DEPARTMENT OF CHEMICAL ENGINEERING

# A prospective comparative lifecycle assessment for green and grey hydrogen production and utilisation in the South African context

Prepared by

Ongezwa Mbaba

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Supervisors

Harro Von Blottnitz

Fadiel Ahjum

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# ABSTRACT

Green hydrogen has gathered increasing interest as a medium in the transition to a carbon-neutral economy, with several large, export-focused projects currently under development in Southern Africa. However, the environmental implications of hydrogen production and utilisation are not well understood. To address this challenge, a comprehensive literature review for hydrogen production and utilisation lifecycle assessment studies was conducted, and two prospective comparative lifecycle assessments are presented for green and grey hydrogen production and utilisation in the South African context. The first LCA aims to quantify the environmental impacts of producing green hydrogen, relative to grey hydrogen, and determine the production route with the least environmental impacts. The scenarios investigated for hydrogen production are water electrolysis powered by wind, solar PV or concentrated solar power, steam methane reforming, and water electrolysis powered by a 2040 grid electricity mix. Furthermore, the impacts of three available electrolysis technologies; viz. polymer electrolytic membrane (PEM), alkaline, and solid oxide electrolysis were compared.

The second LCA aims to compare two systems of utilisation for the green hydrogen that would be produced in South Africa to determine the option where the highest level of decarbonisation could be achieved. The application considered for the assessment is the fuelling of heavy-duty truck transportation. The systems considered are local utilisation for fuelling heavy-duty trucks and hydrogen exportation to Germany also to fuel heavy-duty trucks. These two systems were expanded to include conventional fuel utilisation, making the functional units of the systems equal and thus the systems comparable.

SimaPro was used to conduct the two LCAs, and the ReCiPe 2016 midpoint method was used for the lifecycle impact assessments. Grid-powered water electrolysis is found to have the highest potential impacts across most impact categories, even for the case of the significantly decarbonised 2040 grid mix, with SMR second. Solar PV-powered electrolysis leads to the highest potential human non-carcinogenic toxicity impact caused, by the supply chains of PV panels. Wind-powered water electrolysis is the least impactful option across most categories. However, it has the highest potential human carcinogenic toxicity impact among the renewable production options, though it is less than half compared to the value for non-renewable hydrogen production. This toxicity is caused by the supply chains of wind turbines. Considering optimal electrolyser utilisation, combined wind and solar PV-powered electrolysis is the best option. When comparing the water electrolysis technologies, PEM electrolysis leads to the highest environmental impacts. The energy input for production dominates all the impacts. In terms of utilisation, the environmental impact reductions achievable by the export case outweigh the environmental impact reductions achievable by using the green hydrogen locally, across all impact categories. The highest level of decarbonisation is achieved by replacing the most environmentally harmful fuel; South African coal-based diesel used to fuel heavy-duty trucks.

The results of the first LCA confirm that green hydrogen is indeed significantly less environmentally impactful compared to grey hydrogen, but with one hotspot for each of the PV and wind-powered electrolysis, which require attention by project developers. The environmental impacts of all the production scenarios are dominated by the energy required for the production processes. The main finding for the second LCA is that local hydrogen utilisation for heavy-duty truck transportation leads to a larger environmental benefit compared to hydrogen exportation in the case of usage for heavy-duty truck transportation in another country. The highest level of decarbonisation is achieved by displacing South African coal-based diesel first.

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## LIST OF ACRONYMS

| | |
|---|---|
| AWARE | Available water remaining |
| BEV | Battery electric vehicles |
| BoP | Balance of plant |
| CAC | Critical air contaminants |
| CSIR | Council for scientific and industrial research |
| CSP | Concentrated solar power |
| DCB | Dichlorobenzene |
| DSI | Department of Science and Innovation |
| ESMAP | Energy sector management assistance program |
| ETC | Energy transition commission |
| FCH | Fuel cell and hydrogen |
| FRS | Fossil resource scarcity |

| | |
|---|---|
| FU | Functional unit |
| GHG | Greenhouse gases |
| GW | Global warming |
| HcT | Human carcinogenic toxicity |
| HFCEV | Hydrogen fuel cell electric vehicles |
| HncT | Human non-carcinogenic toxicity |
| HySA | Hydrogen South Africa |
| IA | Impact assessment |
| IEA | International energy agency |
| IRENA | International renewable energy agency |
| IRP | Integrated resource plan |
| ISO | International organisation of standardisation |
| LCA | Lifecycle assessment |
| LCI | Lifecycle inventory |
| NDC | Nationally determined contribution |
| NDP | National development plan |
| NRF | National research foundation |
| PEM | Polymer electrolytic membrane |
| PGM | Platinum group metals |
| PV | Photovoltaic |
| SDGs | Sustainable development goals |
| SRU | Single repeating unit |
| SMR | Steam methane reforming |
| TA | Terrestrial acidification |
| UNFCCC | United Nations framework convention on climate change |

## LIST OF CHEMICAL COMPOUNDS

| | |
|---|---|
| $CH_{0.8}$ | Coal |
| $CH_4$ | Methane |
| CO | Carbon monoxide |
| $CO_2$ | Carbon dioxide |
| DCB | Dichlorobenzene |
| $H_2$ | Hydrogen |
| $H_2O$ | Water |
| KOH | Potassium hydroxide |
| $NH_3$ | Ammonia |
| $O_2$ | Oxygen |
| Sb | Antimony |
| $SO_2$ | Sulphur dioxide |

# 1. INTRODUCTION

## 1.1. Background

Global warming and climate change have been recognised as a threat to the earth and its inhabitants. Reducing carbon emissions toward climate change mitigation and achieving climate neutrality is an urgent global priority. In 2020, the International Energy Agency (IEA) reported that the energy-related global carbon dioxide emissions amounted to 31.5 Gt (IEA, 2021). In South Africa, the total carbon dioxide emissions were 435 Mt (Tiseo, 2021). These emissions mainly result from industry and the utilisation of fossil fuels (Tiseo, 2021). The share of coal in the 2020 South African electricity generation mix was 82% (Calitz and Wright, 2021). Contrarily, the combined share of renewable energy comprising solar PV concentrated solar power and wind power was 5.4% (Calitz and Wright, 2021). South African energy supply is mainly dependent on coal.

In partnership with other countries, South Africa signed the Paris agreement, which is a commitment to keep global warming levels below 2°C and possibly reduce the levels to 1.5°C. The Paris agreement resulted from a United Nations conference in 2015 referred to as the United Nations Framework Convention on Climate Change (UNFCCC) (Modise, 2016). As a response and plan of action in line with the Paris agreement, each country, including South Africa, has a nationally determined contribution (NDC) framework, which outlines the climate change mitigation targets the country has to meet to honour the goals of the Paris agreement. Renewable energy alternatives have a significant role in climate change mitigation due to the energy-related emission reductions that could be achieved, and the lack of fossil fuel dependence associated with them.

Hydrogen is a viable energy alternative that can significantly contribute to a low carbon economy. It is a secondary form of energy that can be produced from primary sources such as coal and natural gas. Different hydrogen types are termed based on their production routes. Grey hydrogen is produced from steam methane reforming. Steam methane reforming is the conventional production route for hydrogen in regions such as the United States and the United Kingdom, as well as in South Africa, and it is highly carbon-intensive.

Hydrogen produced by water electrolysis, powered by renewable energy sources such as wind or solar energy, is green hydrogen. This production route is a potential zero-carbon option, as it does not include the burning of fossil fuels. Other types of hydrogen are blue hydrogen produced via steam methane reforming and accompanied by carbon capture and storage, black hydrogen produced by coal gasification, and brown hydrogen produced from lignite (ESMAP, 2020). Hydrogen has various applications in different sectors. It can be used in the chemical industry as a chemical feedstock. It can be used in the transport sector for hydrogen fuel cell-powered vehicles. It could also decarbonise the steel, cement, and aviation fuel industries, which are high carbon emitters.

### *1.1.1. Hydrogen landscape in South Africa*

The hydrogen landscape in South Africa is currently made up of grey hydrogen production and utilisation. The grey hydrogen is produced by Sasol via the steam methane reforming process. The hydrogen is produced at low quality, and it is primarily used to produce ammonia which serves as a fertiliser (Hoffmann, 2019). There is, however, accelerating traction towards the large-scale production of green hydrogen in South Africa. South Africa is well located and resourced to produce green hydrogen at a large scale due to the wind and solar resources availability (Roos and Wright, 2021). The South African president, President Cyril Ramaphosa, has even mentioned hydrogen as one of the national priorities due to its potential as an energy alternative (Engie Impact, 2021). Additionally, there is a great availability of platinum group metals that are used to manufacture PEM electrolysers and PEM fuel cells. This availability of PGMs in South Africa is one of the reasons, PEM electrolysis among other electrolysis technologies, is the chosen pick for South Africa.

A few authors have studied the potential of green hydrogen production in South Africa. Ayodele and Munda (2019) conducted an assessment of the wind regime of fifteen sites across South Africa to produce wind-powered hydrogen. The electrolyser used for the assessment was the polymer electrolytic membrane (PEM) electrolyser due to platinum availability in South Africa. It was found that Napier, in the Western Cape, has the best potential for wind-powered hydrogen production because it resulted in the highest amount of hydrogen produced. An economic analysis was conducted to determine the costs of wind power. The analysis revealed that the wind turbines with the best capacity factor result in the lowest energy costs (Ayodele and Munda, 2019). Another study was conducted by Hoffmann (2019) and is focused on investigating the feasibility of solar thermal powered hydrogen in South Africa. The sites considered were Upington, Saldanha bay and Sasolburg. This study explored multiple ways to include solar thermal technologies in hydrogen production processes (Hoffmann, 2019). Some of these options were solar and wind-powered low-temperature alkaline electrolysis and solar-powered steam methane reforming. The overall conclusion of this study highlighted that South Africa has the solar PV and wind power capacity to implement carbon-free hydrogen production.

There has also been progress towards research focused on hydrogen knowledge in South Africa. The South African Department of science and innovation (DSI) developed a national fuel cells and hydrogen (FCH) development and innovation strategy termed Hydrogen South Africa (HySA). HySA aims to develop the country's knowledge, skills, resources, and processes towards the realisation of large-scale implementation of FCH technologies (Bessarabov et al., 2017). HySA comprises three centres of competency: HySA Catalysis, HySA Systems and HySA infrastructure. Hydrogen production technologies fall under the HySA infrastructure centre. According to the timeline of the programme, HySA is supposed to be in its third phase, which is the implementation and commercialisation of hydrogen and fuel cell technologies.

Due to the potential of large scale hydrogen production in South Africa, the Department of Science and innovation partnered up with other organisations to create a hydrogen valley feasibility project which outlines locations in South Africa that could be hydrogen production hubs and outlines the potential local demand for the hydrogen that would be produced in these hubs (Engie Impact, 2021). These hubs are Johannesburg which would mostly serve the mobility sector; Mogalakwena, which would mainly serve the mining sector; and Richards Bay, primarily serving as a hydrogen export hub (Engie Impact, 2021). The combined local hydrogen demand that these hubs would fulfil is expected to be 185 kt by 2030 (Engie Impact, 2021). In addition to Richards Bay, other ports considered potential export hubs for hydrogen are Port of Saldanha Bay, Boegoebaai Port and Port of Ngqura.

The department of science and innovation has also launched a hydrogen society roadmap, a framework for the development of hydrogen production and utilisation in various south African sectors (DSI, 2021). This roadmap also outlines how a hydrogen society would economically benefit the country. Some of the outcomes planned to be achieved in 2050, as outlined on the roadmap, are; the decarbonisation of heavy-duty trucks transportation, decarbonisation in industries such as cement, mining, steel and refineries, the development of export demand for the renewable hydrogen produced in South Africa, and the increased utilisation of renewable hydrogen in South African energy systems. (DSI, 2021).

### *1.1.2. Global Hydrogen Landscape*

The global hydrogen landscape is also currently dominated by grey hydrogen. In 2019, 96% of the global market of hydrogen was made up of fossil fuel-based hydrogen production processes, which are oil reforming, steam methane reforming, and coal gasification (ESMAP, 2020). Steam methane reforming made up 48% of the global market. Green hydrogen only made up 4% of the hydrogen market (ESMAP, 2020). Green hydrogen developments and initiatives are taking place all over the world. The Energy Transition Commission (ETC), an international organisation aiming to achieve net-zero carbon emissions by 2050, published a net-zero summary report. This report discussed ways in which a net-zero economy can be achieved, including using renewable hydrogen as a cleaner energy alternative. The application sectors of hydrogen discussed were the shipping and aviation sectors as well as the cement sector due to these sectors being energy-intensive and difficult to decarbonise (Energy Transitions Commission, 2020). The energy transition is expected to contribute to a significant decline in the demand for fossil fuel energy such as oil, natural gas, and coal.

Some countries and regions have released hydrogen roadmaps which entail the energy transition plans and projections of the respective countries towards a hydrogen economy. The Europe hydrogen roadmap estimated that hydrogen could make up 24% of the energy demand in Europe by 2050, and could significantly contribute to employment (Fuel Cells and Hydrogen Joint Undertaking, 2019). The applications for which hydrogen would be used were estimated to be heavy-duty transport and chemical feedstock for industrial processes. The United States roadmap also estimated 2050 as the period to achieve the US goals towards a low carbon energy mix (US hydrogen study, 2020). By 2050, renewable energy sources such as wind, solar and hydropower are expected to fulfil approximately 85% of global electricity demand (PWC South Africa, 2021).

Japan released a hydrogen strategy roadmap intending to achieve a net-zero economy in 2050. Japan is mainly focused on reducing the cost of hydrogen production. Some of the goals outlined in Japan's Hydrogen roadmap are to have large scale hydrogen production in 2030, the utilisation of hydrogen in multiple sectors in 2050, 800 000 hydrogen fuel cell vehicles in 2030 and 900 hydrogen fuelling stations in 2030 (New Zealand Embassy, 2020).

Australia also has a national hydrogen roadmap. The main aim of the national hydrogen roadmap is to implement some of the economic opportunities related to green hydrogen (Bruce et al., 2018). Some of Australia's hydrogen priorities are to have affordable renewable electricity that would power green hydrogen and position hydrogen production plans close to hydrogen utilisation points to minimise hydrogen transportation requirements. And to have joint ventures to invest in hydrogen refuelling stations (Bruce et al., 2018).

Countries across the world are currently forming partnerships to help one another create hydrogen-driven economies. One such partnership exists between Germany and Namibia. These two countries have jointly signed an agreement of intent for a partnership based on the development of green hydrogen technologies (Smith, 2021). Namibia has great potential as a mass producer of hydrogen due to its wind and solar power potential (Naujokaityte, 2021). As part of this agreement, Germany is planning to invest €40 million to aid projects and initiatives towards green hydrogen production in Namibia (Naujokaityte, 2021).

### 1.1.3. *Contribution of green hydrogen to sustainable development*

Green hydrogen production and utilisation have the potential to contribute to long term sustainable development and the achievement of the sustainable development goals (SDGs). The sustainable development goals are seventeen global goals that were set up and agreed upon by 193 countries in the United Nations General Assembly in 2015. These goals are a core part of the 2030 Agenda for Sustainable development that resulted from the General assembly. The adoption of green hydrogen technologies and utilisation in different sectors would contribute to the $7^{th}$, $9^{th}$, and $13^{th}$ SDGs: affordable clean energy, industry, innovation and infrastructure, and climate action, respectively.

Green hydrogen provides a cleaner and more sustainable energy alternative to fossil fuel-based energy systems. The progression of renewables over the years is expected to result in renewables being more affordable. South African research on green hydrogen technologies contributes to industry, innovation, and infrastructure in that it provides valuable South African based information and knowledge about hydrogen production and utilisation. Climate action and clean energy go hand in hand because the energy sector is responsible for a significant portion of greenhouse gas emissions, leading to global warming and climate change. Green hydrogen as an energy alternative could cause a substantial reduction in carbon emissions; therefore, it has the potential to positively contribute to climate change mitigation.

## 1.2. Problem statement

Green hydrogen has gained accelerating interest as a clean energy alternative from various organisations such as government and investors towards environmental sustainability. Several initiatives are being developed for large scale hydrogen production and utilisation in South Africa. Although the potential of green hydrogen in the energy transition is being explored, the main problem observed is that the lifecycle material and energy requirements, and the environmental impacts of green hydrogen production and utilisation are not well understood, due to a lack of South African-based lifecycle assessment studies for hydrogen. Thus, the people and organisations with decision making power towards climate sustainability cannot make fully informed decisions and develop policies to aid the transition to a carbon-neutral economy.

