonstration
H <sub>2</sub> purity	%	>99.5	99.99	99.9

## 4.6 Replacement of Electrolyzer Parts

In this section, it is discussed whether any parts of the electrolyzers need replacement within the expected lifetime used in this thesis.

### AEL

In the source from where the inventory data for the AEL emanates, it is stated that over a period of ten years, no parts of the AEL must be replaced. However, it is expected that after ten years of operation, the stacks along with the KOH solution should be replaced. [36] In this thesis, the expected lifetime of the AEL is 80 000 hours, which adds up to just over nine years of operation. Accordingly, no replacement of AEL parts needs to be done within the expected lifetime.

## MCEC

A source that has performed an LCA of a molten carbonate fuel cell states that the stacks should be replaced every five years. [51] In this thesis, the lifetime of the MCEC is assumed to be 40 000 hours, corresponding to approximately 4.5 years of operation. Therefore, no parts of the MCEC are anticipated to be replaced within the expected lifetime.

### 4.7 Previous LCA's of Electrolyzers

A short review of some previous life cycle analyses of hydrogen production through electrolysis will be provided in this section. Functional unit, system boundaries, and environmental impact categories used in the studies are described when the information is available.

There are many sustainability assessments performed on hydrogen production methods. One study performs a comparative LCA on steam reforming of natural gas and fossil-free production methods based on high-pressure electrolysis run with renewable energy sources (RES); solar (photovoltaic and thermal), wind, hydro, and biomass. The functional unit in the study was 1 MJ energy produced from H<sub>2</sub>. The impact categories studied were global warming potential (GWP), acidification potential (AP), eutrophication potential (EP), and winter smog effect. The results show that electrolysis run with photovoltaic (PV) energy has the worst environmental impact due to the production of the PV panels. Hydrogen produced by electrolysis with solar thermal, wind, and hydropower proved to be the most environmentally sustainable out of the investigated production methods. [52]

## Previous LCA's of Alkaline Electrolyzer

Burkhardt et al. has performed another study that aims to investigate if the assumption that hydrogen produced with electrolysis can be considered to have zero emissions is valid. The EU has made this assumption, based on the supposition that emissions from construction of the hydrogen production plant are negligible. The construction includes the building of wind turbines for electricity production, electrolyzer, and refueling station. An LCA was performed on a hydrogen refueling station in Germany where hydrogen is produced with an alkaline electrolyzer driven by wind power. The functional unit was 1 kg compressed H<sub>2</sub>. Studied environmental impact categories were GWP, AP, EPfw (freshwater), human toxicity (HTP), and terrestrial ecotoxicity. It is concluded that the emissions from the construction of the plant are not negligible. However, it is stated that hydrogen from wind-powered electrolysis still has the potential to reduce the greenhouse gas emissions compared to conventional fuels. [53]

In a study by Koj et al., an alkaline electrolyzer with an asbestos membrane is compared to an alkaline electrolyzer with a newer developed polymer membrane, using LCA. The functional unit in the study was 1 kg H<sub>2</sub> at 33 bar and 40°C. In this study, many impact categories were analyzed, including e.g. GWP, AP, EPsw (salt water), EPfw, HTP, etc. For all studied impact categories, the newer technology with polymer-based membrane has a lower impact. The results of the study show that the disposal of the stack has a very small impact in the studied categories compared to construction and operation. The construction phase has the highest impact in some categories, e.g. EPfw and HTP. Another interesting finding is that during the construction phase, the cell stacks have the highest impact in all categories. The auxiliary equipment such as reformer, pipes, etc., called balance of plant (BOP), have only minor impact in all studied impact categories. [42]

The authors of another study, Spath et al., have performed an LCA of a wind powered electrolysis system, considering the cradle to grave of wind turbines, electrolyzer, and

hydrogen storage. The environmental indicators include GWP and air emissions. The impact from the electrolyzer is small in most of the categories, under 10% of the systems total impact. However, the impact is more severe in categories nitrous oxides (NO<sub>x</sub>) and sulfur oxides (SO<sub>x</sub>), due to the production of benzene that is used in the studied electrolyzer. [54]

Two studies performed by Hake et al. and Koj et al. regard a comparative LCA of a pressurized alkaline electrolyzer with a Zirfon membrane run in three different countries, i.e., with three different electricity mixes. The functional unit in both studies is 1 kg H<sub>2</sub> (33 bar, 40°C and 99.8% purity). The authors of the studies use FC-HyGuide guidelines that interpret the ISO 14040 and ISO 14044 standards specifically for hydrogen systems. The study includes construction and operation of the electrolyzer as well as the BOP including tanks, heat exchangers, etc. Since the authors do not have any information on how the Zirfon membrane will be disposed of, the end of life is not included in the study, rather a cradle-to-gate approach is applied. Impact categories include GWP, AP, EP<sub>sw</sub>, EP<sub>fw</sub>, ozone depletion potential (ODP), etc. The results show that the construction of the alkaline electrolyzer have the highest impact in the impact category ODP, it also has a significant effect on other categories such as AP and EP<sub>fw</sub>. However, it is still concluded that the operation phase with the electricity supply have the highest environmental impact. [35], [36]

In 2014 Bhandari et al. presented a review of the LCA's performed thus far regarding hydrogen production. A finding in the review is that in wind-based electrolysis systems, the electrolyzer unit constitutes only 4% of the total GWP impact. [41] However, this is only one impact category and as the above literature study has shown, electrolyzer construction might have a more dominating impact in other categories. A conclusion in the study is that none of the considered studies compare the environmental impacts of one electrolyzer to the other [41]. The authors also state that a study investigating the environmental impact of individual components in the electrolyzer is needed. [41]

## Previous LCA's of Molten Carbonate Electrolyzer

Regarding MCEC, no published LCA's were found during the literature study performed in this thesis. However, there are some studies investigating the fuel cell counterpart, MCFC, that are reviewed in this section.

In one study an LCA of the production of an MCFC stack is performed by Lunghi et al. The functional unit was chosen as one single cell (1 m<sup>2</sup>). The studied environmental impact categories were ecosystem quality and resources. The results show that the anode production have the highest impact in both impact categories, followed by cathode and matrix production. [55] This study is then built on in another study by Lunghi et al., where an LCA is performed of a whole MCFC system, driven by H<sub>2</sub> produced from natural gas. [56] However, in that study, there is no environmental evaluation of the MCFC unit itself, it is treated as a black box.

In another study, Monaco et. al performs an LCA of the production, operation, and end of life of a 2.5 kW MCFC prototype. Several impact assessment methods were used, and thus many environmental impact indicators were investigated. The results show that the main environmental impact derives from the natural gas used to drive the fuel cell. The manufacturing of MCFC mainly affects AP, HTP, and minerals consumption. [57]

In a study by Raugei, another MCFC prototype is the subject of a comparative LCA. The 500 kW MCFC is compared to three different natural gas turbine plants, the systems intended use is as stationary electricity production. The systems manufacturing and use-phase are investigated. Impact categories in the study include airborne emissions, ecological footprint, and withdrawal of natural resources. A conclusion from the study is that the MCFC system shows lower overall environmental impact than even the most modern gas turbines. [58]

In [59], a comparative LCA is performed by Alkaner et al. on MCFC and diesel engine systems, both to be used for power supply on a ship. The system boundaries include manufacturing, fuel supply, operation, and end of life of both systems. The functional

unit is 1 kWh of electricity produced by the system. Impact categories include AP, EP, GWP, HTP, ODP, winter smog, etc. A conclusion in the study is that the assembly of the MCFC plant (including BOP) has a larger overall impact than that of the diesel engine. The impact is mainly in the category AP due to emissions of NO<sub>x</sub> and sulphur dioxide (SO<sub>2</sub>) from the production of components used in the stack. [59]

Moreover, in [51] Zucaro et al. has performed an LCA on a single MCFC cell, one MCFC stack (125 kW), and one complete system of 4 stacks (500 kW) and BOP. The functional unit varies between the studied systems; for the first two the functional unit is the produced cell and stack, and for the third system the functional unit is produced electricity. The system boundaries include manufacturing and operation, but not the end of life. Environmental indicators were chosen as recommended in the FC-Hy Guide, including AP, EP, GWP, ODP, HTP, etc. The impact categories where the MCFC systems have the highest impact are AP, EP, ODP, HTP, and photochemical oxidation, although a large portion of the impact originates from the natural gas reformer in the BOP. The MCFC stack, where the anode is the largest contributor, mainly impacts ODP and HTP, although impacts in EP, GWP, and abiotic depletion are not negligible. [51]

## Summary of Previous LCA's of Electrolyzers

The literature study performed in this chapter does not contain all previous LCA's of electrolyzers, for example, LCA's of PEMEC and SOEC are not considered. However, from the literature study, it can be concluded that no published LCA was found that compares different types of electrolyzers to each other. Many studies conclude that electrolyzers have less environmental burden than other hydrogen production methods. This shows that electrolyzer as the choice of hydrogen production method should be the preferred method.



Even though there is a substantial amount of LCA's performed on electrolyzers, as mentioned earlier, results from LCA's vary greatly depending on chosen functional units and system boundaries. Therefore, it is not possible to simply compare results from previous studies and draw conclusions on which electrolyzer is more environmentally sustainable. Therefore, the contribution of this thesis together with the concurrent thesis conducted by Lundberg [8] would be to have comparable LCA's of the main technologies for electrolysis.

## Chapter 5. Life Cycle Inventory

As mentioned previously, no primary data were available. Rather, data from the literature and data gathered through contact with writers of earlier LCA's will serve as the basis for the LCA conducted in this study. In this chapter, the inventory data for alkaline electrolyzer is presented, and the inventory data for molten carbonate electrolyzer discussed.

### 5.1 Data for Alkaline Electrolyzer

Data for the alkaline electrolyzer is taken from [36], which was the source found with the most detailed inventory, see Table 5. The studied electrolyzer in the article was a 6 MW pressurized alkaline electrolyzer. [36] The amounts in unit [kg/100 kg H<sub>2</sub>] was calculated from the numbers stated in the original article using a lifetime of 80 000 operating hours, see Appendix 4. Data in pink fields are only included in case "All data" presented in Appendix 1, not in the results of the base case presented in Chapter 6. In Table 5 it is also specified, when possible, what purpose the respective materials serve in the electrolyzer.

*Table 5. Inputs for construction of alkaline electrolyzer. [36]*

Material	kg/100 kg H <sub>2</sub>	Application of material
Copper	1.93*10 <sup>-02</sup>	Cell stack framework
Unalloyed steel	1.93	Cell frames
Nickel	1.83*10 <sup>-01</sup>	Electrodes and cell frames
Aluminum	4.34*10 <sup>-03</sup>	Cathodes
Calendered rigid plastic	7.52*10 <sup>-03</sup>	
Polytetrafluoroethylene	7.52*10 <sup>-04</sup>	Gasket

Acrylonitrile butadiene styrene	$1.54 \cdot 10^{-03}$	Gasket
Polyphenylene sulfide	$3.28 \cdot 10^{-03}$	Membrane
Polysulfones	$2.51 \cdot 10^{-03}$	Membrane
N-Methyl-2-pyrrolidone	$1.25 \cdot 10^{-02}$	Membrane
Aniline	$4.72 \cdot 10^{-04}$	Gasket
Acetic anhydride	$5.20 \cdot 10^{-04}$	Gasket
Terephthalic acid	$8.48 \cdot 10^{-04}$	Gasket
Nitric acid	$3.18 \cdot 10^{-04}$	Gasket
Hydrochloric acid	$1.25 \cdot 10^{-03}$	Gasket
Graphite	$4.14 \cdot 10^{-03}$	Gasket
Lubricating oil	$4.63 \cdot 10^{-06}$	Gasket
Zirconium oxide	$1.06 \cdot 10^{-02}$	Membrane
Carbon monoxide	$1.45 \cdot 10^{-03}$	Cathodes
Decarbonized water	$1.06 \cdot 10^{-01}$	
Deionized water	$8.29 \cdot 10^{-01}$	
Industrial machine production	$1.54 \cdot 10^{-06}$	
Plaster mixing	$7.52 \cdot 10^{-03}$	
Energy                      kJ/100 kg H <sub>2</sub>		
Electricity	347	
Heat	848	
Steam	6.74	

The material ‘calendered rigid plastic’ is not further specified. What type of plastic this refers to is therefore not known. By studying the process of calendering, polyvinyl chloride (PVC) is the main plastic material for which this process is used [60]. It is

therefore assumed that PVC is the intended plastic in the alkaline electrolyzer.

For the operation of the electrolyzer, additional material and energy inputs are required. These are presented in Table 6.

*Table 6. Inputs for alkaline electrolyzer operation. [36]*

Material	Amount	Unit
Electricity	18 000 000	kJ/100 kg H <sub>2</sub>
Deionized water	1 000	kg/100 kg H <sub>2</sub>
Nitrogen	0.0290	kg/100 kg H <sub>2</sub>
KOH	1.90	kg/100 kg H <sub>2</sub>
Steam	11.0	kg/100 kg H <sub>2</sub>

Electricity and deionized water serve as reactants to produce hydrogen. Nitrogen is used for cleaning, while process steam is used during start up to heat up the system. [36]

## 5.2 Data for Molten Carbonate Electrolyzer

Some partly confidential inventory data for MCEC was retrieved by contact with a corresponding author of a previously published LCA of a molten carbonate fuel cell. A combination of partly confidential and unvalidated data lead to the decision to not include inventory data and results for MCEC in this report.

## 5.3 Transports

Two transportations are included in both models; transportation of raw material to electrolyzer manufacturing and transportation of the electrolyzer to the hydrogen production site. Both transports are assumed to be made with a Euro 5 truck (maximum load 22 000 kg and payload 85%). The first transport is assumed to be

1 000 kilometers. The second transport is assumed to be 2 364 kilometers, from Germany where the electrolyzer is assumed to be produced, to a hypothetical hydrogen production site in Sweden.

## 5.4 Data in GaBi

When materials for the different technologies are put into GaBi, European averages are used as far as possible. When European averages are not available, global averages are prioritized second. All datasets used in GaBi are specified in Appendix 2.

## Chapter 6. Life Cycle Impact Assessment

The results from the LCA are presented in this chapter, along with a discussion of the results. The results in this chapter represent the base cases, meaning that some data has been excluded to reach comparable models of all electrolyzer technologies. In Appendix 1 the cases with all retrieved data are presented. The results for AEL are presented in detail and discussed. The results for MCEC are not published since the inventory data contained errors. Moreover, the results for the remaining three technologies, i.e. AEL, PEMEC, and SOEC are compared. All results are presented per functional unit, i.e. 100 kg produced hydrogen gas.

The results are presented for the chosen environmental impact categories; ADP elements, ADP fossil, AP, EP, GWP, and POCP. The environmental impact categories are described in section 3.6. The results show the potential environmental impact for the life cycle steps included in this study; raw material extraction, transport of raw material to electrolyzer manufacturing, energy for electrolyzer manufacturing, transport of electrolyzer to hydrogen production site, and lastly material and energy inputs for hydrogen production.

### 6.1 Alkaline Electrolyzer

The results for the AEL life cycle steps are presented in Figure 6, showing that the energy input for hydrogen production and the raw materials for electrolyzer manufacturing have the highest impact in all chosen impact categories.