## 1.3. Key objectives of the dissertation and research approach

Based on the problem statement, the key objectives of the dissertation are:

- To conduct a comprehensive literature review for the application of the lifecycle assessment methodology to hydrogen production and utilisation studies
- To conduct a prospective lifecycle assessment for various hydrogen production methods in the South African context
- To conduct a sequential prospective lifecycle assessment for hydrogen utilisation of the green hydrogen that would be produced in South Africa

In contributing to building South African based knowledge for hydrogen as an energy alternative, the lifecycle assessment tool is the core of the research approach. Lifecycle assessment is an analytical tool used to quantify a process or a product's material and energy flows throughout its lifecycle and assess its lifecycle environmental impacts. This tool can be used to gain a broader understanding of the implications of a given product and find out which parts of its lifecycle result in the most significant impacts. It can also be used to compare products and processes and make informed decisions on sustainable and environmentally friendly products and processes.

## 1.4. Scope of dissertation

Life cycle assessment studies can be done in three categories: environmental, social, or economic-based. Social life cycle assessments focus on social impact, and the economic-based studies are life cycle costing assessments. The environmentally-focused studies are environmental lifecycle assessments. Given the objectives of the dissertation, the assessments conducted are environmental lifecycle assessments.

## 1.5. Dissertation structure

This dissertation is structured into six chapters. Chapter 1 is the introduction and background, which sets the scene for the importance of carrying out the dissertation objectives. Chapter 2 is the literature review where an overview of hydrogen production and utilisation is given, and lifecycle focused studies for hydrogen production and utilisation are reviewed. Chapter 3 comprises the hypotheses of the dissertation informed by the literature review and dissertation objectives. It also lays out the methodology followed for the dissertation, which entails the goal and scope of each lifecycle assessment. Chapter 4 entails the inventory and impact assessment results of the hydrogen production lifecycle assessment. Chapter 5 entails the inventory and impact assessment results of the hydrogen utilisation lifecycle assessment. Chapter 6 is the concluding chapter of the dissertation. It lays out the conclusions drawn from the lifecycle assessments and recommendations for further research and industrial practice.

# 2. LITERATURE REVIEW

This chapter discusses the different hydrogen production methods available and some applications for green hydrogen. Thereafter, it goes into an overview of the LCA methodology. Next, a critical review is conducted for the application of the LCA methodology to hydrogen production and utilisation studies, and the limitations observed during the critical review are discussed. Lastly, the chapter is summarised.

## 2.1. Hydrogen production

There are various production pathways for hydrogen. The conventional methods to produce hydrogen are steam methane reforming and coal gasification. The steam methane reforming process produces hydrogen from natural gas. Before the steam methane reforming begins, natural gas is treated to remove sulphur compounds such as hydrogen sulphide (Spath and Mann, 2001). After this treatment, the natural gas and steam are fed to a steam reformer. Some of the natural gas is also used to fulfil a portion of the fuel requirement for the reformer. The reactions in the reformer produce synthesis gas. The following steps are to feed the synthesis gas to a high pressure and a low-pressure water gas shift reactor, where carbon monoxide is reacted with water to convert it to carbon dioxide and produce more hydrogen (Spath and Mann, 2001). The hydrogen is then purified in a pressure swing absorption unit to produce a purified hydrogen stream (Spath and Mann, 2001).

The following reaction occurs during the steam methane reforming process (Jakobsen and Åtland, 2016)

$$CH_4 + H_2O \leftrightarrow CO + 3H_2$$

*Equation 2. 1: steam methane reforming reaction*

The following equation represents the water gas shift reaction (Jakobsen and Åtland, 2016)

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

*Equation 2. 2: water gas shift reaction*

The coal gasification process uses coal to produce hydrogen. The coal is oxidised using oxygen and steam in a reactor operating at a high temperature (Acar and Dincer, 2014). A syngas results from this reactor mainly containing hydrogen, steam, carbon monoxide, and carbon dioxide. The syngas undergoes a water gas shift reaction to produce more hydrogen. The resulting hydrogen sulphide is treated using the Claus and SCOT process to remove the sulphur content (Wulf and Kaltschmitt, 2012). Coal gasification is a highly carbon-intensive process because coal has a large percentage of carbon ranging from 60 to 80% (Acar and Dincer, 2014).

The coal gasification reaction is as follows (Mehmeti et al., 2018)

$$CH_{0.8} + O_2 + H_2O \leftrightarrow CO + CO_2 + H_2 + other\ gases$$

*Equation 2. 3: coal gasification reaction*

Hydrogen can also be produced via thermochemical water splitting. Cycles of thermochemical water decomposition are carried out in reactors operating at high temperatures of 500°C or above (Ozbilen, Dincer and Rosen, 2012). There are various types of these cycles, including copper-chloride (Cu-Cl), sulphur-Iodine (S-I), iron-chloride (I-Cl), and vanadium-chloride (V-Cl) cycles. Because these cycles operate at high temperatures, the construction materials are highly specialised and inert (Acar and Dincer, 2014). Each type is named according to the materials used and the number of reaction steps required Ozbilen, Dincer, and Rosen (2012) explain the thermochemical cycles in detail.

The current method of interest for producing hydrogen is water electrolysis. In this process, water is split into oxygen and hydrogen (Ahmadi and Kjeang, 2015). Electric current is used in an electrochemical reaction to carry out the split. The reaction is carried out in an electrolyser, consisting of two electrodes: a cathode and anode, and an electrolyte. The electrolyte separates the anode and cathode.

The overall electrolysis reaction is as follows (Bhandari, Trudewind and Zapp, 2014)

$$H_2O + Electricity \rightarrow H_2 + \frac{1}{2}O_2$$

*Equation 2. 4: water electrolysis reaction*

There are different electrolysis technologies available for hydrogen production. These technologies are alkaline electrolysis, polymer electrolyte membrane electrolysis (PEM), and solid oxide membrane electrolysis. For alkaline electrolysis, the liquid electrolyte is a solution usually made up of 20 to 30% potassium hydroxide (Carmo et al., 2013). A diaphragm is used to separate the anode and cathode and prevent mixing hydrogen and oxygen gas produced on the electrodes. PEM electrolysis uses a solid polymer membrane as an electrolyte, and the electrolysers are manufactured using noble metals such as platinum and iridium. Solid oxide electrolysis operates at higher temperatures (600-900°C) compared to alkaline and PEM electrolysis, and it uses a solid ceramic membrane as an electrolyte (Zhao et al., 2020). Figure 2.1 gives a schematic of an alkaline electrolysis cell. The solid oxide and PEM electrolysis cells look similar except for the liquid electrolyte because these two technologies use a solid electrolyte. Carmo et al. (2013) comprehensively compared the three technologies in terms of advantages and disadvantages. A summary of this comparison can be seen in Table 2.1.

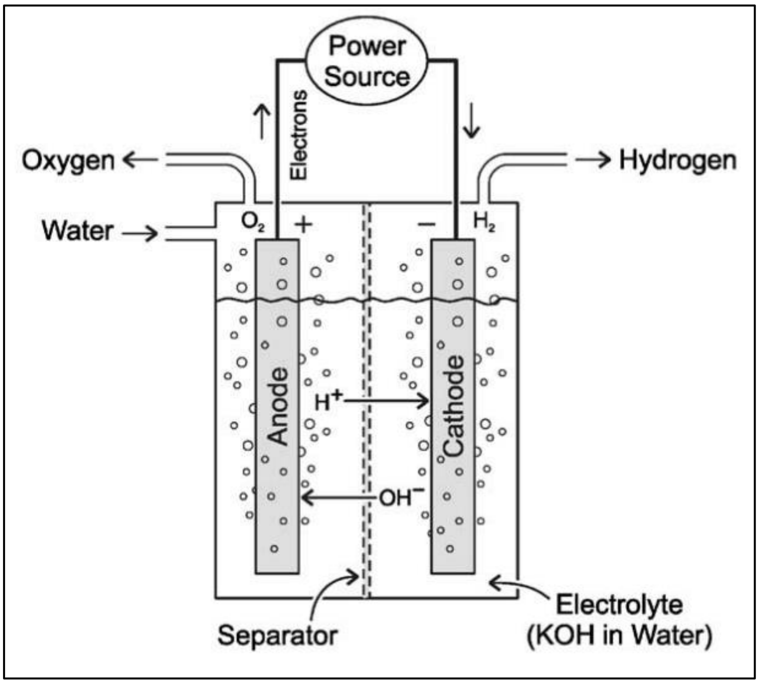


*Figure 2. 1: Schematic of an electrolytic cell (Koroneos et al., 2004)*

*Table 2. 1: Comparison of alkaline, PEM and solid oxide electrolysis (Carmo et al., 2013)*

| **Electrolysis technologies** | **Advantages** | **Disadvantages** |
|---|---|---|
| Alkaline electrolysis | • Mature and established technology<br>• Uses less noble metals<br>• Stability in the long term<br>• Cost-effective | • Operates at low current densities<br>• High gas crossover rates (decreases hydrogen purity)<br>• Liquid electrolyte is corrosive |
| PEM electrolysis | • Operates at high current densities<br>• Quick system response<br>• High hydrogen gas purity is achieved | • Uses expensive noble metals<br>• Presents a corrosive environment<br>• System durability is low |
| Solid oxide electrolysis | • No use of noble metals<br>• Operates at high temperatures (less energy input needed)<br>• High efficiencies up to 100% | • Immature technology (still in the lab and early development stage)<br>• Low durability of ceramic materials |

## 2.2. Hydrogen applications

Hydrogen has multiple applications in various sectors such as road transport, steel, cement, aviation, and the production of chemicals. In South Africa, grey hydrogen is the primary type of hydrogen produced, and it is mainly used to produce ammonia. Numerous initiatives and case studies are presently geared towards the large-scale production and utilisation of green hydrogen. Some of the initiatives focused on hydrogen utilisation have been discussed in Chapter 1 of the dissertation. For road transport, hydrogen can be used to power various types of fuel cell electric vehicles, such as passenger cars, medium and heavy-duty trucks, and buses. In aviation, hydrogen can be used to fuel aircraft by combusting it in a hydrogen burning engine or using it in fuel cell electric motors (Fuel Cells and Hydrogen Joint Undertaking, 2020). For iron and steel production, hydrogen replaces coal as a reducing agent for iron. For the mining industry, hydrogen can be used to fuel mining trucks. Hydrogen can be used in cement production to replace some of the fossil fuels used as energy sources. However, the level of decarbonisation that could be achieved is small because hydrogen cannot be used as a feed or a reactant in the cement production process (Bellona, 2022).

## 2.3. Overview of LCA approach

### *2.3.1. History of LCA*

The first lifecycle focused methods were conducted in the 1960s, and these methods were carried out internally in industry or universities. These methods were named resource profile analyses (Hauschild, Rosenbaum and Olsen, 2018). The first LCA study was presented in 1963, and it was focused on the production of chemical products. In the 1990s, the term lifecycle assessment started to be widely known and used (Hauschild, Rosenbaum and Olsen, 2018). The lifecycle assessment method was initiated and further developed in the United States and Europe.

Initially, the lifecycle assessment method was focused on the lifecycle inventory aspect where inventories regarding material and energy use and emissions from a product were collected. As time went by, just concentrating on the accounting of inventories was not enough, so the impact assessment aspect of the method was developed. The accounted inventories were translated into potential environmental impacts by applying a set of indicators to the inventory results (Hauschild, Rosenbaum and Olsen, 2018).

In the early years of developing the LCA methodology, the studies conducted were focused on whatever the public concern was, and public concerns changed from time to time. This subjectiveness caused a lacking in the development of lifecycle assessment methods because of the inconsistency and standardisation (Hauschild, Rosenbaum and Olsen, 2018). Most lifecycle assessment methods, particularly for the impact assessment, grew and developed in the 1990s and no longer followed the trend of public concerns.

Most lifecycle inventory databases were created in the 1990s and led by different organisations. These databases came with some limitations, such as the difference in data quality and shortage of data. The first ecoinvent database was created and released in 2003, and it brought solutions to the limitations of the initial lifecycle inventory databases (Hauschild, Rosenbaum and Olsen, 2018).

There are two ways of modelling a lifecycle assessment. The first is attributional, and it focuses on attributing the environmental impacts caused by a product's emissions and its resource use (Hauschild, Rosenbaum and Olsen, 2018). The second is consequential, and it is focused on the consequences of the decisions that are made from the results of a lifecycle assessment (Hauschild, Rosenbaum and Olsen, 2018). Due to the difficulties of the modelling lifecycle inventories and conducted impact assessments, LCA software had to be developed. In 1990, the first GaBi and SimaPro software versions were released (Hauschild, Rosenbaum and Olsen, 2018). These software packages have continued to develop and improve over the years, and they are presently widely used to conduct lifecycle assessment studies.

An international standardisation was conducted for LCA methodologies to address inconsistency concerns from companies and industries that wanted to use lifecycle assessment methods to create sustainable and more environmentally friendly products. In 1997 the first LCA standard was created through the international organisation of standardisation (ISO) (Hauschild, Rosenbaum and Olsen, 2018). The standard grew into four main standards: the ISO14040 for the LCA principles, the ISO 14041 for the goal and scope, the ISO 14042 for the impact assessment, and the ISO 14043 for the interpretation phase (Hauschild, Rosenbaum and Olsen, 2018).

### *2.3.2. Application of LCA to sustainability*

The term sustainability encompasses social, environmental, and economic aspects. (Matthews, Hendrickson and Matthews, 2014). Sustainable development refers to current development and provision for the current needs of people, which does not compromise the ability of future generations on earth to meet their needs (Matthews, Hendrickson and Matthews, 2014). People and organisations who have the decision-making power for developing policies towards achieving sustainability, such as the government, do not have all the information required to make these important decisions. Lifecycle thinking and having a systems perspective of products and services can be used as a tool to inform decision makers of the lifecycle consequences of producing and using certain products and services. This information would assist in making more informed decisions towards sustainable products and services.

Lifecycle thinking and lifecycle assessment conduct environmental hotspot analyses for products and services (Matthews, Hendrickson and Matthews, 2014). Hotspots are aspects of the lifecycle that have significant contributions towards the environmental impacts of a particular product or service. These hotspots can be identified for processes across the lifecycle and a wide range of environmental impact indicators such as climate change, human toxicity, and resource scarcity. Additionally, conducting lifecycle assessments helps avoid creating solutions that are only suitable for one aspect of a product's lifecycle but detrimental to another part of the lifecycle (Hauschild, Rosenbaum and Olsen, 2018). The creation of solutions thus considers all aspects of a lifecycle.

Lifecycle assessments are quantitative; they can be used to compare the environmental impacts of different products and services and to make informed decisions on which products are the most sustainable. To generate quantitative results for LCAs, the emissions and resource use of all the processes of a product's lifecycle are mapped, and a range of factors considering relevant cause-effect chains are used to transform these emissions and resource use amounts into quantities of environmental impacts (Hauschild, Rosenbaum and Olsen, 2018).

While lifecycle thinking serves as a helpful tool to support decision making towards sustainability it does not necessarily ensure sustainable products and services. To achieve sustainability in terms of reducing the environmental burdens of products and services, it is essential to use the results and findings from lifecycle studies to change and improve the processes making up a product's lifecycle. The lifecycle assessment tool cannot work as a stand-alone tool. Instead, it can be used with other tools such as risk analysis, cost-benefit analysis, and environmental management (Matthews, Hendrickson and Matthews, 2014). A combination of these tools thus fully addresses the environmental impacts of current products and services and work towards reducing them. Furthermore, it promotes a more sustainable design of products and services.

### *2.3.3. LCA framework*

The lifecycle assessment framework, which complies with the ISO LCA standard, comprises four main phases: the goal and scope definition, the lifecycle inventory analysis, the lifecycle impact assessment, and the lifecycle interpretation. The goal and scope outline the aim and intention behind the LCA. The lifecycle inventory analysis involves modelling the lifecycle material and energy flows of a product or service. The lifecycle impact assessment quantifies the environmental impacts associated with the material and energy flows, and the lifecycle interpretation phase evaluates the results of the assessment.

Goal and scope

According to the ISO LCA standard, the goal statement of an LCA is supposed to explain the aim of the study, the reasons for conducting the study, the target audience of the study and if the results are intended to be published publicly. The scope of the study should contain important information about the key parameters being used in the study. Some of these parameters are the product system, the functional unit, the system boundary considered, important inventory data to be collected, and the impact assessment categories of concern (Matthews, Hendrickson and Matthews, 2014).