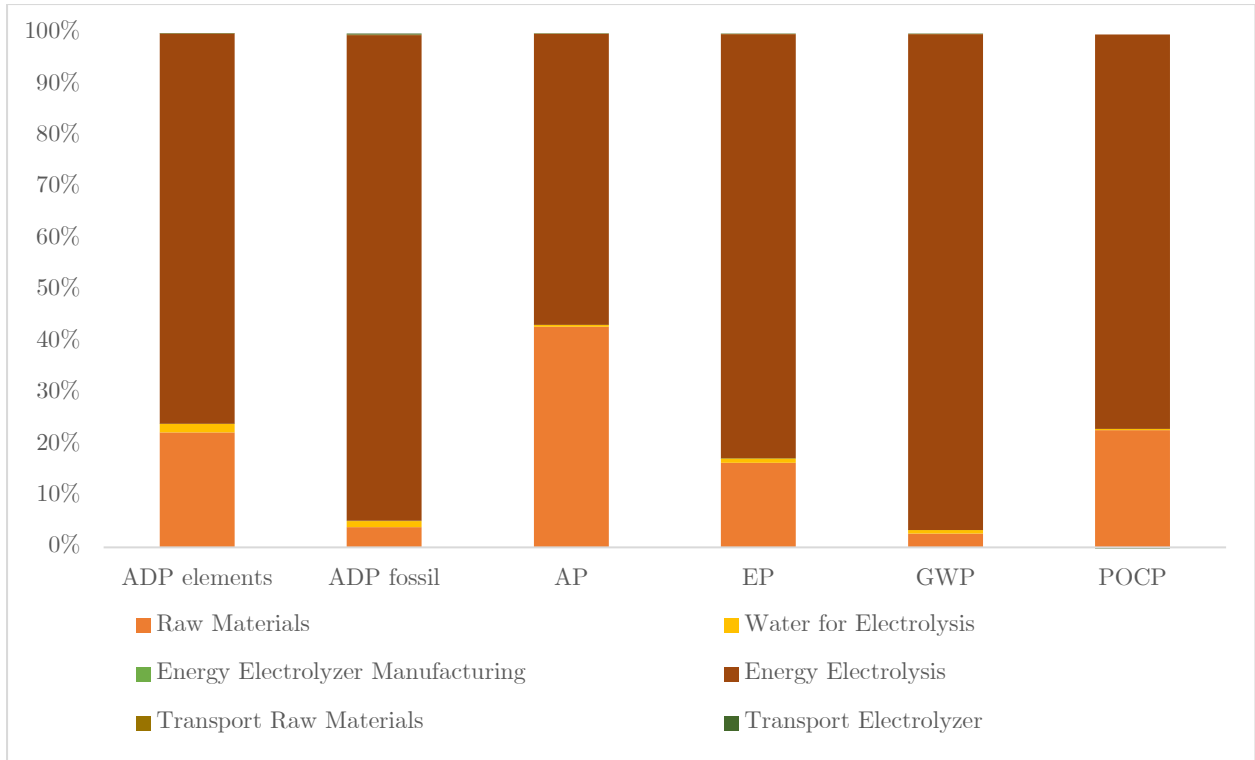
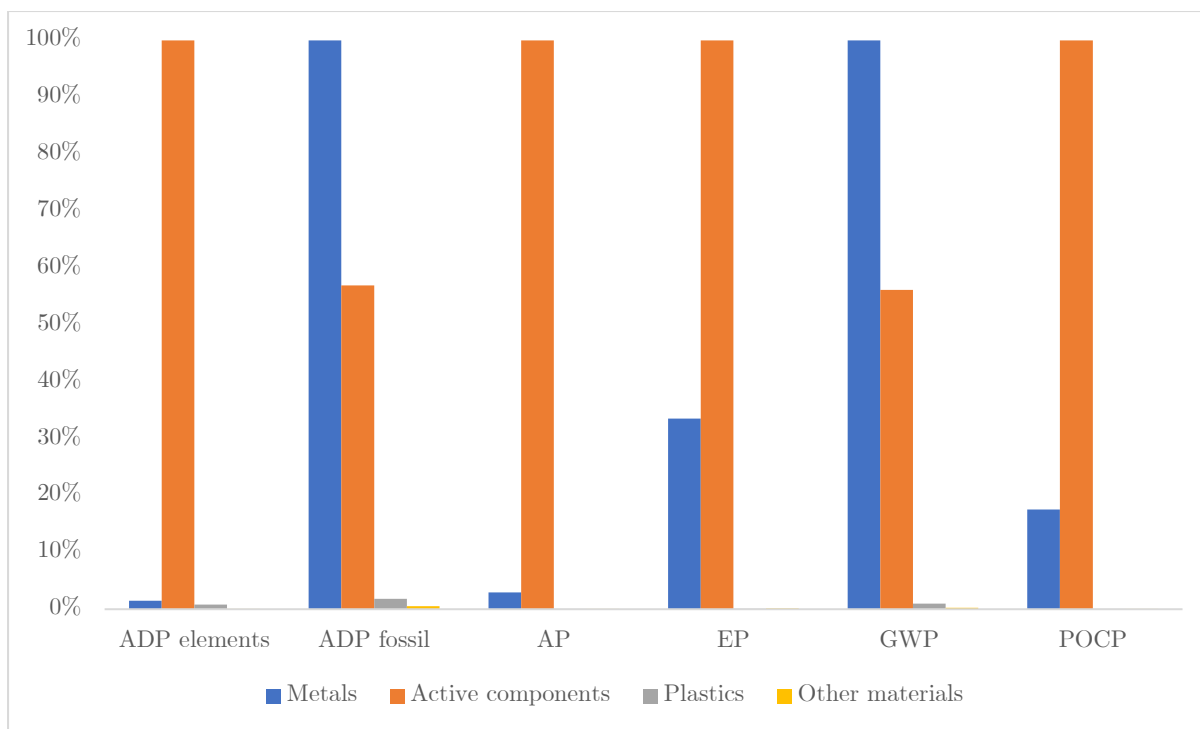


Figure 6. Life cycle results for production of 100 kg H<sub>2</sub> with an AEL.

The other life cycle steps have smaller impact compared to raw materials for electrolyzer manufacturing and electricity for hydrogen production. The energy consumption for the hydrogen production will be discussed more closely in a sensitivity analysis performed in Chapter 7.

To explore the cause of the relatively large impact from the raw materials, Figure 7 shows a more detailed analysis of the raw materials in Figure 6. To reach an effective presentation of the impact from the raw materials, they are categorized into metals, active components (i.e. materials for electrodes etc.), plastics, and other materials which includes e.g. different acids used for gasket manufacturing.



*Figure 7. Breakdown of results for raw material extraction for AEL production. The group of materials with the highest impact in each impact category was set as 100%.*

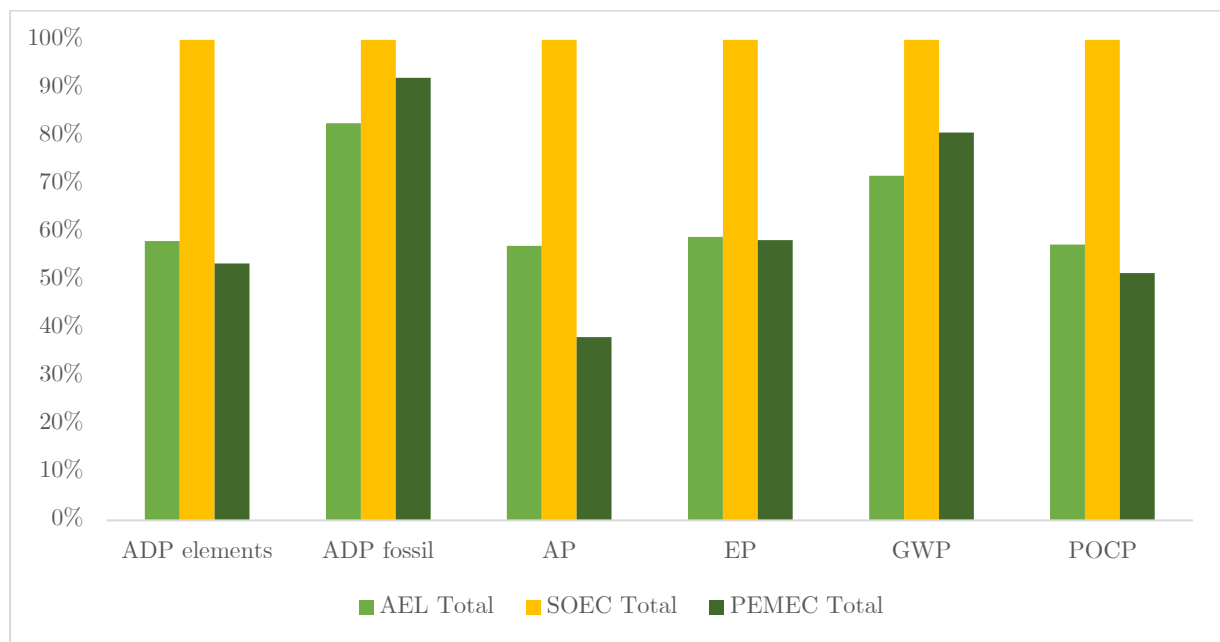
Figure 7 shows that metals and active components have the highest impact in all chosen impact categories. Nickel and steel are the main constituents of both anode and cathode, as well as the cell chamber. Production of both nickel and steel use high amounts of fossil energy sources, which is the reason for the high contributions of these materials in the results. The collected data, found in section 5.1, shows that these materials account for the largest masses, which suggests an explanation for their high impact. Apart from nickel and steel, polytetrafluoroethylene (PTFE), a fluorinated polymer [61], is the largest contributor to the impact category ADP elements, which is included in “plastics” in Figure 7. Looking in depth at the results for PTFE, this could be related to its high use of non-renewable resources. In the other impact categories N-methyl-2-pyrrolidone (NMP) is the dominating material, setting nickel and steel to the side. NMP is included in “other materials” in Figure 7. Production of NMP seems to be connected with extensive use of non-renewable energy resources, which could be the reason for its high impact in remaining impact categories, compared to the other materials.



## 6.2 Comparison of AEL, PEMEC, and SOEC

In this section, the results from the base cases of the three technologies will be compared. Data for PEMEC and SOEC emanates from the concurrent thesis conducted by Lundberg [8].

In Figure 8, the total results for AEL, SOEC, and PEMEC are compared to each other.



*Figure 8. Comparison of total results for AEL, SOEC, and PEMEC. The technology with the highest impact in each impact category was set as 100%.*

Figure 8 shows a relatively distributed result between the technologies. SOEC has the highest impact in all impact categories. The results in Figure 8 indicates that PEMEC is the electrolyzer with the lowest impact in most impact categories out of the investigated technologies.

To further investigate what lies behind these results, Figure 9 shows a comparison of the life cycle steps of AEL, SOEC, and PEMEC. In Figure 9, the life cycle steps are categorized into only material, energy, and transport, to get a more effective presentation of the results. For example, “AEL Material” includes both materials for electrolyzer manufacturing and for hydrogen production.

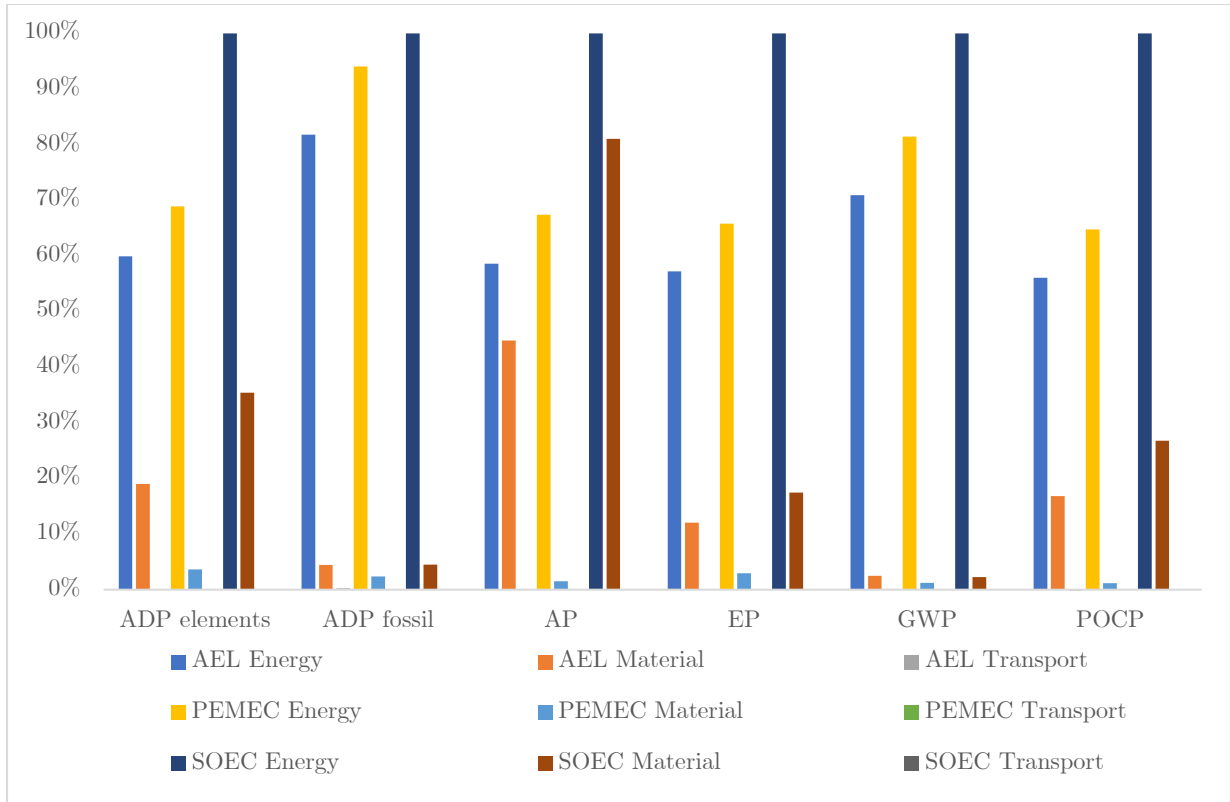


Figure 9. Comparison of life cycle steps for AEL, PEMEC, and SOEC. The step with the highest impact in each impact category was set as 100 %.

Figure 9 shows that the largest contributors in all impact categories are the energy consumption for the three technologies. The exception is the materials for SOEC which has the second highest contribution to the impact category AP. Furthermore, the materials for AEL and SOEC have significant impact in all categories. The potential impact from the transports are not significant compared to the other life cycle steps.

The materials for PEMEC show very low impact compared to the materials for the other technologies. PEMEC is the only one of the studied technologies that use platinum group metals (PGM's) for the active components of the electrolyzer, while the other technologies use nickel. The studied PEMEC uses iridium and not platinum, but platinum is used since the LCA software did not have data for iridium. Figure 10 shows a comparison of the potential impacts in chosen environmental impact categories from 1 kg of platinum compared to 1 kg of nickel. Platinum has the highest impact in all categories and was set as 100%.

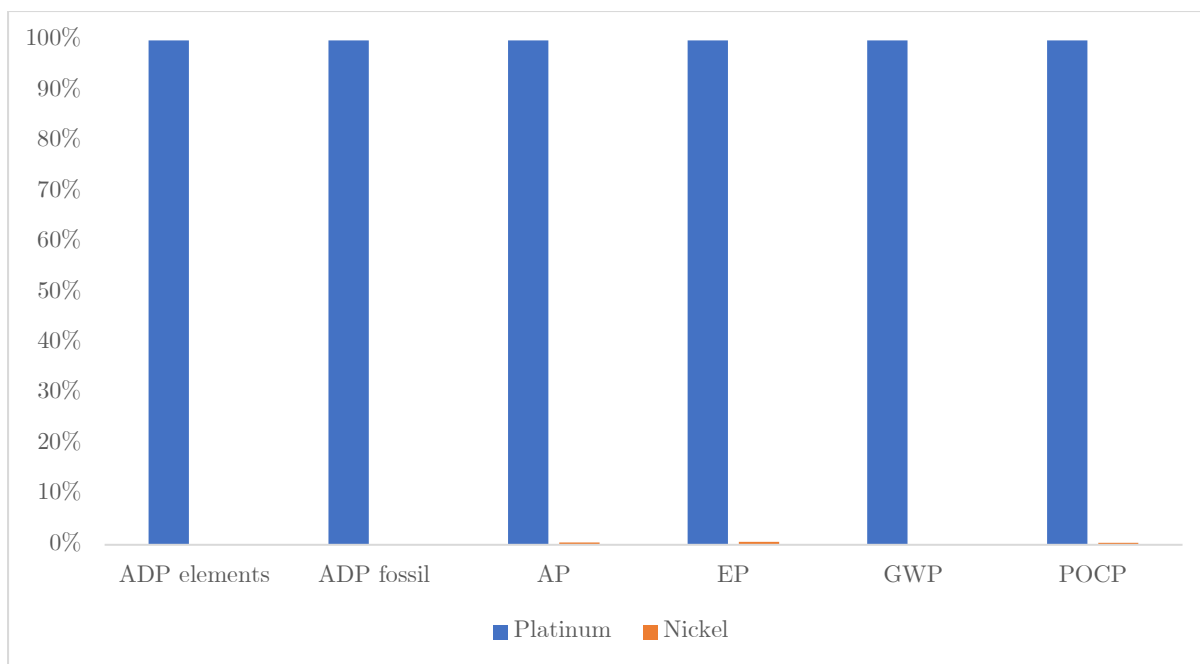


Figure 10. Comparison of potential environmental impacts from 1 kg of platinum and 1 kg of nickel.

Figure 10 shows that the potential impact in all studied environmental impact categories is substantially higher than that of nickel. Nickel is the material that has the highest contribution in all environmental impact categories in all other technologies, where nickel is used as part of the active components. This, together with the results for PEMEC shown in Figure 9, could suggest that the amount of nickel needed to reach the desired properties of the active components is large enough to give higher environmental impact than if PGM's would be used.

## Chapter 7. Sensitivity Analysis

In this chapter, a sensitivity analysis of the alkaline electrolyzer will be presented. The electricity used for hydrogen production by AEL will be changed and the results analyzed. Moreover, a discussion of electricity grid mixes in different countries will be presented.

### 7.1 Electricity for AEL manufacturing

As is readily seen from the results presented in Chapter 6, the energy used for operation of the electrolyzer is a significant contributor to the electrolyzers life cycle impact. The electricity used for electrolyzer manufacturing does not significantly contribute to the results. However, it might still be interesting to look at the impacts for some different countries' electricity mixes.

Germany was chosen as the geographic location for the electrolyzer production in this study since it is a country with a lot of industrial production. Different electrolyzer technologies are included in this study, with several producers of at least alkaline electrolyzers. Accordingly, Germany might not be the actual location of the electrolyzer production. For example, the largest producer of alkaline electrolyzers is located in Norway; Nel Hydrogen [62]. Therefore, in Figure 11, a comparison of electricity mixes from Europe (average over 28 countries), Germany, Sweden, and Norway are presented.

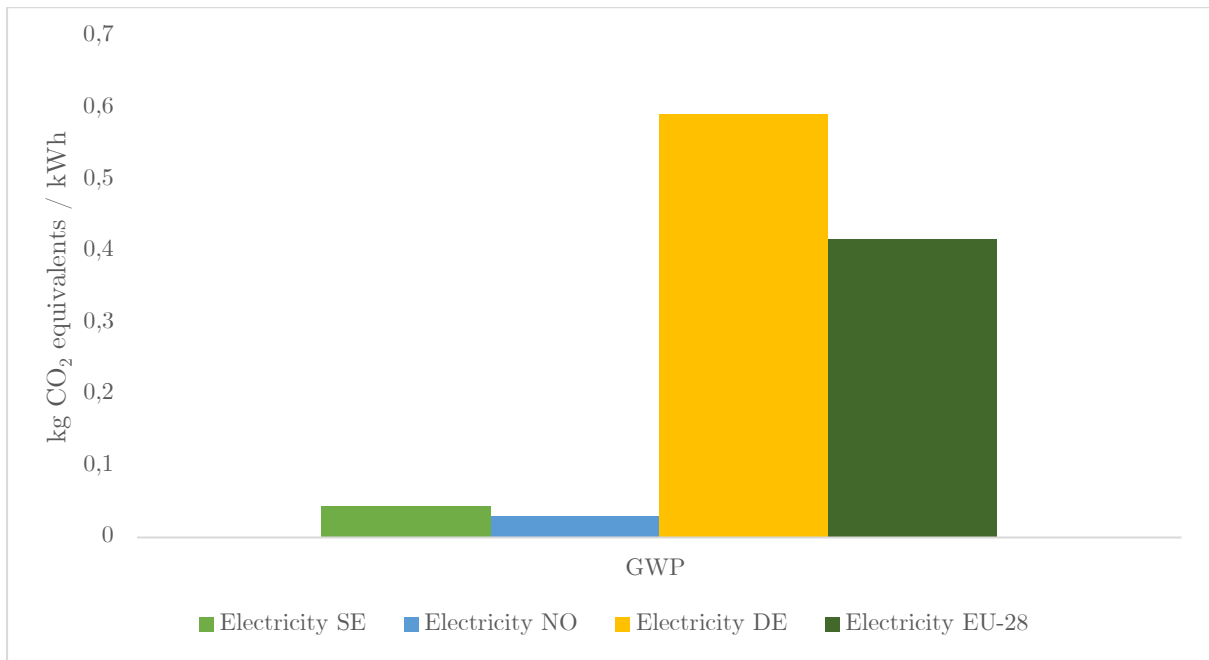


Figure 11. Comparison of GWP impact for Swedish, Norwegian, German, and EU average over 28 countries.