The product system refers to the input flows and processes making up the product or service being studied. The functional unit states a defined quantity that relates the function fulfilled by the product system to the input and output flows that make up the product system. The system boundary outlines the inputs and processes related to the studied product system. It is usually shown as a block flow diagram or process flow diagram. The inventory data collection states the important lifecycle material and energy flows making up the lifecycle inventory model. Lastly, the impact categories relevant to the goal and scope of the study are explained.

Lifecycle inventory analysis

According to the ISO standards, the steps that should be followed to conduct the lifecycle inventory analysis are preparing to collect the inventory data, data collection, data validation, data allocation, linking the collected data to the unit processes, relating collected data to the functional unit and data aggregation (Matthews, Hendrickson and Matthews, 2014). To prepare for data collection, the goal and scope need to be consulted, particularly the system boundary, to determine the unit processes for which data should be collected. Figure 2.2 shows the inputs and outputs of a unit process.

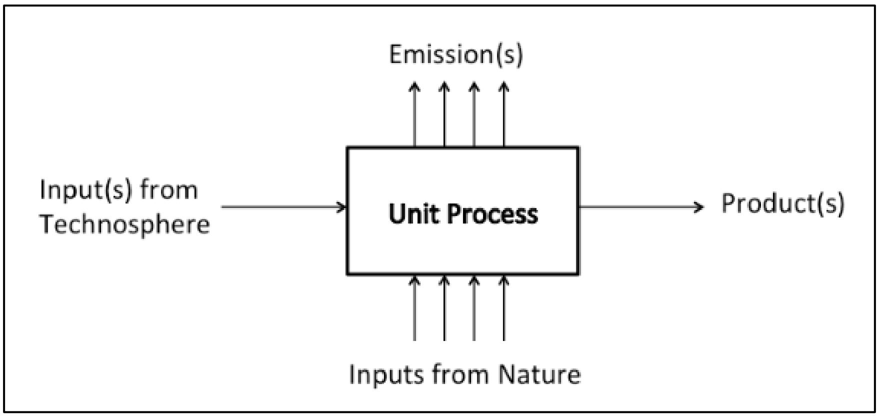


*Figure 2. 2: diagram of a unit process*

During data collection, the flows required are quantified in different ways for all the unit processes making up the system boundary. These flows could be determined via calculation or estimation. For this step, it is recommended to organise the collected data in the form of a spreadsheet in order to manage the data sufficiently (Matthews, Hendrickson and Matthews, 2014). The data collected should match the data quality requirements of the study. The collected data should be validated to ensure that there are no discrepancies. The allocation approach used for the inventory analysis should be explained. Allocation refers to assigning amounts of inputs and outputs to a certain product (Matthews, Hendrickson and Matthews, 2014). This is relevant mainly for product systems where multiple products are produced.

The collected data should be related to the amounts required for the unit processes making up the system boundary. The data should also be related to the chosen functional unit for the product system being studied. All the flows should be referenced against the functional unit. The data should be aggregated to represent single inputs and outputs related to the functional unit. This means that the various material or energy inputs of a certain material or energy source along different life cycle stages would be added together to form one overall input.

Lifecycle impact assessment

The lifecycle impact assessment translates the lifecycle inventory results or emissions to environmental impacts associated with humans, ecosystems or resources (Matthews, Hendrickson and Matthews, 2014). The impact assessment results can either be focused on midpoint impacts or endpoint impacts. The midpoint methods are problem-focused and typically consider impacts such as global warming potential, acidification potential, and toxicity. In contrast, the endpoint methods are damage-focused and look at impacts on human health, resource depletion and the quality of ecosystems (Meijer, 2014).

The lifecycle impact assessment phase has elements that are compulsory and optional. The compulsory elements are the selection of impact categories, classification, and characterisation. The optional components are normalisation, grouping and weighting (Matthews, Hendrickson and Matthews, 2014).

Classification is a quantitative step where the lifecycle inventory results are classified into suitable impact categories. The characterisation steps change the classified inventory results to quantifiable impact flows using characterisation factors. The normalisation step changes the characterised impact result into a unitless impact score using a reference value. Different reference values could be chosen for each impact category. An example of a reference value would be the average annual impact of a person in a particular region. The normalisation step contextualises the impact assessment results and makes it possible to analyse and compare the significance of each impact category.

Grouping refers to sorting or ranking the lifecycle impact results following a specific criterion of priorities related to the goal and scope of the study (Matthews, Hendrickson and Matthews, 2014). This optional step is subjective as each lifecycle assessment practitioner could prioritise the impact categories differently. Grouping is usually done when a significant number of impact categories are considered in the study. Weighing uses a set of weighting factors to create weighted impact results (Matthews, Hendrickson and Matthews, 2014). The weighted impact results add up to make a single impact score. This step is also subjective because each practitioner would use different weighting factors for the impact results. There are various ways to determine the weighting factors for the weighting step. One of the approaches is panel methods, where a group of people, experts, or stakeholders are chosen to determine the factors.

Interpretation phase

The interpretation phase serves to evaluate the results of the lifecycle inventory analysis and impact assessment and to provide conclusions and recommendations (Matthews, Hendrickson and Matthews, 2014). Interpreting the results also refers to assessing and discussing the uncertainty associated with the results and conducting sensitivity analyses of key parameters. This phase is iterative with the other three phases and should be carried out throughout the lifecycle assessment.

There are three components that make up a lifecycle assessment model. These components are data and inputs, methods and results (Matthews, Hendrickson and Matthews, 2014). All these components contribute to a level of uncertainty. Data uncertainty refers to the uncertainty of a value or amount of a particular data point. Examples of data uncertainty are measurement uncertainty for measured data, parameter uncertainty such as incomplete data, geospatial uncertainty relating to data specific for a particular location, and temporal uncertainty where the data used could be outdated (Matthews, Hendrickson and Matthews, 2014). Method uncertainty refers to the uncertainty related to the methods used to conduct the assessment (Matthews, Hendrickson and Matthews, 2014). There are different approaches to conducting a lifecycle inventory analysis and a lifecycle impact assessment. An example of this is software uncertainty, where modelling and results generated by one software package may differ from the modelling techniques and results produced by another software package. Another example is database uncertainty, where other databases used for the lifecycle inventory could generate different results.

## 2.4. Application of LCA approach to Hydrogen Production

This part of the literature review is the critical review and analysis of six hydrogen production life cycle assessment studies. This review summarises the studies and critically reviews the studies in terms of how each study applied the LCA methodology. Furthermore, the key findings for these studies were highlighted, and the limitations were discussed. Reviewing this literature is essential for learning about the state-of-art for hydrogen life cycle assessments.

(Koroneos et al., 2004) compared six hydrogen production methods: steam methane reforming and alkaline water electrolysis powered by five renewable energy sources. These renewable energy options were wind power, solar thermal energy, solar photovoltaics, biomass gasification, and hydropower. There was an expectation for hydrogen to be part of a sustainable energy system in future (Koroneos et al., 2004).

Steam methane reforming is currently the primary production method for hydrogen globally. Hydrogen production via water electrolysis results in no carbon monoxide or carbon dioxide emissions and thus has the potential to be used in the long term (Koroneos et al., 2004). The main objective was to conduct a comprehensive lifecycle study for the production processes using the lifecycle assessment tool and determine the most environmentally benign process. The global emission model for integrated systems (GEMIS) database was used to conduct the comparative assessment.

Hydrogen is regarded as a clean fuel, but its production processes have various environmental impacts. For the impact assessment, four impact categories were considered by Koroneos et al. (2004). These categories were global warming potential, acidification potential, winter smog effect, and eutrophication potential. Among the renewable energy options, it was found that water electrolysis powered by solar PV electricity was the worst-performing production route. This was due to the manufacture of the PV modules, which had high environmental impacts across all the considered impact categories (Koroneos et al., 2004). Hydrogen produced from natural gas via steam methane reforming was found to have the highest carbon dioxide emissions and thus the highest global warming potential. Hydrogen from wind power, solar thermal energy, and hydropower had the least environmental impacts and thus were the most favourable.

(Acar and Dincer, 2014) compared environmental, social, and economic impacts for various hydrogen production methods. The methods considered were steam methane reforming, coal gasification, thermochemical water splitting, high-temperature electrolysis, and water electrolysis powered by wind and solar PV. This study was similar to the (Koroneos et al., 2004) study, with added hydrogen methods to investigate. The coal gasification process consists of coal oxidation in high pressure and temperature conditions to produce carbon monoxide, hydrogen, steam and carbon dioxide containing syngas (Acar and Dincer, 2014). The thermochemical water-splitting cycles consist of a series of reactions at high temperatures to produce hydrogen and oxygen. The copper chloride (Cu-Cl) cycles in nuclear-powered reactors are the assessed thermochemical water-splitting cycles in this study. The efficiency of this process is estimated to be 40% (Acar and Dincer, 2014).

Biomass gasification consists of the oxidation of biomass resources to produce hydrogen. This process could be powered by agricultural waste (Acar and Dincer, 2014). High-temperature electrolysis is like conventional electrolysis, except it has higher efficiency due to the reactors being operated at higher temperatures. In this study, high-temperature electrolysis powered by nuclear energy was considered. Following the lifecycle assessment framework, a comparative assessment was conducted. The Koroneos et al. (2004) study was used by Acar and Dincer (2014) to obtain data for hydrogen production from fossil fuels and renewable energy sources.

The environmental impact categories considered were global warming potential, acidification potential, production costs, energy and exergy efficiency and the social cost of carbon. The social cost of carbon was a new environmental impact indicator developed in this study, which represents the cost of environmental damage caused by the carbon dioxide emissions of a particular process (Acar and Dincer, 2014). Based on the assessment results, nuclear-based thermochemical cycles and wind-powered electrolysis have a low global warming potential and social cost of carbon. When comparing capital costs, it was found that steam methane reforming required lower costs compared to the other methods. Wind-powered electrolysis had the least environmental impacts for three of the considered impact categories: global warming potential, acidification potential, and social cost of carbon.

Patterson et al. (2014) conducted a lifecycle assessment aimed to determine the environmental impacts of electrolytic production and utilisation of hydrogen from renewable energy technologies and grid electricity. For hydrogen production, the polymer electrolytic membrane (PEM) electrolyser, also known as the proton exchange membrane electrolyser, was chosen. The system boundary for this study consisted of energy sources for the PEM electrolyser, hydrogen production, hydrogen compression and storage, transportation of hydrogen fuel to a refuelling station, and the operation of fuel cell-driven vehicles (Patterson et al., 2014). For the utilisation modelling, hydrogen was used to fuel an 85-kW fuel cell-driven vehicle (Patterson et al., 2014). The utilisation aspect from this paper is covered further in the review of hydrogen utilisation LCAs. The lifecycle impact assessment revealed that crude oil extraction to produce petrol had lower climate change impacts but still resulted in high fossil fuel burdens. However, the climate change impact for crude oil did not account for the embedded carbonation for the crude oil. Only the carbon emitted upon utilisation was accounted for. Additionally, it was found that hydrogen production from electrolysis powered by grid electricity is not the best option due to the reliance on fossil fuels to generate electricity (Patterson et al., 2014).

(Karaca, Dincer and Gu, 2020) conducted a study aimed to compare nuclear-based hydrogen production methods through a lifecycle assessment. The production methods compared were conventional water electrolysis, high-temperature water electrolysis and three to five-step Cu-Cl thermochemical water-splitting cycles. The effect of reactor type on the impact assessment results was also analysed. The reactors considered were the pressurised water reactor and the boiler water reactor. The geographic boundary of the study was stated as North America and the time period for the study was 2010. The system boundary considered was the input of uranium into a nuclear power plant to produce energy, the production of hydrogen and oxygen, and hydrogen storage (Karaca, Dincer and Gu, 2020). The thermal energy requirements were sourced from a nuclear power plant.

High-temperature electrolysis is similar to conventional electrolysis, except that it uses heat from the nuclear power plant to reduce the electricity consumption of the electrolysis process (Karaca, Dincer and Gu, 2020). It has different operating conditions to conventional electrolysis and uses a different electrolyte. The conventional Cu-Cl water splitting cycle consists of five steps. The four-step cycle combines two of the steps and thus requires less energy (Karaca, Dincer and Gu, 2020). The three-step cycle combines three of the five steps and requires less energy than the four-step process.

High-temperature electrolysis yielded the lowest environmental impacts across all the impact categories considered. This is due to the low thermal energy input required for the process compared to conventional electrolysis and Cu-Cl cycles. The favourable reactor was the boiling water reactor, which yielded lower environmental impacts across the impact categories except for ozone depletion potential (Karaca, Dincer and Gu, 2020).

The lifecycle assessment by Lotrič et al. (2021) was aimed at comparing the environmental impacts of fuel cell and hydrogen (FCH) technologies. The technologies considered were alkaline electrolysis, polymer electrolytic membrane (PEM) electrolysis, a high-temperature PEM fuel cell, and a low-temperature PEM fuel cell. An additional objective was to show how the end-of-life phase of critical materials impacts the manufacturing phase. The end-of-life phase was modelled with and without recycling critical materials to display the significance of recycling critical materials. The critical materials for the considered technologies were platinum group metals (PGMs).

The system boundary consisted of manufacturing the electrolysers and the end-of-life phase of PGMs. The hydrogen production phase was left out because of its high expected contribution to environmental impacts (Lotrič et al., 2021). That high contribution would make it hard to observe how the recycling of PGMs affects the manufacturing phase. The LCA study was carried out according to the guidelines of the FC-HyGuide project (Lotrič et al., 2021).

The study results revealed that the PEM electrolyser had a greater environmental impact compared to the alkaline electrolyser. This was due to the presence of platinum in the PEM technology, which had a higher environmental impact compared to other PGMs used to manufacture electrolysers (Lotrič et al., 2021). For the fuel cell technologies, the high-temperature PEM fuel cell had a higher environmental impact than the low-temperature PEM fuel cell. This impact was due to the other balance of plant (BoP) components used for the high-temperature technology (Lotrič et al., 2021). The analysis of critical materials recycling showed that the recycling of PGMs significantly decreases the environmental impacts of the technologies, especially the PEM technologies, which include the use of platinum (Lotrič et al., 2021).

#### *2.4.1. Critical analysis and synthesis of the literature*

Important aspects of the life cycle assessment framework were used to analyse the literature. The aspects were the goal and scope of the study, the functional unit used, the system boundary considered, the software used to model the assessment, the impact assessment method used, and the impact categories assessed.

The goal of an LCA serves to reveal the nature of the study and why it is being done. Additionally, it should state the sponsor of the study. The reviewed studies had a similar goal: to compare the lifecycle impacts of different hydrogen production methods and determine the most environmentally benign option. However, Lotrič et al. (2021) had a different goal: to compare fuel cell and hydrogen technologies and reveal the importance of recycling critical materials as an end-of-life phase strategy.

The functional unit serves as a function related basis of comparison. The functional unit used by Acar and Dincer (2014), and Karaca, Dincer and Gu (2020) was 1 kg of hydrogen produced; thus, the function considered was the production of hydrogen using different production pathways. The function considered by the Koroneos et al. (2004) study was the production of energy from hydrogen with a corresponding functional unit of 1 MJ of energy produced. Patterson et al. (2014) considered the function of transporting a passenger in a hydrogen-fuelled passenger vehicle, corresponding to a functional unit of 100 passenger-km of transportation. The Lotrič et al. (2021) study considered the function of electrical energy production from water electrolysers and hydrogen fuel cells, corresponding to a functional unit of 50 kW electric power for electrolysers and 5 kW electric power for fuel cells. The functional units covered by the reviewed studies are based on the function of the product system studied.

Most of the studies assessed a cradle-to-gate system boundary encompassing all activities from raw material extraction to the end of product fabrication. Patterson et al. (2014) added the utilisation of hydrogen as a vehicle fuel to its system boundary. Lotrič et al. (2021) took a different approach by considering the manufacture of equipment for fuel cell and hydrogen technologies and the end-of-life phase for critical materials such as PGMs. The impacts of using recycled critical materials instead of virgin materials were discussed.

The most used software for modelling the LCAs was SimaPro, with one exception being the Gabi Thinkstep software used in the Lotrič et al. (2021) study. The least recent study, undertaken in 2004, did not mention any software used for the assessment. This shows the progression and development of the LCA methods over the years. Both software packages are compliant with the ISO 14044 LCA standard, and their performance is similar, except for some differences in the inventory and impact assessment databases. A lifecycle impact assessment can either take a midpoint approach, which considers earlier impacts in the cause-effect chain or an endpoint approach, which looks at impacts at the end of the cause-effect chain (Meijer, 2014). The impact assessment methods mostly used throughout the studies were Eco-indicator 95 and CML 2001, which are outdated methods.