As can be seen in Figure 11, the German electricity mix has the largest potential impact to the category GWP, second comes the average over 28 EU countries. The Swedish and the Norwegian grid mixes have quite similar results, even though the Norwegian grid mix has somewhat lower potential impact. To further investigate what lies behind these results, a breakdown of the different electricity mixes constituents is presented in Figure 12.

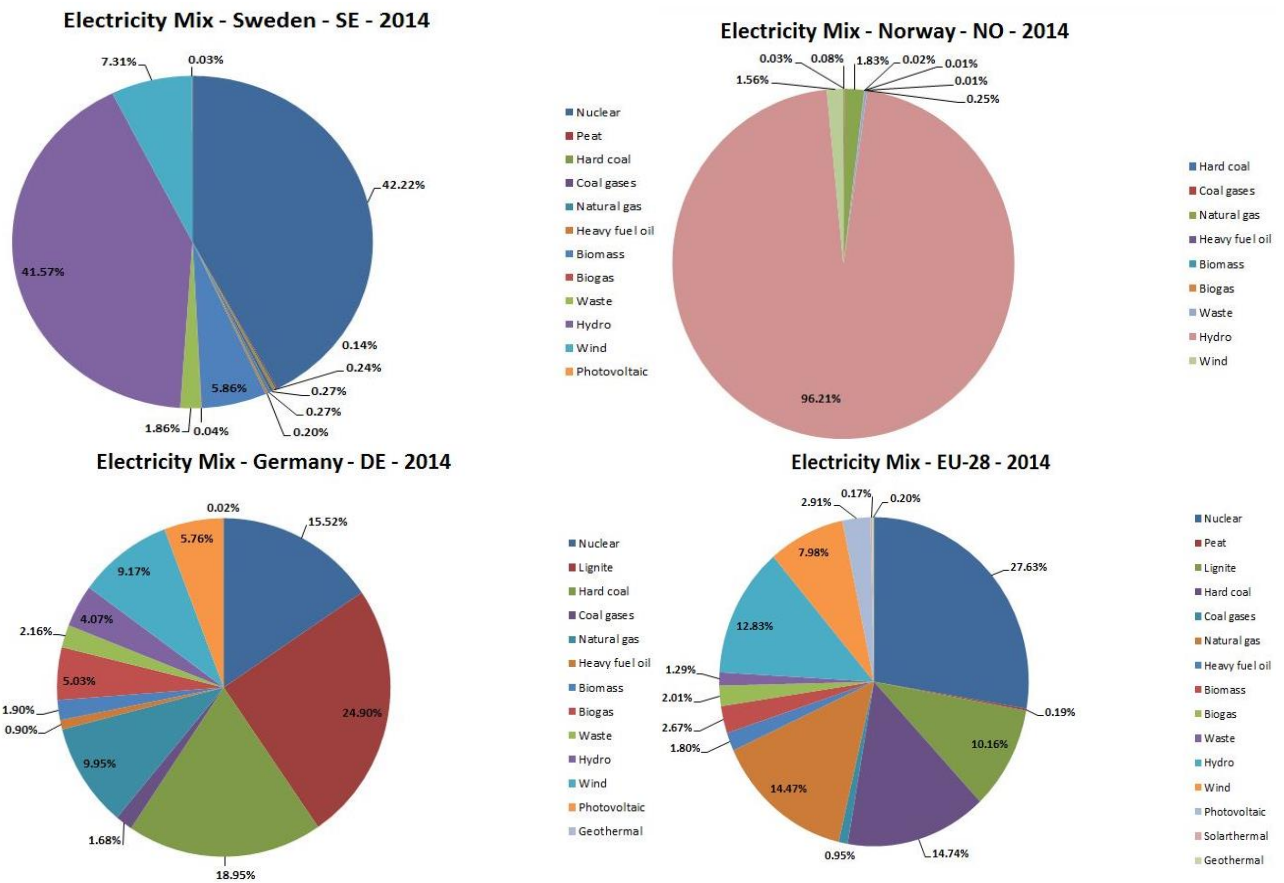


Figure 12. Constituents of analyzed grid mixes.

Norway has over 96% hydro power in its grid mix, which explains its low impact in GWP per kWh. Sweden also has a significant share of hydro power, almost 42%, but also a large share nuclear power, just over 42%. Nuclear power cause close to no GHG emissions, while the production of the fuel is connected with some emissions. However, the results for nuclear power will most definitely be higher in other impact categories. Looking at the pie chart for Germany and the European average, it is obvious that these electricity mixes have large shares of non-renewable energy sources. For example, the German electricity mix consists of coal for up to 45%. Note that these numbers are from 2014, and the electricity mixes will have changed to some extent over the last five years.

## 7.2 Sensitivity Analysis – Electricity for Hydrogen Production by AEL

The electrolyzer operation, i.e. the H<sub>2</sub> production, is in this study chosen to be set in Sweden. In the base case results presented in Chapter 6, the electrolyzer is run with Swedish electricity grid mix, which constituents is presented in Figure 12. The Swedish grid mix will most likely change over time. One possibility is that nuclear power will be phased out and renewable electricity sources such as wind and/or hydro power will increase. Moreover, there is a possibility that the electrolyzers will be operated with electricity from only one specific power source, such as wind power. Therefore, a comparison of the possible impacts from some Swedish electricity types are compared in Figure 13.

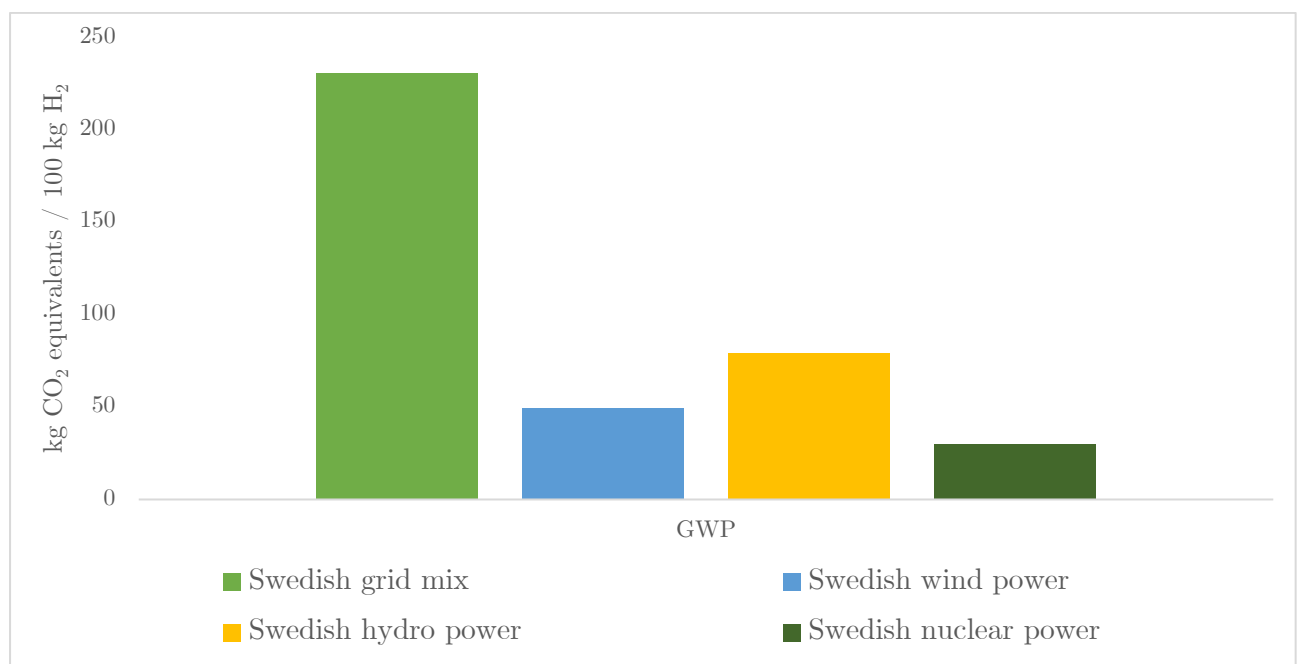


Figure 13. Comparison of total GWP impact for AEL base case with alternating electricity sources.

Figure 13 shows the total impact per 100 kg produced hydrogen in the category GWP from the AEL base case with alternating electricity sources for the production of hydrogen. Wind power, hydro power, and nuclear power all have lower potential impact compared to the Swedish grid mix.

## Chapter 8. Interpretation

In this chapter, some sources of uncertainty are brought up and discussed. Moreover, suggestions for future studies are presented. Lastly, conclusions are drawn based on the results presented in this thesis.

### 8.1 Further Discussion and Sources of Uncertainty

- Dependence on set system boundaries and functional unit

All results depend on the system boundaries (cradle to gate) and the functional unit (100 kg produced hydrogen gas) set in this study. Changing the functional unit or system boundaries would impact the results.

- Lack of accurate inventory data for the molten carbonate electrolyzer

Since only one source of inventory data for MCEC was available for this study, it was not possible to double check the validity of the inventory data with other sources. Due to partly confidential and unvalidated inventory data, the results for the MCEC are not included in this report.

- Dependence on current density and lifetime of electrolyzers

The current densities of the specific electrolyzer technologies that the inventory data was collected for are unknown. The amount of material needed to construct an electrolyzer is directly proportional to the current density (current per unit of electrode area [ $\text{A}/\text{cm}^2$ ]) and may therefore strongly influence the results from the LCA. General current densities for the technologies are presented in Table 4 but will be repeated here; for AEL the range is 0.2-0.4  $\text{A}/\text{cm}^2$ , for PEMEC the range is 0.6-2.0  $\text{A}/\text{cm}^2$ , for SOEC the range is 0.3-2.0  $\text{A}/\text{cm}^2$ . The current density for a molten carbonate fuel cell is typically around 0.16  $\text{A}/\text{cm}^2$ , and it is assumed to be the same



for the molten carbonate electrolyzer.

Thereby, the electrolyzer technology with the highest current density is PEMEC. This correlates well with the total results of the technologies; PEMEC the lowest potential environmental impact. Regarding AEL and SOEC it is likely the difference in expected lifetime used in this study that shows up in the results.

To calculate the material amounts per functional unit, the amount of hydrogen each electrolyzer technology is expected to produce during its lifetime must be taken into consideration. Therefore, the expected lifetimes of the electrolyzer technologies are relevant for this study. The expected lifetime in operating hours used in this study were 80 000 hours for AEL, 40 000 hours for PEMEC (and MCEC), and 10 000 hours for SOEC.

The current density and the lifetimes of the electrolyzers have significant impact on their environmental performance per 100 kg of produced hydrogen gas.

- Future development of the electrolyzer technologies

The results in this thesis shows that the differences in potential environmental impacts from AEL, SOEC, and PEMEC are not very large. The potential environmental impacts seem to largely depend on the current densities and the lifetimes of the technologies. Therefore, which electrolyzer technology is the best one to choose for future hydrogen production depends largely on the development potential that the different technologies have with regards to current density, lifetime, and partly also efficiency.

- Electricity used for hydrogen production

The life cycle step that shows up as the highest contributor to the total potential environmental impact of the AEL, SOEC, and PEMEC is the electricity used for hydrogen production. Therefore, the electricity used to perform the electrolysis with should come from renewable sources and be chosen carefully.

- Different sources of data

Data for the four technologies emanates from four different sources. Moreover, all data is secondary data with no possibility of controlling the detail level on the data. An attempt to reach comparable models was made by excluding some data from the technologies that was obviously not obtained for all technologies, such as water use for electrolyzer manufacturing. However, it cannot with certainty be said that the detail level is the same for all technologies even after that. For example, one technology had a lot of binders included in its LCI, which no other technology had. Since no direct contact with electrolyzer manufacturers was established, there was no way of controlling if the other technologies simply did not use binders during manufacture, or if this data was lacking. Accordingly, some difference in detail level on the LCI might be present. However, it is assumed that the results from the models presented in this thesis still are comparable to the extent that the larger trends can be trusted.

- Temperature, pressure, and purity of the hydrogen gas

The AEL, MCEC, PEMEC, and SOEC would all deliver hydrogen at different temperatures, pressures, and purities. That is not considered in this thesis, since including e.g. the purity of the hydrogen gas in the functional unit would result in having to consider the auxiliary equipment (BOP) of the electrolyzer. Accordingly, for real cases where the area of use of the hydrogen gas is decided, desired temperature, pressure, and purity must be decided and the BOP for each technology needed to reach those parameters included.

- The effect of the BOP

For all technologies, the BOP is excluded from the study. As mentioned in section 3.7, some earlier studies have established that the BOP only have minor impact on

the total results in LCAs of electrolyzers. However, the BOP would differ between the technologies, even though in this study the BOP was assumed to be the same for all technologies. Therefore, it cannot with certainty be said that including the BOP for all four technologies would not give effect on the results.

## 8.2 Future Studies

- Retrieve first hand data for all technologies. A future study should be performed in collaboration with electrolyzer manufacturers, to obtain first hand data that can be assured to be correct and comparable.
- Collect reliable inventory data for MCEC. In this thesis, the results for the MCEC are excluded from the published report due to partly confidential and unvalidated inventory data. In a future study, the inventory data for MCEC and all other technologies should be double checked to ensure comparability.
- Include oxygen as a resource. For every 100 kg of H<sub>2</sub> produced by an electrolyzer, almost 800 kg O<sub>2</sub> could potentially be produced (see Appendix 4). In this study, the oxygen produced in the electrolyzer is treated as an emission. In a future study, it would be interesting to include oxygen as a resource that has its own area of use, for example as an oxidant during steel production, as mentioned in [63].
- In a future study, one scenario could be to investigate how the different electrolyzer technologies are predicted to change in the future. The maturity level of the different electrolyzers is very varying, why some technologies might be expected to evolve a lot in the future. For example, the efficiency might be expected to increase, material amounts expected to decrease, etc.

- As was mentioned in Chapter 6, PEMEC is the only electrolyzer using PGM's in its active components, whereas the other technologies use nickel. In the results of this report the amount of nickel needed to reach the desired properties of the active components is high enough to give a much higher impact in all chosen impact categories. Therefore, a future study could investigate how the environmental impact from the electrolyzers would change if PGM's were used in all technologies instead of nickel. Of course, there is a financial parameter to consider as well, which could also be included in the study.

### 8.3 Conclusions

A conclusion from this thesis is that the lifetime and the current density of the electrolyzer technologies has significant impact on their potential environmental impacts. Therefore, when choosing electrolyzer technology for future hydrogen production, the importance of these parameters should be emphasized.

Another conclusion, that has also been brought up in previous LCA's of electrolyzers, is that the electricity used for hydrogen production has the highest impact out of the electrolyzer life cycle steps. Therefore, it is important that the electricity used for hydrogen production by electrolysis should come from renewable sources and be chosen carefully. The impact from the electricity used for hydrogen production in the impact category GWP was investigated in a sensitivity analysis. The results from the sensitivity analysis show that the impact from hydrogen production by electrolysis would significantly decrease if the source of electricity was changed from the Swedish electricity mix to e.g. Swedish wind power.

For the alkaline electrolyzer, the energy for hydrogen production have the highest impact in all chosen impact categories. The raw materials for electrolyzer production also significantly contribute to the impact in most categories, especially in ADP

elements, AP, and POCP. The raw materials with the highest impact in the AEL are nickel and steel.

For the molten carbonate electrolyzer, not enough accurate inventory data have been found to allow a fair comparison with the other technologies. To achieve comparable models of all four electrolyzers, it is important that the inventory data for every technology is correct and comparable. LCA results for the MCEC are therefore not included in the published report and will not be further commented on.

Comparing the remaining three electrolyzers to each other; AEL, SOEC, and PEMEC the differences between the technologies are not that large. However, the comparison shows that the PEMEC has the lowest environmental impact in most of the included impact categories. An explanation to this result is the current density and the materials of the PEMEC technology. For all other technologies, the raw materials for electrolyzer manufacturing have significant impact in most impact categories, while for PEMEC the energy for hydrogen production is the main contributor in all impact categories. Another contributing factor is the relatively high lifetime of the PEMEC, making the material masses per functional unit lower. The comparison of the three electrolyzer also show that SOEC has the highest potential environmental impact. This can in part be explained by the low lifetime of the SOEC.

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## Appendix 1. Results, case “All data”

To reach models of all electrolyzers that are comparable, some data was left out of the models presented in Chapter 6. In this appendix, the results of the AEL model with all retrieved data will be presented.

### Alkaline Electrolyzer – All Data

For the alkaline electrolyzer, there were some data excluded for the base case presented in Chapter 5, e.g. water flows and some energy for electrolyzer manufacturing. To see the full list of what is included in which cases, see section 5.1. The results for AEL with all data included is presented in Figure 14.