The impact categories considered the most were global warming potential and acidification potential. Acar and Dincer (2014) added a new impact indicator: the social cost of carbon (SCC). This indicator represented the cost of environmental damage caused by carbon dioxide emissions. The other impacts typically considered were human toxicity potential, abiotic depletion potential and ozone depletion potential. The Patterson et al. (2014) study used a different impact assessment method and assessed endpoint impacts. These were fossil fuel burdens, climate change, ecotoxicity, carcinogens, and respiratory inorganics. Of these impact categories, the ones relevant to the scope of the dissertation would be global warming potential and human toxicity.

### *2.4.2. Key LCA findings in the studies*

Wind-powered water electrolysis was found to be the most favourable and attractive production option, as stated by Koroneos et al. (2014) study, Acar and Dincer (2014), and Patterson et al. (2014). This option resulted in low equivalent emissions for the impact categories considered and a low impact score overall (Koroneos et al., 2004, Acar and Dincer, 2014).

Hydrogen production from wind and solar PV power resulted in the highest production costs due to the construction of the required infrastructure such as wind turbines and solar PV panels (Patterson et al., 2014). The best performing production option for production costs was steam methane reforming. Acar and Dincer (2014) stated that, even though wind power production costs six to ten times more than fossil fuel options, a drastic cost reduction of 50% or more is expected in the future. Recently, the green hydrogen and power fuels report released by EU-SA stated that the expansion of solar PV and wind energy capacity has led to renewable energy plants being cheaper and cost-competitive with building new fossil fuel-based plants (Roos and Wright, 2021). The prediction made by Acar and Dincer (2014) was indeed correct.

Steam methane reforming was reported as the worst environmentally performing production option, followed by solar PV powered electrolysis, according to Koroneos et al. (2004). Solar PV powered electrolysis resulted in high sulphate equivalent emissions due to the construction of solar PV cells, causing a high acidification potential. However, Acar and Dincer (2014) disputed this result, as they ranked solar PV electrolysis the second-best environmentally performing option, resulting in similar impacts to wind-powered electrolysis. This shows that solar PV technology has undergone advancements over the years. When comparing solar PV technologies, it was reported that the use of crystalline silicon materials to produce solar cells resulted in higher acidification and climate change potential, whereas using thin-film polymer technology to produce solar cells resulted in lower impacts (Tyagi et al., 2013). Steam methane reforming had the highest carbon dioxide emissions, which resulted in a high global warming potential (Koroneos et al., 2004, Acar and Dincer, 2014); hence it remains the least favourable option in terms of environmental impacts.

The highest contributing factor for nuclear-based hydrogen production impacts was the amount of thermal energy required for each process. Nuclear-based high-temperature electrolysis required the lowest amount of energy amongst the options investigated by Karaca, Dincer and Gu (2020); hence it was the most favourable. When nuclear-based production was compared to other options, it ranked competitively with wind-powered electrolysis in terms of global warming potential and acidification potential (Acar and Dincer, 2014). However, nuclear-based energy requires coal and natural gas burning for energy production (Karaca, Dincer and Gu, 2020). It resulted in a high abiotic depletion potential and human toxicity due to uranium tailings disposal (Karaca, Dincer and Gu, 2020). It is thus not a sustainable option. Nuclear-based hydrogen is beyond the scope of this dissertation and thus will not be discussed any further.

### *2.4.3. Limitations*

All the studies reviewed, from the earlier studies to the most recent, used the same impact assessment methods. The studies did not include an impact assessment method analysis or justify their choice of impact assessment methods. Given that there are various impact assessment methods to select, impact assessment method analyses from the studies would have been valuable.

Patterson et al. (2014) conducted a Monte Carlo uncertainty analysis for the impact assessment comparison of hydrogen fuel produced from wind electrolysis and other alternative fuels. The rest of the studies did not include an uncertainty analysis or a sensitivity analysis for the impact assessment results.

Some of the studies reviewed were dated, especially the Koroneos et al. (2004) study. It was, therefore, noted that some of the impact assessment results provided by such studies may no longer be relevant. The impact assessment methods used may also not be suitable to be used in a recent study. The production technologies have undergone changes and improvements over the years, which would lead to lower environmental impacts and better costs. However, these studies are still valuable for this literature review as they provide a structure and understanding of hydrogen production lifecycle assessments.

Lastly, the impact assessment results in terms of the best environmentally performing hydrogen production technologies were based on regions in Europe, the United States, and the United Kingdom. These results may or may not be the same for South Africa or other African countries. A South African-based lifecycle study analysing different hydrogen production technologies would serve as a better basis for deciding on the best-suited hydrogen production route for South Africa.

### *2.4.4. Review of water electrolysis focused lifecycle studies*

Given that water electrolysis was found as the best environmentally performing production method, it is essential to learn about the different electrolysis technologies available, their infrastructure and their environmental impacts. Studies analysing various electrolysis technologies were reviewed and analysed. The main objective of the first study was to compare the environmental impacts of critical materials used for the available electrolysis technologies in a life cycle assessment. The commercially available technologies are polymer electrolyte membrane electrolysis (PEME), alkaline electrolysis (AE) and solid oxide electrolysis (SOE) (Zhao et al., 2020).

This study analysed and compared the electrolysis stacks of the different technologies. A stack consists of a single repeating unit (SRU) and balance of plant (BoP) components, although the impacts for the BoP components were not included. An SRU comprises a hydrogen electrode, an oxygen electrode, an electrolyte, an interconnect and a frame (Zhao et al., 2020). The SRU setup was used as a framework to compare the critical material used for each technology and the resulting impacts. A cradle-to-grave system boundary was considered, and Denmark was the geographical boundary. The functional unit used was 1 $m^2$ of the stack area.

PEM electrolysis cells have the largest stacks compared to other cells. The PEME stacks consist of platinum used for the hydrogen electrode and iridium used for the oxygen electrode. PGM coated titanium is used for the interconnects, and stainless steel is used for the frames (Zhao et al., 2020). AECs used nickel for the electrodes and electrolytes. Nickel alloys and PGMs were used for coating, and stainless steel was used for the frames (Zhao et al., 2020). For SOECs, zirconia and nickel were used for the hydrogen electrodes. Lanthanum strontium cobalt ferrite (LSCF) was used for the oxygen electrodes. The interconnects were made from stainless steel (Zhao et al., 2020).

The ReCiPe 2016 impact assessment method was used to assess the impacts of the various materials used in these technologies, and sixteen impact categories were considered, with the significant ones being the global warming potential (GWP) and the mineral resource scarcity potential (MRSP). The PEME cells' impacts for global warming potential were sixteen times higher than the impacts of SOE and nine times higher than the impacts of AE cells (Zhao et al., 2020). This was due to the high impacts of platinum and iridium used in the PEM technology, with the platinum impacts being much higher than those of iridium.

The MRSP impact was also due to metals used for the cells. PEME cells were thus the worst environmentally performing option due to the platinum-related environmental impacts. AEC was ranked second due to the amount of nickel used. SOECs used were ranked as the most environmentally benign option based on material use. Zhao et al. (2020) stated that solid oxide electrolysis plants require less pure water than PEM electrolysis and alkaline electrolysis plants, making it even more favourable.

An impact assessment was conducted for hydrogen production from the different electrolysis stacks using 1 kg of hydrogen produced as the functional unit. This analysis compared the environmental impacts caused by the electrolysis stack, the electricity, and the water consumption. The results showed that, for all three technologies, electricity consumption (during the production process) had the highest contributions to global warming and mineral resource scarcity impacts. This result highlighted the significance of the production phase when assessing which process in the lifecycle causes the least environmental harm. PEMECs and AECs received the same overall impact score for both GWP and MRSP. Solid oxide electrolysis received a lower overall environmental score for GWP and a similar but slightly lower overall score for MRSP, thus maintaining its first rank. Regardless of being first, the solid oxide technology was reported to be in the early research and development stages and immature compared to alkaline electrolysis and PEM electrolysis (Zhao et al., 2020).

Mehmeti et al. (2018) conducted a life cycle analysis for hydrogen production pathways to determine their environmental impacts using the ReCiPe 2016 impact assessment method. Among the pathways were PEM electrolysis and solid oxide electrolysis. The available water remaining (AWARE) impact assessment method was also used as a stand-alone indicator to quantify the water scarcity footprint of the production process. The impacts of grid electricity-powered electrolysis were higher than those of the fossil fuel-driven production pathways: steam methane reforming and coal gasification (Mehmeti et al., 2018). This study highlighted the importance of using renewable electricity for electrolysis technologies to make them environmentally favourable.

Contrary to the results reported by Zhao et al. (2020), solid oxide electrolysis, according to Mehmeti et al. (2018), had a higher global warming potential compared to PEM electrolysis. The global warming potential impacts for solid oxide electrolysis and PEM electrolysis, reported for a functional unit of 1 kg of hydrogen, were 5.1 and 2.2 kg $CO_2$ eq, respectively (Mehmeti et al., 2018). These impacts may be due to the different materials and design configurations used in different regions for the technologies. However, for all the other ReCiPe 2016 midpoint impact categories, PEM electrolysis resulted in higher impacts. Lotrič et al. (2021) also confirmed this result as the authors concluded that PEM electrolysis caused high environmental impacts, compared to alkaline electrolysis, due to the use of PGMs.

The Zhao et al. (2020) study was recent and brought relevant information about the materials of construction used for the different technologies and their environmental impacts. The production phase of hydrogen was also included in the impact assessment. The Mehmeti et al. (2018) study was also recent and it brought valuable insights about the PEM and solid oxide electrolysis technologies. These studies used the ReCiPe 2016 method to conduct impact assessments and stated that it was the state-of-art method for conducting life cycle impact assessments.

## 2.5. Application of LCA approach to Hydrogen Utilisation

Lifecycle focused studies for hydrogen utilisation were critically reviewed. The articles were sourced from peer-reviewed journals. The studies found in the literature primarily assess the utilisation of hydrogen as a transportation fuel.  These studies were critically reviewed in terms of the goal of the LCA, the system boundary, the functional unit used, the inventory methods used, the impact assessment methods, the key findings, and the interpretation phase. Tables 2.2 and 2.3 are the critical synthesis tables for the studies reviewed. The limitations observed from reviewing the studies were also discussed.

*Table 2. 2: Critical synthesis table for hydrogen utilisation LCA studies #1*

| Source | Goal | System Boundary | FU | Inventory method | IA method and Impact categories | Key findings |
|---|---|---|---|---|---|---|
| (Melamu, 2008) | Compare hydrogen utilisation scenarios for transport and electricity generation | Cradle to gate and utilisation phase | Energy in MJ and vehicle mileage achieved from hydrogen from 3.68 tons of maize | System expansion conducted | CML 2 baseline 2000<br>Climate change<br>Human toxicity<br>Freshwater aquatic ecotoxicity<br>Acidification<br>Eutrophication | Hydrogen is most beneficial when used in electricity production than transport due to coal-based electricity |
| (Bartolozzi, Rizzi and Frey, 2013) | "Evaluate environmental impacts of hydrogen chain scenarios in Tuscany" | "Extraction of raw materials, fuel production, transportation, manufacture, use, maintenance, and end-of-life of plants used for electricity and hydrogen production and of vehicles" | "200 km at nominal full load" | Ecoinvent database<br>No allocation procedures | "CML 2000 method abiotic depletion, acidification, eutrophication, global warming, ozone layer depletion, human toxicity, freshwater ecotoxicity, marine ecotoxicity, terrestrial ecotoxicity, photochemical oxidation" | -High environmental impacts for hydrogen produced by grid-powered electrolysis.<br>-Least environmental impacts for BEVs compared to HFCEVs |
| (Patterson et al., 2014) | Assessing electrolytic production and utilisation | Energy input, production, compression, storage, refuelling station, vehicle operation | 100 pkm | Ecoinvent Database<br>No allocation procedures | Eco-indicator 99 H/A human health, resources, ecosystem quality | -Hydrogen from wind-powered electrolysis had the least impacts |

*Table 2. 3: Critical synthesis table for hydrogen utilisation LCA studies #2*

| Source | Goal | System Boundary | FU | Inventory method | IA method and Impact categories | Key findings |
|---|---|---|---|---|---|---|
| (Ahmadi and Kjeang, 2015) | Comparison of hydrogen-fuelled and gasoline-powered cars | Full lifecycle of vehicle and fuel (Production, distribution, and utilisation of vehicle and fuel, and vehicle disposal) | 1 km of vehicle travel | No allocation procedures | Greenhouse gas emissions<br>Criteria air contaminant emissions | -Thermochemical water splitting was the best performing $H_2$ production route<br>-HFCEV had a higher energy efficiency than gasoline cars |
| (Bekel and Pauliuk, 2019) | "Comparison of fuel cell and battery electric vehicles", considering environmental impacts and lifecycle costing | "Vehicle production, electricity production and distribution, Charger production" for BEVs, $H_2$ production, vehicle usage, end-of-life phase | 1 km driven | Ecoinvent database<br>No allocation procedures | ReCiPe 2016<br>Global warming<br>Human toxicity<br>Surplus ore potential and particulate matter formation potential | -BEVs had the least impacts<br>-FCEVs are better for longer distances |
| (Chang, Liao and Chang, 2019) | Comparative assessment of conventional buses and buses fuelled by alternative fuels including hydrogen | "Raw material acquisition phase-manufacturing-bus service-waste disposal stage" | 1 pkm | No allocation procedures | SimaPro<br>Carbon dioxide emissions | -Replacing public buses with $H_2$ fuelled buses leads to high environmental benefits |
| (Siddiqui and Dincer, 2021) | "Assessment of alternative fuels for the aviation sector" | Well to wake system - Airport operation and maintenance, Fuel production,<br>Aircraft operation | 1 tkm | Ecoinvent database<br>Economic allocation applied for modelling biodiesel | ReCiPe 2016<br>Global warming potential<br>Terrestrial acidification<br>Ionising radiation potential<br>Freshwater eutrophication<br>Photochemical ozone formation<br>Freshwater ecotoxicity<br>Land use occupation | -For green $H_2$ comparison, $H_2$ produced from solar PV powered electrolysis resulted in the highest toxicity and global warming impacts |

### 2.5.1. Goal

Most of the studies assessed the utilisation of renewable hydrogen as a vehicle fuel. The main goal of the lifecycle assessments was to compare the environmental impacts of hydrogen-fuelled vehicles against the impacts of battery electric vehicles and conventional vehicles. Ahmad and Kjeang (2015) compared the hydrogen-fuelled vehicles for hydrogen produced from renewable and non-renewable methods. Alternatively, Siddiqui and Dincer (2021) investigated the environmental impacts and benefits of using hydrogen as aviation fuel. A master's thesis conducted by Melamu (2008) explored the production of hydrogen via the Aqueous Phase Reforming technology. The thesis further explored how hydrogen could be used in different industries. The two primary industries considered by Melamu (2008) for hydrogen utilisation were road transportation and electricity generation.

The system boundary considered mainly by the studies is a cradle to grave system. This system comprises the raw material extraction, production, distribution, use, and disposal phase of a product. These studies considered both the lifecycle of the fuel and the lifecycle of the vehicle where the fuel would be used. Some authors, such as Melamu (2008), Patterson et al. (2014), and Siddiqui and Dincer (2021), considered a cradle to gate system for hydrogen production and the utilisation of hydrogen as fuel. A cradle to gate system ends at the production phase before the product leaves the production plant "gate". Siddiqui and Dincer referred to the system as a well to wake, which considers raw material extraction, fuel production, transportation, dispensing of fuel and fuel utilisation in an aircraft. The impact assessment of the cradle to grave studies focused on the impacts of both the vehicle and the fuel, hydrogen, or conventional fuel, while the impact assessments of cradle to gate (plus hydrogen utilisation) studies were more focused on the impacts of the fuel utilisation phase.

### 2.5.2. Functional units and inventory methods

The functional unit used as a basis of comparison for the studies was mostly km of vehicle usage. For passenger vehicles and buses, pkm was used as the functional unit. For an aircraft, 1tkm was the functional unit used by Siddiqui and Dincer (2021). Melamu (2008) considered both an energy unit (MJ) and a transport unit (km). Based on this observation, the type of vehicle considered directly informs the functional unit used. Most of the studies did not discuss the methods used to model the lifecycle inventories. In lifecycle inventory, there are two methods used to deal with multi-functional and multi-output processes. These methods are system expansion and allocation. System expansion refers to the allocation of a product system with the avoided functions and productions that would take place elsewhere in the technosphere (Hauschild, Rosenbaum and Olsen, 2018). Allocation refers to the division of inputs and outputs of a process between the multiple functions or products of the process (Hauschild, Rosenbaum and Olsen, 2018). Two out of the six sources discussed inventory modelling methods. Siddiqui and Dincer (2021) used economic allocation to model the production of biodiesel, one of the alternative aviation fuels assessed. Melamu's thesis applied the method of system expansion to aid the comparison of two systems that were initially incomparable (hydrogen utilisation in transport and hydrogen utilisation in electricity generation).

### 2.5.3. Impact assessment methods

The SimaPro software was mostly used to model the lifecycle assessments for the studies. The most used impact assessment method used to conduct the impact assessment was ReCiPe 2016. Other impact assessment methods used were CML 2000 and Eco-indicator 99 H/A. ReCiPe 2016 and CML 2000 impact categories consider midpoint impacts. The Eco-indicator 99 H/A considers endpoint impacts at the end of the cause-effect chain. Impact assessment results for endpoint impact categories are prone to higher uncertainty due to the aggregated data used to generate the impact results (Goedkoop et al., 2016).

Global warming potential is the most frequently assessed impact category for the studies reviewed. Bartolozzi, Rizzi and Frey (2013) and Siddiqui and Dincer (2021) considered a comprehensive list of impact categories, including terrestrial acidification, human toxicity, eutrophication, ecotoxicity, and photochemical oxidation. The rest of the reviewed studies focused on a shorter list of impact categories, and Chang, Liao and Chang (2019) focused on carbon footprint only. Considering multiple impact categories is linked to the nature of the lifecycle assessment methodology; however, the chosen impact categories depend on the objectives and scope of each lifecycle study.

#### *2.5.4. Key findings*

Most of the studies found in the literature considered the utilisation of hydrogen as a fuel for road transport. The environmental impacts of hydrogen utilisation for fuel cell electric vehicles were compared with those of battery electric vehicles and vehicles powered by conventional fuels such as petrol and diesel. Battery electric vehicles were reported to cause the least environmental impacts compared to hydrogen fuel cell electric vehicles (Bartolozzi, Rizzi and Frey, 2013), (Patterson et al., 2014), (Bekel and Pauliuk, 2019). However, according to Chang, Liao and Chang (2019), hydrogen fuel cell electric vehicles have lower carbon footprints than battery electric vehicles. Patterson et al. (2014) and Bekel and Pauliuk (2019) both concluded that the best way forward is to integrate the utilisation of hydrogen fuel cell electric vehicles and battery electric vehicles powered by an electricity grid with a high renewable energy share.

Ahmadi and Kjeang (2015) compared hydrogen-fuelled vehicles for hydrogen produced in renewable and non-renewable methods. Hydrogen produced from thermochemical water splitting was the fuel causing the least environmental impacts. In aviation, renewably produced hydrogen fuel was generally less impactful than conventionally produced hydrogen. The Siddiqui and Dincer (2021) study included ammonia as another clean fuel for aviation; however, hydrogen and ammonia were not compared to determine the fuel with the least environmental impacts. Melamu (2008) found that the best environmental benefit is achieved by replacing coal-based electricity with hydrogen-based electricity than using the hydrogen for transport. This finding confirmed that for a scarce low-impact resource, it is best to use it to displace the most harmful fuel, which was coal-based electricity in the case of Melamu (2008). Lifecycle studies for hydrogen utilisation in other applications such as steel and petrochemicals production were limited.

#### *2.5.5. Interpretation*

Interpretation is the last phase of the lifecycle assessment framework. It is not included in the critical synthesis table; however, it is an equally essential element for LCA studies. It aims to assess the uncertainty associated with the results, the sensitivity of the results to key parameters, and give substantial conclusions and recommendations. Patterson et al. (2014) conducted the most comprehensive interpretation phase, with a sensitivity analysis of important parameters and an uncertainty analysis. The parameters used for the sensitivity analysis were the capacity factors of solar PV and wind by selecting a location with better solar and wind availability and another lifecycle impact assessment methodology. The increase of capacity factors, particularly for wind, led to lower environmental impacts associated with hydrogen fuel produced from wind electrolysis (Patterson et al., 2014). The change in results for increasing the solar PV capacity factor was not as apparent (Patterson et al., 2014). The Monte Carlo uncertainty analysis tool on SimaPro was used to conduct a quantitative uncertainty for all the impact assessment results. The uncertainty analysis confirmed that electric vehicles powered by a prospective 2030 grid were the least impactful; however, the hydrogen fuel cell electric vehicles were the least impactful when considering fossil fuel burdens (Patterson et al., 2014).

Bekel and Pauliuk (2019) conducted a sensitivity analysis using the electricity mix used to fuel battery electric vehicles, vehicle lifetime, and vehicle range in km as the key parameters for the analysis. The rest of the studies did not include a sensitivity analysis or an uncertainty analysis for the impact assessment results. However, all the studies provided clear and substantial conclusions and recommendations which is also an essential part of the Interpretation phase.

Melamu (2008) gave great insight into using the lifecycle assessment tool when deciding how to allocate a scarce low impact resource to competing environmentally harmful options. Melamu (2008) conducted a system expansion to compare different utilisation options for hydrogen and found that it is best to use the limited renewable energy resource, hydrogen, to displace the "dirtiest fuel".

#### *2.5.6. Limitations of LCA application for hydrogen utilisation*

A major limitation observed during the search and collection of literature for hydrogen utilisation-focused LCAs is the lack of African and South African based studies for hydrogen utilisation. All the articles found are for the United Kingdom, The United States of America or Europe. The exception to this is the thesis conducted by Melamu (2008) which is South African based. This lack may be attributed to the lack of access to information and data regarding hydrogen production in Africa. It may also be due to a lack of resources and knowledge required to conduct a comprehensive lifecycle assessment. Lastly, this may also be attributed to the fact that hydrogen, mainly green hydrogen, has just gathered interest in recent years. Most plans and developments regarding hydrogen production and utilisation in African countries are still under development.

In the course of reviewing the studies, another limitation observed, particularly for the methodologies followed, was the omission of the reasoning behind the impact assessment methods chosen for the assessments. The studies did not explain why a particular method was used and why it was the most suitable compared to other available methods. Lastly, a limitation observed regarding the LCA framework was the lack of uncertainty analyses and sensitivity analyses for the interpretation phase.

## 2.6. Chapter Summary

This literature review discussed the available hydrogen production methods and technologies in detail. The applications of hydrogen, mainly green hydrogen, were briefly discussed. An overview of the lifecycle assessment methodology was given, including the history and development of the tool and the contribution of lifecycle assessment studies to sustainability. Thereafter, a critical review was conducted for lifecycle assessment studies focused on hydrogen production and utilisation. The limitations observed from reviewing the hydrogen lifecycle assessments were discussed. The literature review serves as a basis for the methodology followed to achieve the objectives of the dissertation.

# 3. METHODOLOGY

The research approach and methodology stems from the objectives of the dissertation and the literature review. The literature review was used to refine the objectives of the dissertation and form the key hypotheses. Similar to the objectives of the dissertation and the structure of the critical review in Chapter 2, the key hypotheses were defined for both hydrogen production and hydrogen utilisation.

## 3.1. Hypothesis for hydrogen production

Based on the results of most of the reviewed literature for hydrogen production lifecycle studies done for other regions, it is hypothesised that the environmental impacts of the energy required to produce hydrogen far outweigh the environmental impacts associated with the infrastructure and equipment used to produce the hydrogen for all production routes. To test this hypothesis, the environmental impacts of hydrogen production are analysed in terms of the environmental impact contributions of the processes making up the hydrogen product systems. These processes are different for green and grey hydrogen production. The contributions are quantified and compared.

From the hypothesis, the following key questions are formulated:

- What energy sources are likely to be used to produce hydrogen in South Africa?
- Are the lifecycle datasets to model these energy sources available?
- What electrolyser technologies are likely to be used for hydrogen production in South Africa?

## 3.2. Hypothesis for hydrogen utilisation

Based on the learnings of the hydrogen utilisation aspect of the literature review, it is hypothesised that the most environmentally beneficial way to utilise the hydrogen produced in South Africa, which would initially be a scarce resource, would be to use it to displace the most environmentally harmful fuel. This hypothesis stems from the idea that a scarce low-impact renewable resource should first be used to decarbonise the dirtiest fuel, as stated by Melamu (2008). This hypothesis is tested by defining two hydrogen utilisation systems and comparing the environmental impacts of each expanded system.

The following key questions are developed to aid the investigation of the hypothesis:

- How do environmental benefits of exported hydrogen compare to local utilisation?
- How can hydrogen be used to achieve substantial environmental benefits through decarbonisation?
- Can the utilisation of hydrogen to fuel heavy duty truck transportation be used as a case study to compare utilisation in South Africa versus utilisation in a country that might import hydrogen from South Africa?
- How is system expansion conducted in LCA for the allocation of a scarce, low-impact resource?

The methodology used to carry out the objectives is the lifecycle assessment tool. This tool is defined and discussed in detail in Chapter 2, Section 2.3. The framework of the tool comprises four elements: the goal and scope, the lifecycle inventory analysis, the impact assessment and the interpretation phase. The goal and scope of an LCA form part of the methodology. Given that two lifecycle assessments were conducted, two goal and scope sections were defined.

## 3.3. Approach and Resources

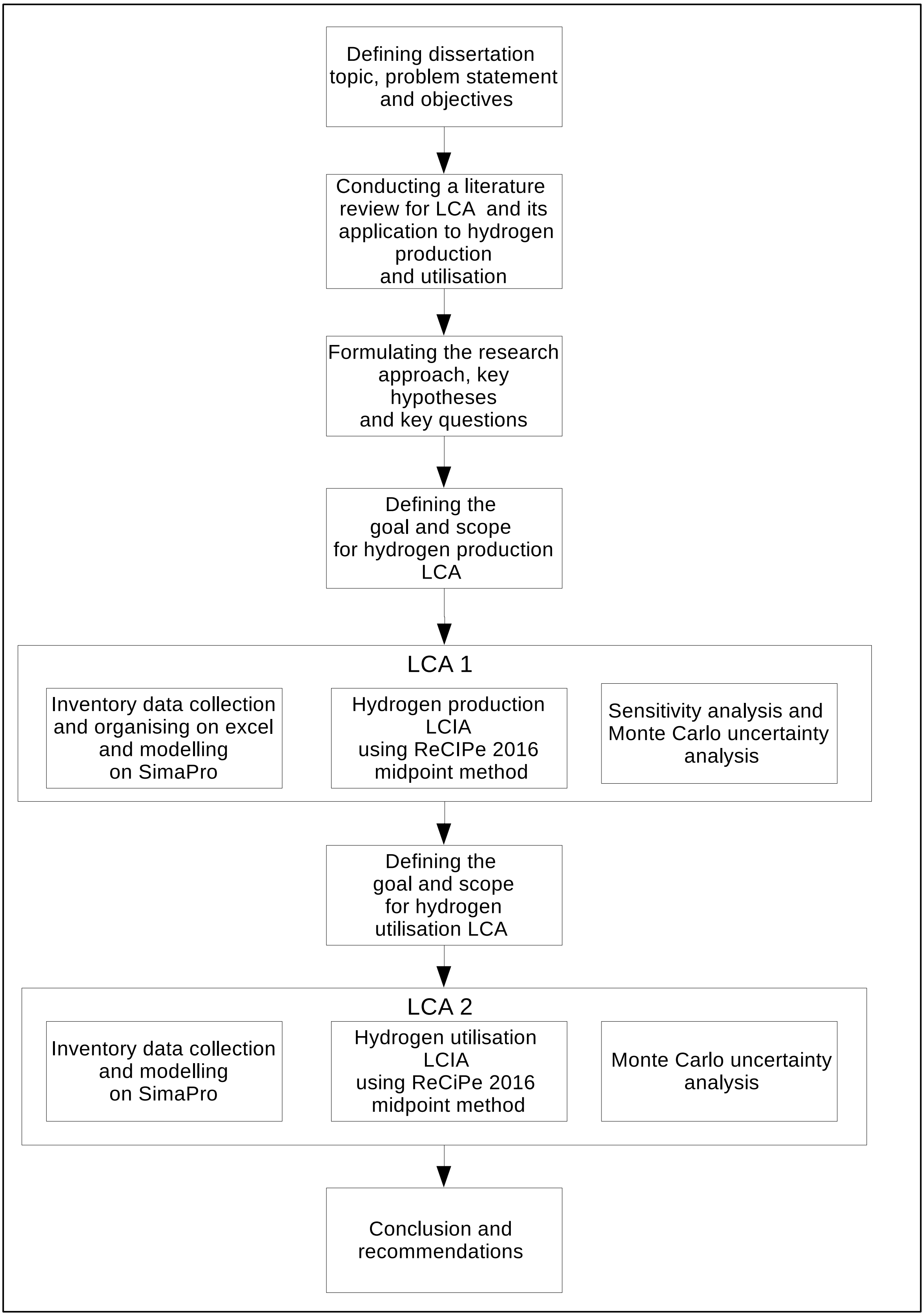


*Figure 3. 1: Flowchart of research approach and methodology*

Figure 3.1 illustrates the research approach followed for the dissertation in a flowchart. The SimaPro software version 9.1.1.7 was used to model the two comparative lifecycle assessments, and the ecoinvent database version 3.6 was used to model the lifecycle inventories. Microsoft Excel was used prior to the modelling to calculate the reference flows of the inputs based on the functional units.

## 3.4. Goal and scope for hydrogen production LCA

### *3.4.1. Goal*

This lifecycle assessment intends to compare renewable and non-renewable hydrogen production technologies and determine the hydrogen production option with the least environmental impacts. The assessment aims to produce valuable results that would prospectively influence South African policy decision-making towards achieving a renewable hydrogen-driven economy. Inspired Evolution Investment Management Pty (Ltd.) and the National Research Foundation (NRF) are the funding organisations for this LCA.

Limitations

This study is an environmental LCA; thus, the impact categories are focused on environmental impacts. The study results are limited to the data available for the lifecycle inventory data compilation and the available lifecycle impact methods on SimaPro version 9.1.1.7.

Target audience

The target audiences of this LCA are industrial and energy system planners, academics, and policy and investment analysts working towards climate change mitigation and a low carbon economy in South Africa. Additionally, it is targeted at the sponsors of the LCA which are mentioned above.

### *3.4.2. Scope*

The production technologies to be compared are steam methane reforming and water electrolysis. Water electrolysis is powered by solar PV power, solar thermal power, wind power or grid electricity. Five hydrogen production pathways are compared, as seen in Table 3.1.

*Table 3. 1 Hydrogen production processes*

| **Production processes** | |
|---|---|
| **Non-renewable energy-based** | **Renewable energy-based** |
| Steam methane reforming | Wind-powered water electrolysis |
| Grid electricity-powered water electrolysis | Solar PV-powered water electrolysis |
| | Concentrated solar-powered water electrolysis |

Functional unit

The function considered by most of the hydrogen LCA studies reviewed was the use of various renewable and non-renewable production technologies to produce hydrogen. This correlated with a functional unit of 1 kg of hydrogen produced. The same functional unit of 1kg is used for this lifecycle assessment. All the reference flows were calculated to produce 1 kg of hydrogen.

Data sources and quality

The data for the inputs to the system was sourced from the ecoinvent database available on the SimaPro software. Data was also sourced from the reviewed literature. Where South African input data was not available, global and European data points were used and adapted as much as possible to the South African context.

Time period

Relevant sources were consulted to determine the suitable prospective year to base this lifecycle assessment. A report released by the international renewable energy agency (IRENA) stated that Southern Africa is expected to meet about 63% of its electricity demand using renewable electricity in 2040 (IRENA, 2021). The 2011 South African national development plan (NDP) estimated that the energy transition would be in full effect by 2030, and the power mix will be fully diversified by then (National Planning Commission, 2011). The Paris agreement for climate change, which South Africa has signed, estimated that a carbon-neutral world would be achieved by mid-century (UN, 2015). Based on the sources above, 2040 is the year chosen as a middle ground to base this assessment.

Geographical Boundary

South Africa is the geographical region of interest for this assessment. This includes all the locations which are within the South African borders. All data used were South African based or adapted as much as possible to the South African context.

System Boundary

A cradle to gate system is considered for this assessment. The main processes that make up the system boundary are the extraction of raw materials and feedstock production, the transportation of the feedstock where necessary, the location of production, the supply of energy to the production processes, and lastly, the production of hydrogen. The primary infrastructure materials are also included in the system boundary. For a more straightforward comparison, it is assumed that all the production plants, i.e., the water electrolysis plants and the steam methane reforming plant, would be located at the same place. The system boundary is illustrated in Figure 3.2.