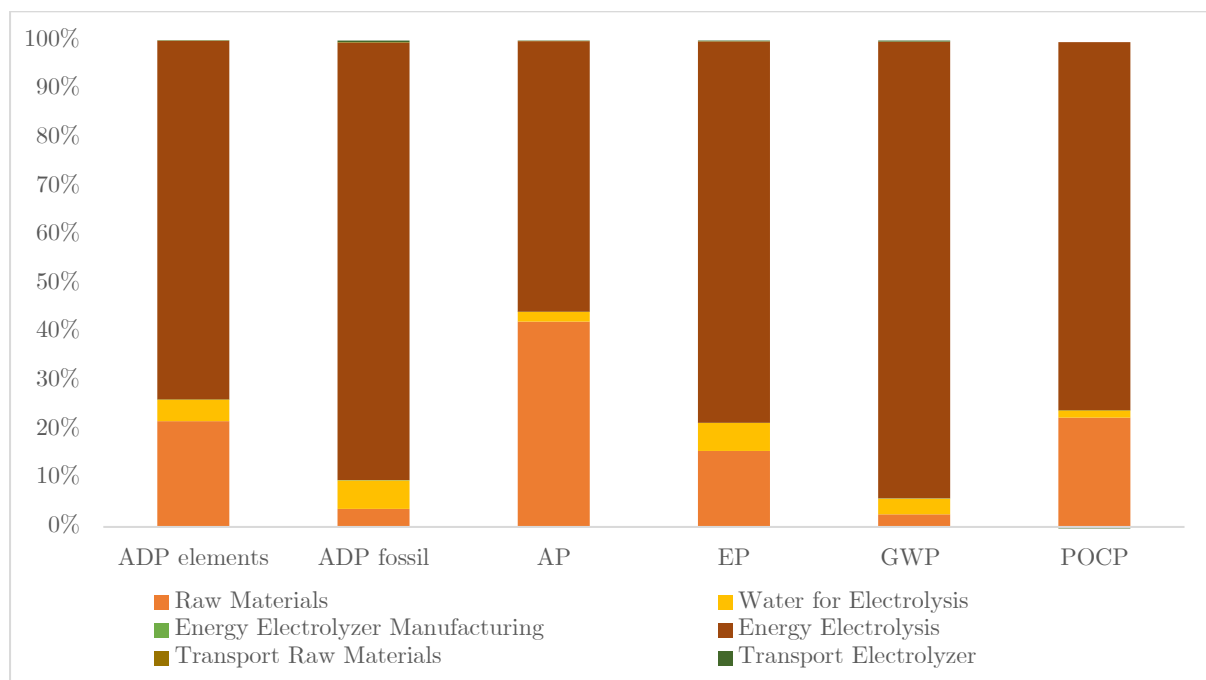


Figure 14. Life cycle results for production of 100 kg H<sub>2</sub> with an AEL - all data included.

Comparing Figure 14 to Figure 6 presented in section 6.1, it is mainly the “Material 2” that show some difference. The steam used for heating during run-up of the system and the deionized water used as reactant are the main contributors in the material

for hydrogen production.

Figure 15 shows a comparison of the results for the AEL in the base case and in the case with all included data.

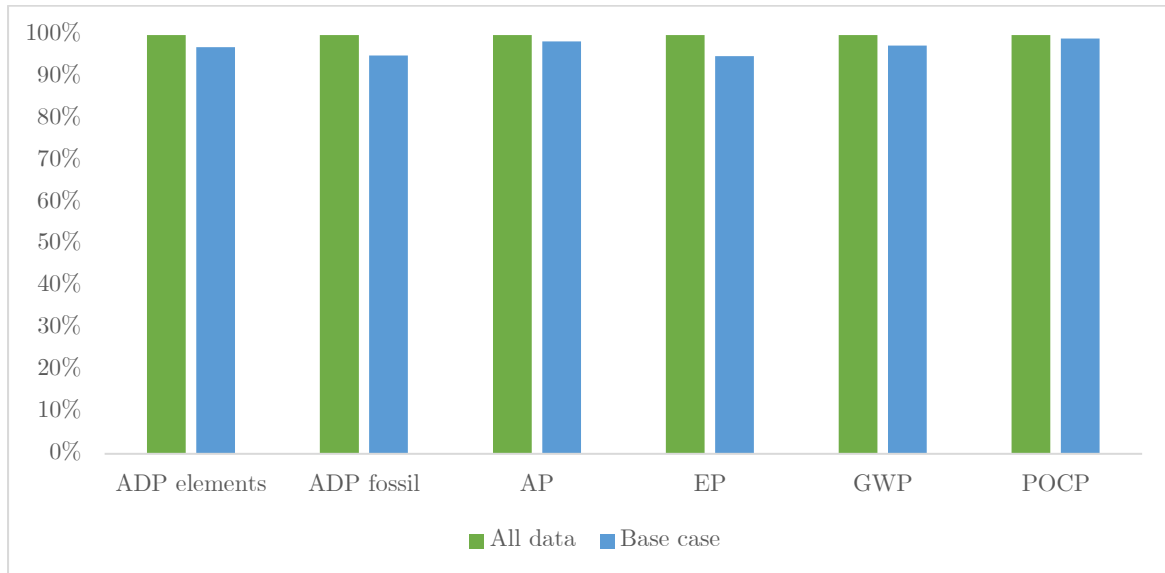


Figure 15. Comparison of results for AEL - base case (with some excluded data) and case with all retrieved data included.

The difference between the two cases is not very large. This indicates that the data included for the base case of AEL shows an acceptable simplification of the technology, even with some data excluded.

# Appendix 2. Data in GaBi

## Datasets for AEL

Table A 1. Datasets in GaBi for AEL. Fields in pink are included for case "all data", not in base case. Fields in green are used for the sensitivity analysis.

Material	Dataset in GaBi	Nation	Source	Parent Folder
Copper	Copper Sheet Mix	EU-28	DK/MECI	Copper
Unalloyed steel	Market for steel, unalloyed	GLO	ecoinvent 3	Manufacture of basic iron and steel
Nickel	Market for nickel, 99.5%	GLO	ecoinvent 3	Manufacture of basic precious and other non-ferrous metals
Aluminium	Aluminium sheet mix	EU-28	ts	Metal production
Calendered rigid plastic	Polyvinyl chloride sheet (PVC)	RER	PlasticsEurope	PlasticsEurope
Polytetrafluoroethylene	Polytetrafluoroethylene granulate (PTFE) Mix	DE	ts	Plastic production
Acrylonitrile butadiene styrene	Acrylonitrile butadiene styrene (ABS)	EU-28	PlasticsEurope	PlasticsEurope
Polyphenylene sulfide	Market for polyphenylene sulfide	GLO	ecoinvent 3	Manufacture of plastics and synthetic rubber in primary forms
Polysulfones	Market for polysulfone	GLO	ecoinvent 3	Manufacture of basic chemicals
N-Methyl-2-pyrrolidone	N-Methyl-2-pyrrolidone production	RER	ecoinvent 3	Manufacture of basic chemicals
Aniline	Market for aniline	GLO	ecoinvent 3	Manufacture of basic chemicals
Acetic anhydride	Market for acetic anhydride	RER	ecoinvent 3	Manufacture of basic chemicals
Terephthalic acid	Terephthalic acid	RER	PlasticsEurope	PlasticsEurope
Nitric acid	Nitric acid (38% HNO3)	EU-28	FertilizersEurope	FertilizersEurope
Hydrochloric acid	Hydrochloric acid mix (100%)	DE	ts	Inorganic intermediate products
Graphite	Graphite production	RER	ecoinvent 3	Other mining and quarrying n.e.c.
Lubricating oil	Market for lubricating oil	GLO	ecoinvent 3	Manufacture of refined petroleum products
Zirconium oxide	Market for zirconium oxide	GLO	ecoinvent 3	Manufacture of basic chemicals
Carbon monoxide	Market for carbon monoxide	RER	ecoinvent 3	Manufacture of basic chemicals
Decarbonized water	water production and supply, decarbonized	RER	ecoinvent 3	Water collection, treatment and supply
Deionized water	Water (deionized)	EU-28	ts	Water
Industrial machine production	industrial machine production, heavy, unspecified	RER	ecoinvent 3	Manufacture of machinery for mining, quarrying and construction
Plaster mixing	market for plaster mixing	GLO	ecoinvent 3	Manufacture of cement, lime and plaster
Electricity	Electricity grid mix	DE	ts	Electricity grid mix
Heat	Thermal energy from Natural gas (EU-28) (plan)	EU-28	ts	Thermal energy (fuel prod/combustion)
Steam	Process steam from Natural gas 30% (EU-28)	EU-28	ts	Steam (fuel prod/combustion)
Material	Dataset in GaBi - flows into AEL production	Nation	Source	Parent Folder
Copper	Copper (valuable)		ts	Metals
Unalloyed steel	Steel (valuable)		ts	Metals
Nickel	Nickel (valuable)		ts	Metals
Aluminium	Aluminium (valuable)		ts	Metals
Calendered rigid plastic	Polyvinylchloride-sheet (PVC)		ts	Plastic parts
Polytetrafluoroethylene	Polytetrafluoroethylene granulate (PTFE) (valuable)		ts	Plastics
Acrylonitrile butadiene styrene	Acrylonitrile butadiene styrene (ABS) (valuable)		ts	Plastics
Polyphenylene sulfide	Polyphenylene sulfide granulate (PPS) (valuable)		ts	Plastics
Polysulfones	Polysulfone (PSU) (valuable)		ts	Plastics
N-Methyl-2-pyrrolidone	n-Methyl pyrrolidone (valuable)		ts	Organic intermediate products
Aniline	Aniline (valuable)		ts	Organic intermediate products
Acetic anhydride	Acetic anhydride (valuable)		ts	Organic intermediate products
Terephthalic acid	Terephthalic acid (valuable)		ts	Organic intermediate products
Nitric acid	Nitric acid (38%) (valuable)		ts	Inorganic intermediate products
Hydrochloric acid	Hydrochloric acid (100%) (valuable)		ts	Inorganic intermediate products
Graphite	Graphite (valuable)		ts	Inorganic intermediate products
Lubricating oil	Lubricating oil (valuable)		ts	Operating minerals
Zirconium oxide	Zirconium oxide (valuable)		ts	Inorganic intermediate products
Carbon monoxide	Carbon monoxide (valuable)		ts	Inorganic intermediate products
Decarbonized water	Water (decarbonized, softened) (valuable)		ts	Operating minerals
Deionized water	Water (deionized)		ts	Operating minerals
Industrial machine production	Industrial machine, heavy, unspecified		EI	Allocatable product
Plaster mixing	Plaster mixing		EI	Allocatable product
Electricity	Electricity (valuable)		ts	Electric power
Heat	Thermal energy from heating (MJ) (valuable)		ts	Thermal energy
Steam	Steam (MJ) (valuable)		ts	Steam
Material	Dataset in GaBi - transport	Nation	Source	Parent Folder
Transport	Templates by IVL - Transport			
Material	Dataset in GaBi - processes into hydrogen production	Nation	Source	Parent Folder
Electricity	Electricity grid mix	SE	ts	Electricity grid mix
Deionized water	Water (deionized)	EU-28	ts	Water
Nitrogen	Nitrogen (gaseous)	EU-28	ts	Inorganic intermediate products
KOH	potassium hydroxide production	RER	ecoinvent 3	Manufacture of basic chemicals
Steam	Steam production, in chemical industry	RER	ecoinvent 3	Steam and air conditioning supply
Electricity	Electricity from nuclear	SE	ts	Electricity from nuclear power
Electricity	Electricity from hydro power	SE	ts	Electricity from hydro power
Electricity	Electricity from wind power	SE	ts	Electricity from wind power
Material	Dataset in GaBi - flows into hydrogen production	Nation	Source	Parent Folder
Electricity	Electricity (valuable)		ts	Electric power
Deionized water	Water (deionized) (valuable)		ts	Operating minerals
Nitrogen	Nitrogen gaseous (valuable)		ts	Inorganic intermediate products
KOH	Potassium hydroxide (potash) (valuable)		ts	Inorganic intermediate products
Steam	Steam, in chemical industry		EI	Allocatable product
Hydrogen (output)	Hydrogen (valuable)		ts	Other fuels
Oxygen (output)	Oxygen		ts	Inorganic emissions to air