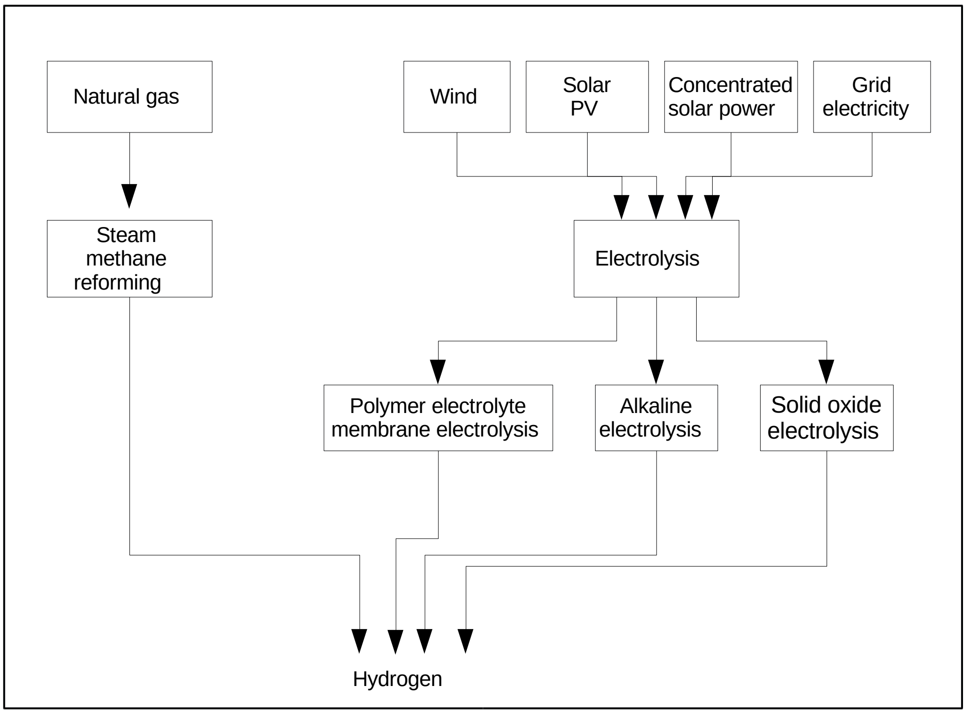


*Figure 3. 2 Hydrogen production system boundary*

Impact categories of concern for the LCA

The critical impact categories in the South African context are global warming potential, water footprint and human toxicity. Global warming potential is significant because it is essential to determine the potential greenhouse gas emission reductions that could be achieved by shifting from grey hydrogen to green hydrogen. The water footprint is significant because South Africa is a water-scarce country, and the water electrolysis technologies use water as a primary feed. Water is also used in the production processes of the energy required to power these processes. Therefore, the water footprint of green hydrogen production would be a matter of concern for the target audience. Human toxicity, especially carcinogenic toxicity is critical to address because carcinogens cause cancer in humans; thus, it would be necessary to understand and quantify the potential health risk posed by green hydrogen production.

Lifecycle Inventory (LCI) modelling framework

An LCI modelling framework can be either attributional or consequential. Attributional LCI modelling isolates the product system from the technosphere and attributes the environmental impacts to the product (Hauschild, Rosenbaum and Olsen, 2018). Consequential LCI modelling focuses on the changes or consequences brought by the process system (Hauschild, Rosenbaum and Olsen, 2018). The attributional LCI modelling framework is followed for this LCA, as it allows for the environmental impacts to be attributed to the produced hydrogen. The oxygen gas produced during water electrolysis is thus considered an emission instead of a product.

## 3.5. Goal and scope for hydrogen utilisation LCA

### *3.5.1. Goal*

The goal and scope of the hydrogen utilisation LCA are informed by the outcomes of the hydrogen production LCA. The hydrogen produced from the least impactful production route in the first LCA is used as an input for the hydrogen utilisation LCA. Chapter 4 gives the results of the hydrogen production LCA. The goal and scope are as follows:

The goal of this comparative lifecycle assessment is to investigate the most environmentally beneficial and efficient way to use the green hydrogen produced in South Africa. The aim is to determine the highest level of decarbonisation that could be achieved by using hydrogen to fuel heavy-duty trucks. Two cases of hydrogen utilisation are considered: The first is using hydrogen for heavy-duty truck transportation locally, the second is exporting the hydrogen for usage in heavy truck transportation in Germany. Germany was chosen for this assessment because it is one of the countries that has expressed interest to import green hydrogen from Southern Africa. The results of this study are intended to reveal the most effective way to use the limited renewable energy resource produced in South Africa, and hence the limited green hydrogen which would be produced from the renewable energy.

Similar to the production LCA, this assessment's target audiences are industrial and energy system planners, academics, and policy and investment analysts working towards achieving a low carbon economy. Other audiences could be environmentally focused organisations and individuals in civil society. As for the first LCA, the sponsors of this assessment are Inspired Evolution Investment Management Pty (Ltd.) and the National Research Foundation.

### *3.5.2. Scope*

Functional unit

The function considered for this assessment is using hydrogen to either fuel local heavy-duty truck transportation or exporting hydrogen to Germany also to fuel heavy-duty truck transportation. According to the South African hydrogen valley report, the local green hydrogen demand for medium and heavy-duty trucks in 2030 is predicted to be 70 kt (Engie Impact, 2021). Based on a hydrogen fuel consumption of 0.0044 kg/tkm for hydrogen-fuelled trucks (as explained in Section 5.1.2), 70 kt of hydrogen results in 15.9 billion tkm of truck transport activity. Based on this amount, a comparative functional unit of 16 billion tkm transport activity is used for this assessment. Contrary to the hydrogen production lifecycle assessment, this functional unit is set to a more realistic scale to reflect the current developments and plans related to hydrogen production and utilisation in South Africa.

Data sources and quality

Journal articles from the reviewed literature were used to source the data to model this lifecycle assessment. The ecoinvent database available on SimaPro was also used. The quality of this data was sufficient in terms of carrying out the goal of the LCA.

Time period

The time period considered for this lifecycle assessment is linked to the functional unit. Given that the functional unit is based on a 2030 prediction for the hydrogen utilisation in the South African mobility sector, mainly truck transportation, the time period for this assessment is the year 2030.

Geographical boundary

The geographical boundary contains two regions, given the goal of this assessment. The first location is South Africa, for the case of using hydrogen locally to decarbonise heavy-duty truck transportation. The second is Germany for the case of exporting hydrogen to decarbonise heavy duty truck transportation in another country.

System Boundary

The system boundary for the local utilisation case is set to a pump-to-wheels system which refers to fuel consumption during the operation of heavy-duty trucks. For the export case, the system boundary consists of the conversion of hydrogen (liquefaction or ammonia synthesis), shipping, reconversion, and fuel consumption during truck transport activity. The distribution of hydrogen to refuelling stations in both cases is considered negligible in terms of lifecycle environmental impacts; therefore, it was not included in the analysis. Figure 3.3 is an illustration of the system boundary.

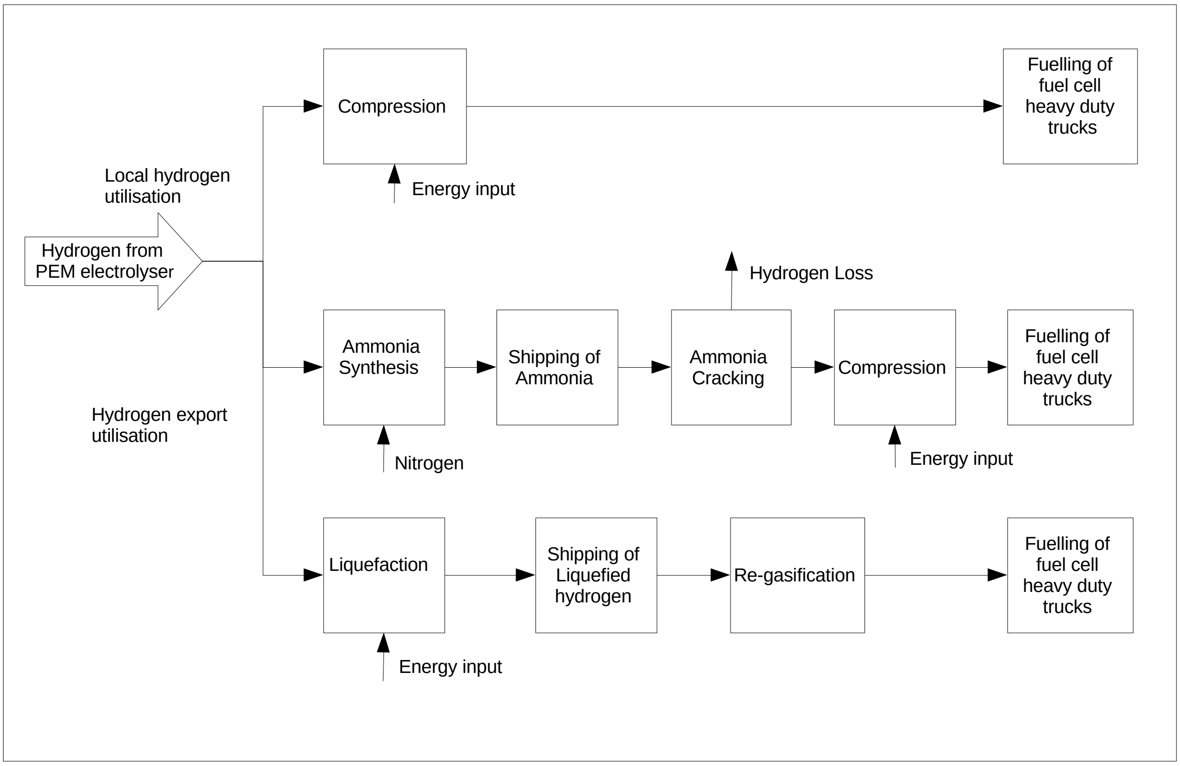


*Figure 3. 3: System boundary for hydrogen utilisation*

Impact categories of concern

The ReCiPe 2016 midpoint method was used to conduct the lifecycle impact assessment. The impact categories relevant to the scope of this study are the same as the ones used for the first lifecycle impact assessment. The impact categories are global warming, terrestrial acidification, human carcinogenic and non-carcinogenic toxicity, fossil resource scarcity, and water consumption.

Impact assessment methods

The impact assessment quantifies the potential environmental impacts and resource use of the lifecycle inventories. The impact assessment method used to determine the environmental impacts associated with hydrogen production and utilisation in South Africa is the ReCiPe 2016 method; the detailed definition and discussion of this method can be found in (Huijbregts et al., 2017). This method is an update of the ReCiPe 2008 method, and it assesses 18 midpoint impact categories and 3 endpoint impact categories. The midpoint impact categories are focused on the problem associated with a particular emission from the lifecycle inventory. In contrast, the endpoint impact categories are focused on the damage that could result. Figure 3.4 shows the relation between the midpoint and endpoint impact categories. Only the midpoint/ problem-oriented impact categories were considered for the lifecycle assessment modelling for this dissertation. The six impact categories assessed in the lifecycle assessments conducted are briefly explained below.

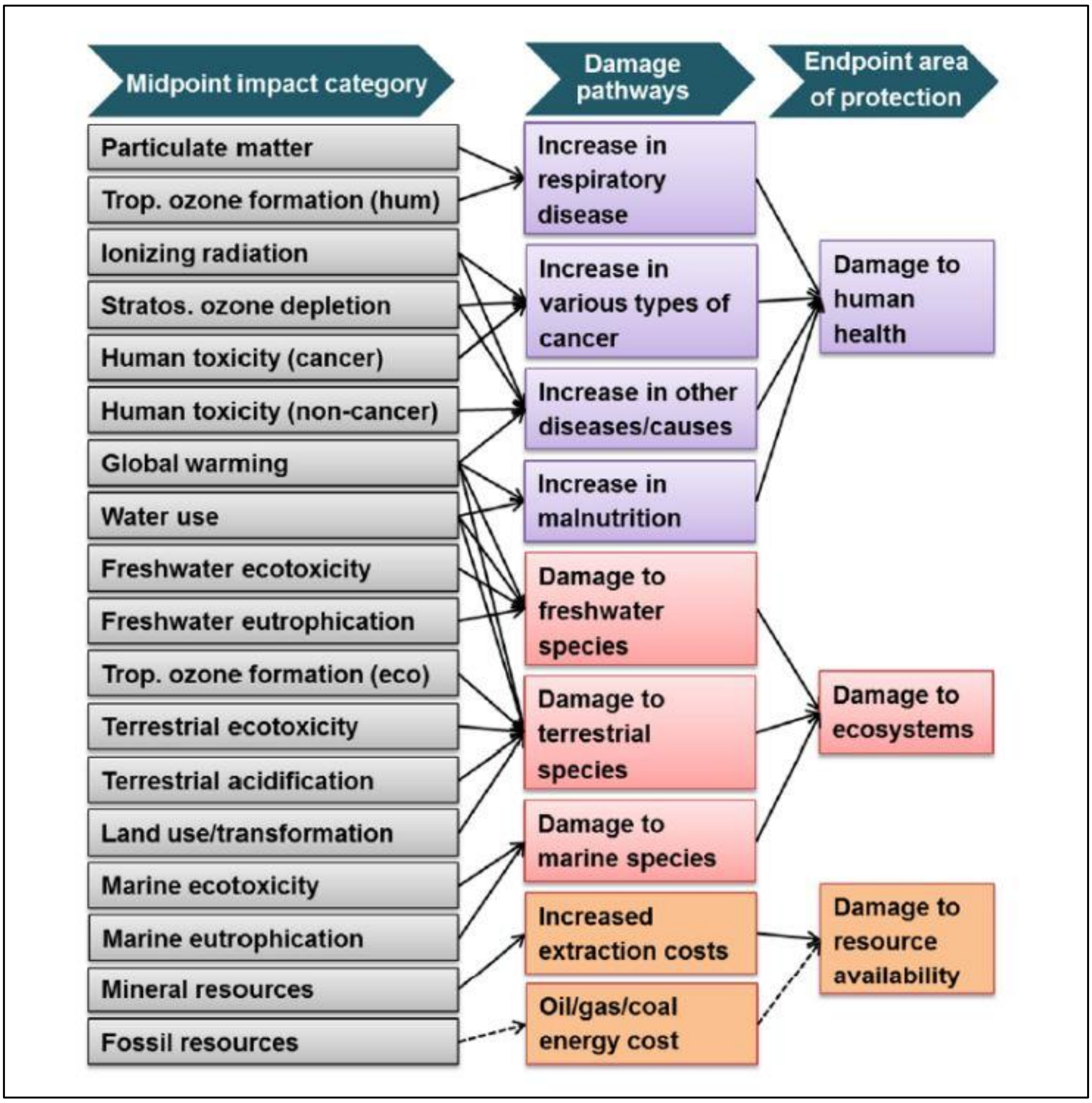


*Figure 3. 4 ReCiPe impact assessment method (Huijbregts et al., 2017)*

Global warming

The global warming impact concerns the emissions of harmful greenhouse gas emissions to the atmosphere. It is characterised by the global warming potential, and its unit is kg of $CO_2$ equivalents (Goedkoop et al., 2016).

Terrestrial acidification

Terrestrial acidification concerns the emission of chemicals and gases which would cause acidification on soil, water, and the environment, such as sulphur dioxide (Goedkoop et al., 2016). The unit used for acidification potential is 1 kg of $SO_2$ equivalents.

Human toxicity

The toxicity impacts concern the emission of toxic chemicals and substances into the atmosphere that could cause harm to human beings upon enough exposure. Carcinogenic toxicity refers to chemicals that could potentially cause cancer in humans, and non-carcinogenic toxicity refers to non-cancerous toxic chemicals (Goedkoop et al., 2016). The unit for the toxicity impact is 1.4 kg-dichlorobenzene.

Fossil resource scarcity

Fossil resource scarcity refers to the depletion of fossil fuel resources. This impact is characterised by the number of fossil fuels extracted (Goedkoop et al., 2016). The unit for this impact is 1 kg of oil equivalent.

Water consumption

The water consumption impact refers to the depletion of fresh water. The unit for this impact is $m^3$ of water consumed.

Normalisation

The normalisation factors for ReCiPe are based on the global population in 2010, which was 6.89 billion (National Institute for Public Health and the Environment, 2020). So, each impact is normalised against the yearly impact caused by an average person from the global population.

## 3.6. Research Ethics

It is essential to consider proper research ethics principles when conducting research. It was thus important to receive ethics clearance from the Faculty of Engineering and the Built Environment before commencing the research work. Ethics clearance was applied for and granted by the faculty. Proof of ethics clearance for this dissertation can be found in Appendix 8.5. The work of this dissertation did not involve any relation to interacting with humans or animals; therefore, there was no possible harm to human beings, animals, or the environment. The literature sources used throughout the dissertation were acknowledged through in-text citations and a reference list following the UCT Harvard referencing method. The assistance and guidance provided by the supervisors were appropriately acknowledged in the Acknowledgements section. Lastly, there is a potential bias towards the results of this dissertation coming from the researcher based on the expected results or conclusions. The LCA tool counteracts any potential bias because of its holistic lifecycle view. All results, including the unfavourable results, were taken seriously and reported.

# 4. HYDROGEN PRODUCTION INVENTORY AND IMPACT ASSESSMENT

## 4.1. Inventory Analysis

A process-based approach was taken to develop the LCI model. This approach builds the LCI model using information about the industrial processes throughout the product's lifecycle and the material and energy flow connected to those processes (Hauschild, Rosenbaum and Olsen, 2018). The LCI analysis is structured below in four steps.

### *4.1.1. Processes identified for the LCI model*

Based on the literature review and analysis for hydrogen production LCAs, these main processes were identified for the lifecycle inventory model.

- The extraction and preparation of raw material input required (including transport where necessary)
- The production of the required energy input
- The construction of the main plant equipment for the production processes

The main processes that make up the LCI model for hydrogen produced via water electrolysis are the deionised water feed, the construction of the electrolysis stack, and the production of the electricity required. The main processes for steam methane reforming are the pipeline transportation of natural gas, the input of natural gas to be used as the feed and fuel, and the plant's construction. Natural gas is sourced by Sasol from the Pande and Temane gas fields in Inhambane, Mozambique (Gqada, 2012). The natural gas is transported via an 865 km long pipeline to Secunda (Gqada, 2012).

### *4.1.2. Planning and collecting data*

The first step in collecting inventory data was to scan the ecoinvent database on SimaPro to see what material and energy processes were available concerning the main processes identified for the LCI models. Journal articles from reputable journals were used to source the data inputs and amounts needed for each unit process making up the LCI models. The ecoinvent database was used to model the lifecycle product stages on SimaPro for the thirteen scenarios. Data was collected for 2020, 2030 and 2040.

The raw material feed required for water electrolysis is deionised water. To produce 1 kg of hydrogen, 9 kg is needed, based on stoichiometry calculations. The deionised water process available on SimaPro, which was not a country-specific process, was adapted to a South African water process by adjusting the water and energy input to South African specific processes. For alkaline electrolysis, an additional feed required was the liquid alkaline electrolyte which was a 30 wt.% potassium hydroxide (KOH) solution (Brauns and Turek, 2020). A ratio of 1 mg per $Nm^3$ of hydrogen (Jopek, 2015) was used to calculate the amount of KOH solution required to produce 1 kg of hydrogen.

The raw material required for steam methane reforming is natural gas and water. The amounts of the raw materials required were determined stoichiometrically, and peer-reviewed journal articles were used to check and confirm these values. The materials are shown in Table 4.1.

*Table 4. 1: Raw materials (Mehmeti et al., 2018)*

| Raw material inputs | Values in kg (mg) |
|---|---|
| Steam methane reforming | |
| Natural gas | 3.5 |
| Water | 5.9 |
| Water electrolysis | |
| Deionised Water | 9 |
| 30 wt.% KOH solution (for alkaline electrolysis) | (37) |

The Cetinkaya, Dincer and Naterer (2012) study was used to source the plant construction materials needed to produce 1 kg of hydrogen via steam methane reforming. These materials are shown in Table 4.2. The main plant equipment for water electrolysis is an electrolyser or an electrolysis stack. An electrolysis stack single unit comprises two electrodes, an electrolyte, interconnect plates and frames. The stacks are made up of different materials for each electrolysis technology. Zhao et al. (2020) provided the mass amounts of the materials required to construct a 1 $m^2$ single unit stack for the three technologies. These materials and corresponding amounts are shown in Table 4.3. The energy needed for each electrolysis system to produce 1 kg of hydrogen and the lifetime energy input for each stack was used to determine the portion of the stack required to model the 1 kg hydrogen product system. This information was used to model the stack assemblies on SimaPro.

*Table 4. 2: SMR materials of construction corresponding to 1 kg of hydrogen produced (Cetinkaya, Dincer and Naterer, 2012)*

| Materials of construction | Amounts in grams |
|---|---|
| Steam methane reforming | |
| Concrete | 12.6 |
| Iron | 0.05 |
| Aluminium | 0.03 |
| Steel | 4.03 |

*Table 4. 3: Electrolyser materials of construction for 1kg of hydrogen produced (Zhao et al., 2020)*

| Main materials of construction | Amounts in grams |
|---|---|
| PEM electrolysis | |
| Stainless steel | 1185 |
| Nafion (PFTE and sulfuric acid) | 167 |
| Platinum | 22 |
| Iridium | 13 |
| Titanium | 9689 |
| Alkaline electrolysis | |
| Nickel | 6947 |
| Stainless steel | 2328 |
| Zirfon diaphragm – Zirconium oxide and polysulfone | 112 |
| Solid oxide electrolysis | |
| LSCF | 72 |
| Yttria stabilised zirconia | 150 |
| Stainless steel | 4170 |
| Ceramic glass | 20 |

Water electrolysis requires electricity input to produce hydrogen. Four electricity sources were considered: wind, solar PV, concentrated solar power (CSP), and grid electricity. Unit processes for South African renewable electricity were available on SimaPro. The grid electricity production mix available was for 2016. This unit process was used as a guide to create unit processes for the grid electricity inputs required for 2020 and 2040. The CSIR meridian economics technical report, which analyses ambitious $CO_2$ emission scenarios for the South African electricity system, was used to extract data for the electricity generation mix in 2020, 2030 and 2040 (Wright and Calitz, 2020). The IRP updated scenario was used for this study. The data shown in Table 4.4 was used to model the electricity production mix unit processes on SimaPro.

*Table 4. 4: 2020, 2030 and 2040 generation and storage mix for 1 kWh of electricity (Wright and Calitz, 2020)*

| **2020, 2030 and 2040 generation and storage shares for 1 kWh electricity production** | | | |
|---|---|---|---|
| **Technology** | **2020 Value** | **2030 Value** | **2040 Value** |
| Biofuel | 0.00765 | 0.00667 | 0.0115 |
| Coal | 0.779 | 0.515 | 0.241 |
| Concentrated solar power | 0.00945 | 0.00995 | 0.00878 |
| Hydropower | 0.0519 | 0.0989 | 0.0632 |
| Natural gas | 0.00906 | 0.00775 | 0.0174 |
| Nuclear | 0.0608 | 0.0532 | 0.0461 |
| Peaking | 0.00373 | 0.00158 | 0.00548 |
| Solar PV | 0.0279 | 0.105 | 0.190 |
| Wind | 0.0327 | 0.193 | 0.399 |
| Pumping storage | 0.0171 | 0.00288 | 0.0106 |
| Battery storage | 0.00102 | 0.00654 | 0.00709 |
| **Total** | **1** | **1** | **1** |

### 4.1.3. Updating the solar PV electricity process available on ecoinvent.

The solar PV electricity process found on the ecoinvent database for South Africa was based on a 2009 source with outdated technologies solar PV electricity production. An update of solar PV lifecycle inventory data was provided by (Frischknecht et al., 2020) and used to model an updated version of the solar PV electricity process on the ecoinvent database. The following changes were applied to correct the outdated process.

- Removal of electronic-grade silicon from casted silicon production mix inputs
- Removal of silicon carbide from silicon wafer production inputs
- Removal of polystyrene from silicon wafer production inputs
- Reducing the water input for silicon wafer production
- Reducing electricity input required to produce casted silicon

### 4.1.4. Constructing the LCI models

A Product stage on SimaPro is where a product can be defined by its assemblies, material inputs, and energy inputs (Hauschild, Rosenbaum and Olsen, 2018). Electrolysis stack assemblies were created on SimaPro under product stages for alkaline, PEM and solid oxide electrolysis. The electrolysis-based hydrogen product stages comprise an electrolysis stack assembly, water feed, and electricity requirement. The steam methane reforming-based hydrogen product stage includes the natural gas pipeline transportation, the natural gas feed, the water requirement, and the construction of main plant equipment. The product stages are illustrated in Figure 4.1 and 4.2 below.

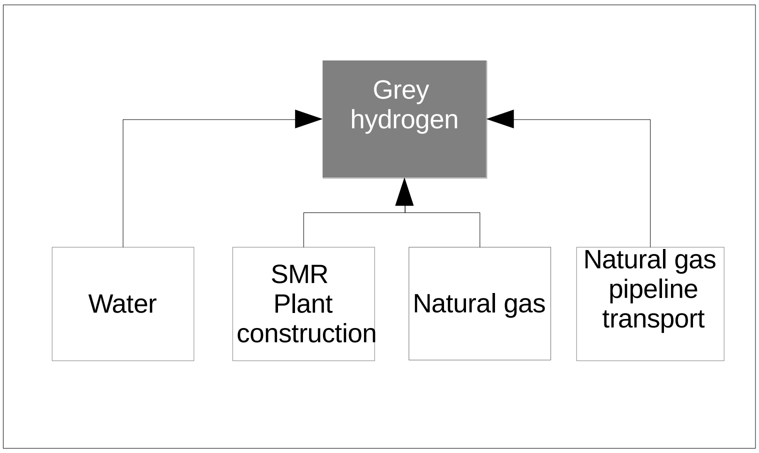


*Figure 4. 1: The grey hydrogen product system as modelled on SimaPro*

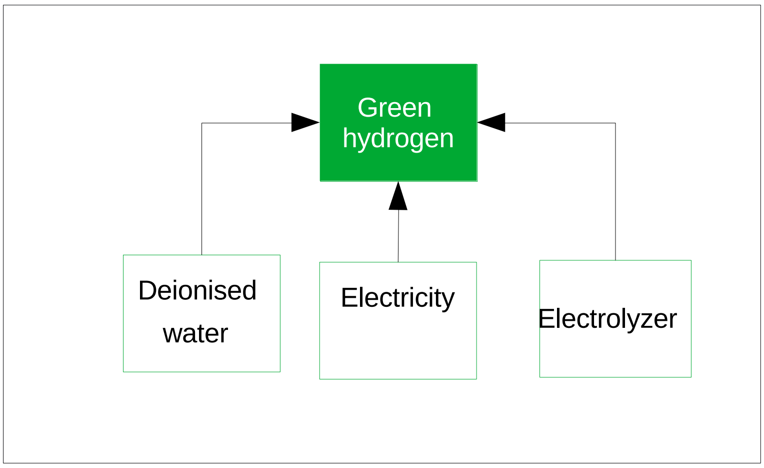


*Figure 4. 2: The green hydrogen product stage as modelled on SimaPro*

## 4.2. Lifecycle Impact assessment

The ReCiPe 2016 impact assessment method was used to conduct the lifecycle impact assessment. Various environmental impact comparisons are conducted for the hydrogen production scenarios mentioned in the scope and their respective energy inputs. The diagrams show the characterisation results for the potential environmental impacts of the hydrogen production scenarios comparisons. Normalisation results are only shown, in Figure 4.8, for the environmental impact results of the five hydrogen production scenarios.

### *4.2.1. Analysis of water electrolysis environmental impacts*

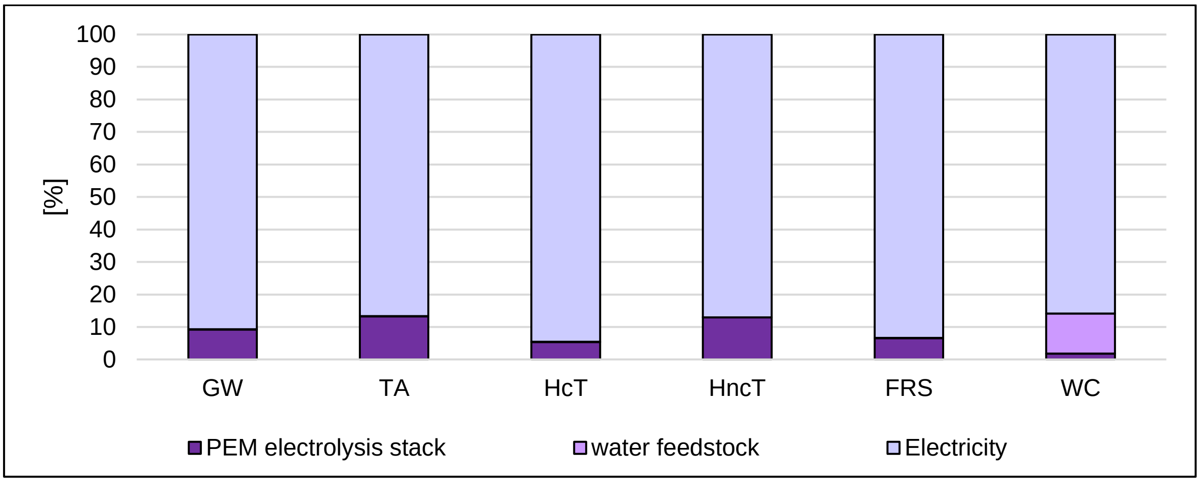


*Figure 4. 3: The environmental impacts contributions of producing hydrogen from water electrolysis powered by solar PV*

Figure 4.3 shows the environmental impact contributions of the main inputs making up the green hydrogen assembly modelled on SimaPro. The most significant environmental impact contributor across all the impact categories was the electricity input, with contributions ranging from 85% to 95%. The water feed did not significantly contribute to most environmental impact categories except for water consumption, where it contributed 12% of the total water consumption for water electrolysis. The PEM electrolyser portion required to produce 1 kg of hydrogen had miner environmental impact contributions ranging from 1.8% for water consumption to 13% for terrestrial acidification.

### *4.2.2. Analysis of hydrogen production via steam methane reforming*

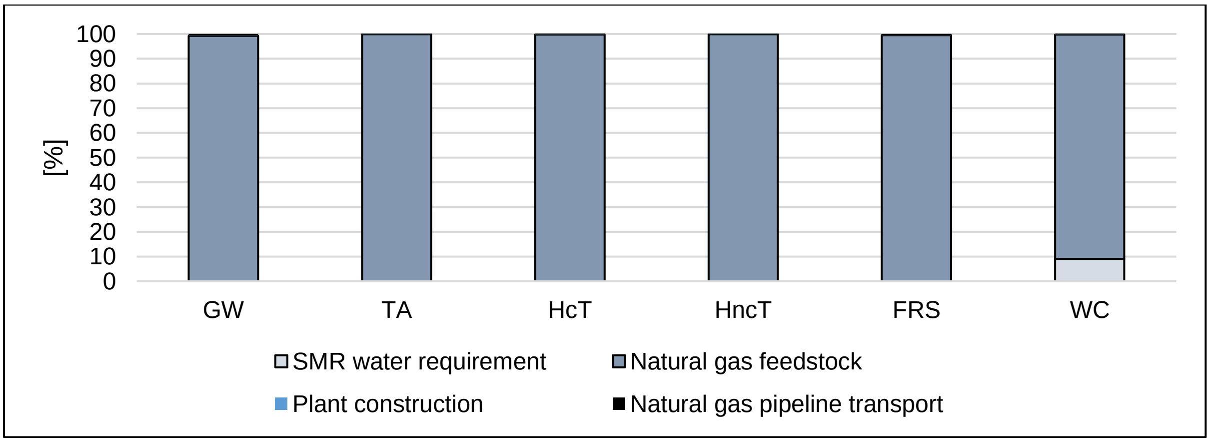


*Figure 4. 4: The environmental impacts contributions of producing hydrogen from Steam Methane reforming*

Figure 4.4 shows how the different inputs for the grey hydrogen production assembly modelled on SimaPro contribute to the total environmental impacts of steam methane reforming. The significant contributor to all the impact categories was the natural gas feed, which is both a feed and fuel input for steam methane reforming, with contributions ranging from 90% to 99.9%. The water feed contributed 9% to the total water consumption of steam methane reforming and negligible impacts in other categories, with contributions ranging from 0.005% to 0.02%. The contributions of the natural gas pipeline transport and the steam methane reforming plant construction materials were also relatively small, ranging from 0.02% to 0.7%.