## Other Datasets

Datasets for the material comparison in Figure 10 are presented in Table A 3.

*Table A 3. Chosen datasets for comparison of nickel and platinum.*

<b>Dataset in GaBi</b>	<b>Nation</b>	<b>Source</b>	<b>Parent Folder</b>
market for nickel, 99.5%	GLO	ecoinvent	Manufacture of basic precious and other non-ferrous metals
Platinum mix	GLO	ts	Metal production

Datasets for the comparison of electricity grid mixes in Figure 11 are presented in Table A 6.

*Table A 4. Chosen datasets for comparison of electricity grid mixes.*

<b>Dataset in GaBi</b>	<b>Nation</b>	<b>Source</b>	<b>Parent Folder</b>
Electricity grid mix	DE	ts	Electricity grid mix
Electricity grid mix	NO	ts	Electricity grid mix
Electricity grid mix	EU-28	ts	Electricity grid mix

## Appendix 3. Assumptions for Materials

*Table A 5. Assumptions for materials not found in GaBi. The table states the material in data source, i.e. what material is in the electrolyzer. The table also shows what was chosen instead of that material and a short explanation of the assumption.*

Technology	Material in data source	Chosen dataset in GaBi	Source /explanation
AEL	Calendered rigid plastic	Polyvinylchloride-sheet (PVC)	The main material produced with the calendering process is PVC sheets. [60]

## Appendix 4. Calculations

Some smaller calculations have been performed within this thesis, which will be presented in this appendix.

### Capacity MCFC to capacity MCEC

For the MCEC, all data was obtained for a molten carbonate fuel cell with a capacity of 135 kW. To use the data for an MCEC instead, the capacity must be converted to apply for an electrolyzer rather than a fuel cell. This is done using Faraday's law.

$$Q = n * F$$

Where F is Faraday's constant, 96 485 [C/mol] and Q is the charge [Coulomb] and n is the amount of mole produced. For a fuel cell with a capacity of 135 kW, assumed to be run at 0.9 V (typical cell voltage for fuel cells [46]), the current is calculated.

$$135\,000 \left[ \frac{J}{s} \right] * \frac{1}{0.9} \left[ \frac{A * s}{J} \right] = 150\,000 \text{ A}$$

The unit  $\left[ \frac{A*s}{J} \right]$  is another way of expressing voltage, V, which can also be expressed as 150 000 C/s ([C] = [As]). The molar flow of hydrogen gas can then be calculated.

$$n = \frac{Q}{F} = 150\,000 \left[ \frac{C}{s} \right] * \frac{1}{96\,485} \left[ \frac{mol}{C} \right] * \frac{1}{2} = 0.77732.. mol H_2/s$$

The capacity needed in an electrolyzer to reach the same molar flow must now be calculated. The electrolyzer is assumed to be run at 1.1 V (typical cell voltage for electrolyzers [46]). The current must be the same as the fuel cell, 150 000 A.

$$150\,000 [A] * 1.1 \left[ \frac{J}{A * s} \right] = 165\,000 \frac{J}{s} = 165 \text{ kW}$$

In other words, 135 kW capacity for the molten carbonate fuel cell translates into 165 kW for the molten carbonate electrolyzer, which is then used as basis for further calculations for the MCEC.

### Produced hydrogen during lifetime

To convert the inventory data for the electrolyzers given in [kg] to per functional unit, i.e. [kg / 100 kg H<sub>2</sub>], the amount of hydrogen that the electrolyzer is assumed to produce during its lifetime must be calculated. This calculation was made for both AEL and MCEC. To show how the calculations were made, AEL will be presented as the example. The capacity of the electrolyzer that the data was retrieved for was 6 MW, or 6 000 kJ/s. The capacity is defined as electricity input into the electrolyzer. The parameters needed for the calculations are given in Table A 6. The information on efficiency and lifetime is taken from several sources, and the number used is in the middle of the range that was obtained from these sources.

*Table A 6. Parameters for unit conversion AEL.*

Parameter	Value	Unit
H <sub>2</sub> energy content [6]	119 800 (LHV)	kJ/kg
Capacity AEL [36]	6 000	kJ/s
Efficiency AEL [6], [38], [44], [50]	72	%
Lifetime AEL [37], [39], [40]	80 000	h

The energy per second out from the electrolyzer is calculated using the efficiency of the electrolyzer.

$$6\,000 \left[ \frac{kJ}{s} \right] * 0.72 = 4\,320 \frac{kJ}{s}$$



Then, the amount of hydrogen that translates to is calculated.

$$4\,320 \left[ \frac{kJ}{s} \right] * \frac{1}{119\,800} \left[ \frac{kg}{kJ} \right] * 3\,600 \left[ \frac{s}{h} \right] = 130 \frac{kg\ H_2}{h}$$

Lastly, the amount of hydrogen that adds up to over the lifetime of the electrolyzer is calculated.

$$130 \left[ \frac{kg\ H_2}{h} \right] * 80\,000 [h] = 10\,378\,378\ kg\ H_2$$

That is, the specific AEL that data was retrieved for during this study is assumed to produce 10 378 378 kg of hydrogen gas during its lifetime.

The amount of hydrogen that the specific MCEC is assumed to produce during its lifetime was calculated in the same way. The information lifetime is taken from several sources, and the number used is in the middle of the range that was obtained from these sources, i.e. 40 000 operating hours for MCEC. The efficiency for MCEC is assumed to be 100%.

## Produced Oxygen

The functional unit in this study is 100 kg H<sub>2</sub>. To perform a mass balance over the system, the amount of produced O<sub>2</sub> for every 100 kg of H<sub>2</sub> must be calculated. The molar weights of hydrogen and oxygen gas are presented in Table A 7.

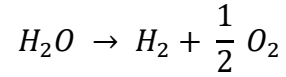
*Table A 7. Molar weights of H<sub>2</sub> and O<sub>2</sub>. [64]*

Molar Weight	Value	Unit
H <sub>2</sub>	2.02	kg/kmol
O <sub>2</sub>	32.0	kg/kmol

First, 100 kg H<sub>2</sub> is converted to moles

$$100 \text{ [kg]} * \frac{1}{2.02} \left[ \frac{\text{kmol}}{\text{kg}} \right] = 49.6 \text{ kmol } H_2$$

The main reaction taking place during electrolysis is the following



I.e., for every mole of hydrogen gas produced, one half mole of oxygen gas is produced.

Therefore, the molar ratio of O<sub>2</sub> to H<sub>2</sub> is 0.5. Knowing this, the amount of produced O<sub>2</sub> per 100 kg H<sub>2</sub> is readily calculated.

$$0.5 * 49.6 \text{ [kmol]} * 32.0 \left[ \frac{\text{kg}}{\text{kmol}} \right] = 794 \text{ kg } O_2$$

Accordingly, for every 100 kg of H<sub>2</sub> produced, 794 kg O<sub>2</sub> is produced.