### *4.2.3. Comparison of current and future grid-based electrolysis*

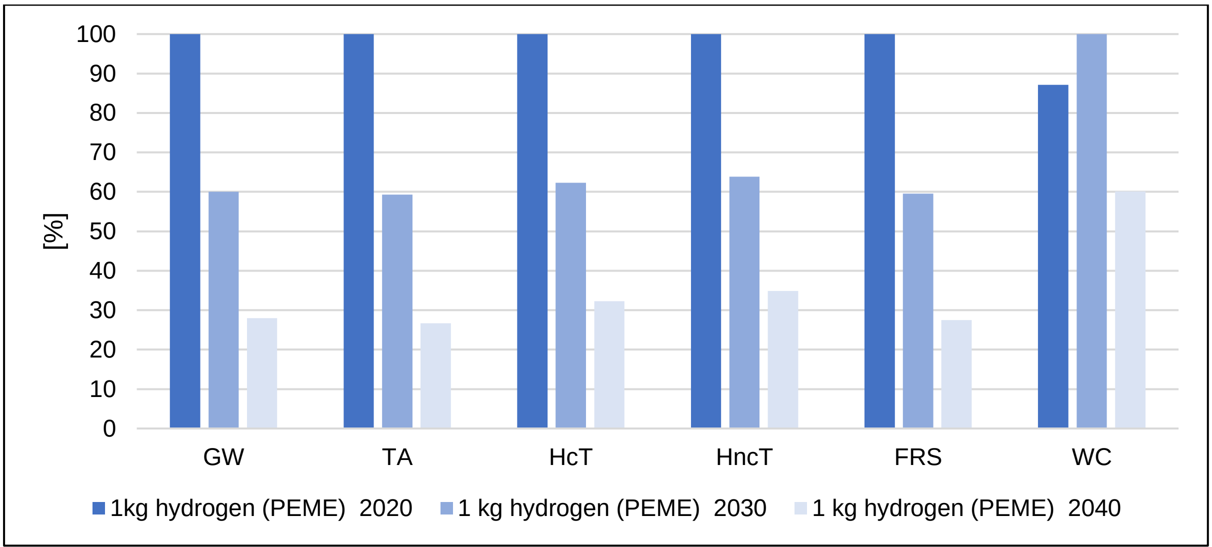


*Figure 4. 5: The environmental impacts of current and future grid electricity-powered electrolysis.*

Figure 4.5 illustrates the environmental impacts of 1 kg of hydrogen produced by water electrolysis powered by the 2020, 2030, and the 2040 grid electricity mix for South Africa. The hydrogen produced in 2020 resulted in the highest environmental impacts across all the impact categories except for water consumption. The global warming impacts for 2020, 2030, and 2040 grid electricity-powered electrolysis were 0.91, 0.61, and 0.33 kg$CO_2$ eq., respectively. The grid electricity input was the main contributor to the environmental impacts across all the impact categories for all three options.

The global warming and terrestrial acidification impacts are caused mainly by the share of electricity produced from coal. The human toxicity impacts also originate from coal-based electricity, particularly the treatment of coal ash from coal mining. The supply chain of coal also causes the fossil resource scarcity impact. According to the scenario used, the 2030 grid electricity mix has a higher share of hydropower than the 2020 and 2040 grid electricity mixes. The 2030 water electrolysis option thus, had the highest water consumption out of the three options (0.0042 $m^3$/kg of hydrogen produced).

This reduction in emissions across all impact categories reflects the increase in renewable energy shares for the 2030 and 2040 grid electricity mix and the reduction of coal shares in the future grid electricity mixes. For the 2020 grid electricity mix, the combined solar PV and wind energy shares are 6.06%. For the targeted 2030 grid electricity mix, the shares are 29.8%, and for the targeted 2040 grid electricity mix, the shares are 58.9%. The coal-based electricity shares for the 2020, 2030, and 2040 grid electricity mix are 78%, 52% and 24%, respectively. This figure shows that the improvement of the grid electricity, particularly the reduction of fossil fuel-based electricity reduces not only global warming-related impacts but also reduces environmental impacts in other impact categories.

#### *4.2.4. Comparison of 2020 2030 and 2040 wind-powered electrolysis*

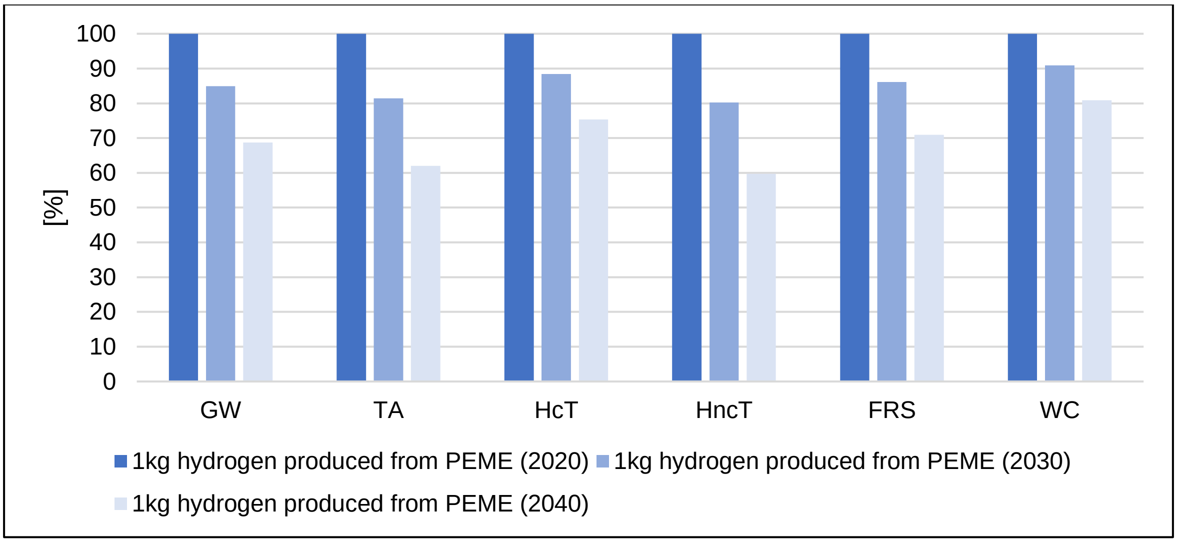


*Figure 4. 6: The environmental impacts of current and future renewable energy powered electrolysis*

Figure 4.6 compares the environmental impacts of producing 1 kg of hydrogen via wind-powered PEM electrolysis in 2020, 2030 and 2040. Wind power was chosen solely to compare current and future PEM electrolysis powered by the same renewable energy source. Similarly to the previous comparison, a steady reduction in environmental impacts from the 2020 production scenario to the 2030 and 2040 production scenario can be seen. The absolute values for the global warming impacts of 2020, 2030 and 2040 PEM electrolytic production were 2.62 kg$CO_2$ eq., 2.22 kg$CO_2$ eq., and 1.8 kg $CO_2$ eq., respectively.

This emission reduction is due to the anticipated improvements in hydrogen production efficiency via water electrolysis. The current system efficiency related to the electricity required to produce 1 kg of hydrogen from PEM electrolysis is 67 kWh/kg, and it is targeted to drop to 50 kWh/kg in 2050 (IRENA, 2020). This expected drop explains the gradual reduction in environmental impacts across all impact categories. Another aspect that would cause additional emission reductions is the future improvement and development of the technologies that make up the supply chain of wind turbines and wind electricity from 2020 to 2040. However, these improvements were not reflected in the modelling as most of the information and data for future improved technologies is unavailable.

### 4.2.5. Comparing future green hydrogen production and current grey hydrogen

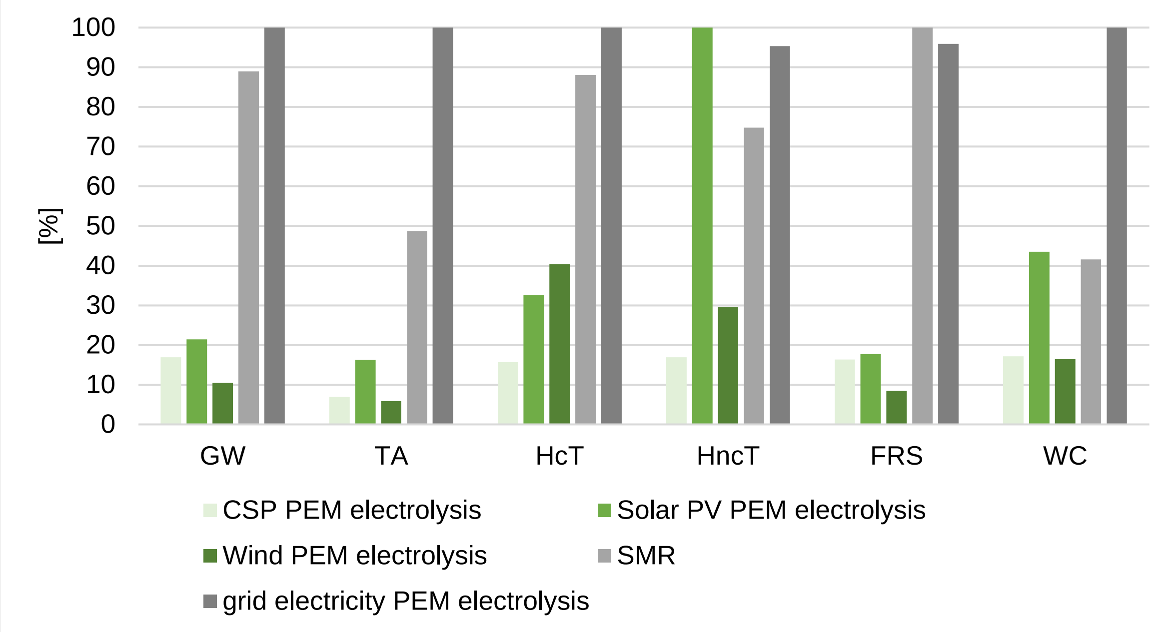


*Figure 4. 7: the characterisation impact results of producing 1kg of hydrogen in 2040 for five production scenarios*

*Table 4. 5: Absolute environmental impact results of producing 1 kg of hydrogen from five production scenarios*

| Impact category | Unit | PEME (CSP) | PEME (solar PV) | PEME (wind powered) | Steam methane reforming | PEME (grid powered) |
|---|---|---|---|---|---|---|
| Global warming | kg $CO_2$ eq. | 2.89 | 3.68 | 1.79 | 15.2 | 17.1 |
| Terrestrial acidification | kg $SO_2$ eq. | 0.0109 | 0.0255 | 0.00922 | 0.0767 | 0.157 |
| Human carcinogenic toxicity | kg 1,4-DCB | 0.213 | 0.441 | 0.546 | 1.19 | 1.35 |
| Human non-carcinogenic toxicity | kg 1,4-DCB | 4.61 | 27.2 | 8.05 | 20.4 | 25.9 |
| Fossil resource scarcity | kg oil eq. | 0.852 | 0.927 | 0.443 | 5.22 | 5.01 |
| Water consumption | $m^3$ | 0.0272 | 0.0689 | 0.0260 | 0.0659 | 0.158 |

Figure 4.7 above compares the environmental impacts of producing 1 kg of hydrogen from five hydrogen production scenarios. The renewable hydrogen production scenarios are PEM electrolysis powered by concentrated solar power, solar PV and wind. The non-renewable production scenarios are steam methane reforming and PEM electrolysis powered by the 2040 grid electricity mix. Table 4.5 shows the absolute characterised impact results for the production scenarios. Hydrogen produced from renewable energy powered electrolysis was

significantly less impactful compared to hydrogen produced from steam methane reforming and grid electricity-powered electrolysis across five out of the six impact categories considered.

The global warming impacts for CSP, solar PV and wind-powered PEM electrolysis were 2.89, 3.68, and 1.79 kg $CO_2$ eq., respectively. The global warming impacts of producing hydrogen from steam methane reforming and grid electricity-powered electrolysis were approximately a factor of 10 more impactful than the electrolytic production scenarios, at 15.2 kg $CO_2$ eq. and 17.1 kg $CO_2$ eq., respectively. Grid-based electrolysis had the highest global warming impact even with an improved 2040 grid electricity mix, with a renewable energy share of 58.9%. Therefore, it is vital to power water electrolysis with renewable electricity such as wind and solar PV electricity for it to be a low carbon hydrogen production option.

Grid-based electrolytic production also had a high acidification impact (0.157 kg $SO_2$ eq.) originating from the coal-based share of the grid electricity mix. Steam methane reforming resulted in the highest fossil resource scarcity impact (5.22 kg oil eq.), which was an expected result because of the coal-based natural gas used for the steam methane reforming process. For the sixth impact category, human non-carcinogenic toxicity, solar PV powered electrolysis had the highest impact compared to the other production scenarios. Human non-carcinogenic toxicity is primarily caused by sulfidic tailings resulting from copper mining. Copper is one of the materials used to manufacture photovoltaic panels.

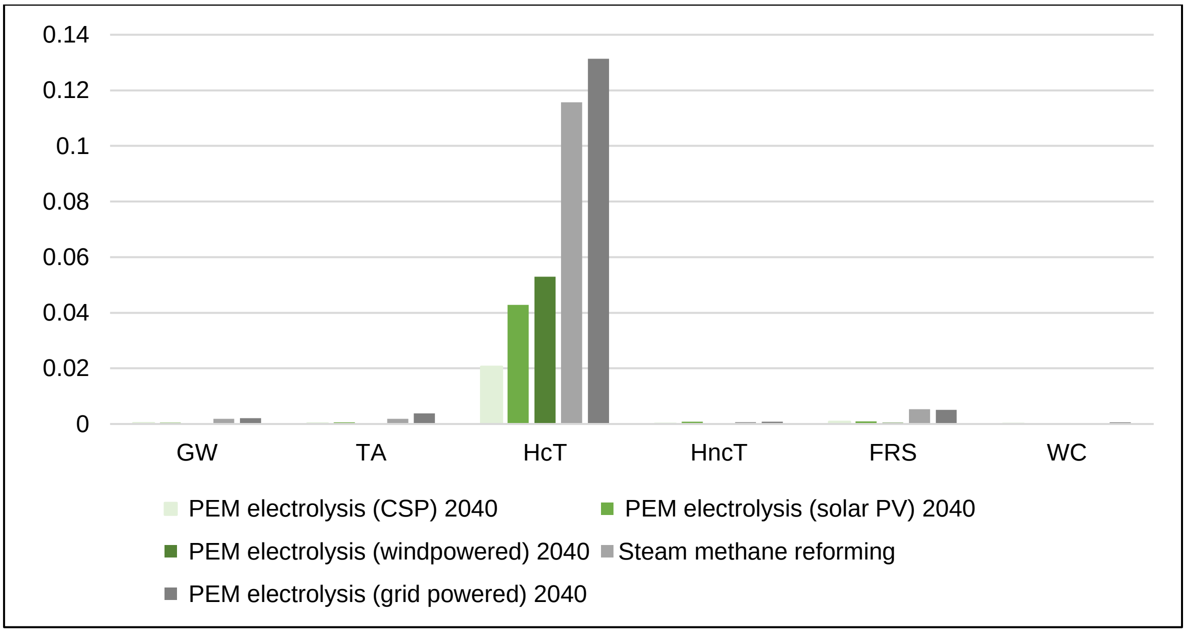


*Figure 4. 8: The normalised environmental impacts of producing 1 kg of hydrogen from five production scenarios (Method: ReCiPe 2016 midpoint method)*

*Table 4. 6: the normalised impact results for producing 1 kg of hydrogen from five production scenarios*

| Impact category | PEM electrolysis (CSP) | PEM electrolysis (solar PV) | PEM electrolysis (wind powered) | Steam methane reforming | PEM electrolysis (grid powered) |
|---|---|---|---|---|---|
| Global warming | 0.000362 | 0.00046 | 0.000225 | 0.00191 | 0.00214 |
| Terrestrial acidification | 0.000266 | 0.000623 | 0.000225 | 0.00187 | 0.00384 |
| Human carcinogenic toxicity | 0.0206 | 0.0428 | 0.053 | 0.116 | 0.131 |
| Human non-carcinogenic toxicity | 0.000147 | 0.000871 | 0.000258 | 0.000652 | 0.000831 |
| Fossil resource scarcity | 0.000869 | 0.000946 | 0.000452 | 0.00533 | 0.00511 |
| Water consumption | 0.000102 | 0.000258 | 0.0000975 | 0.000247 | 0.000594 |

Figure 4.8 shows the normalised impact results for producing 1 kg of hydrogen via the five methods shown in the diagram. The normalisation set is based on a 2010 world population, and the results are normalised against the average yearly impact of one person from the world population in 2010. The human carcinogenic toxicity impact category stood out with the highest normalised scores for each production scenario.

The normalised human carcinogenic toxicity impacts of steam methane reforming and grid-powered water electrolysis were 0.116 and 0.131, respectively. These scores mean that the toxicity impact of producing 8.62 kg of grey hydrogen or 7.63 kg of grid powered electrolytic hydrogen would equate to one person's annual human carcinogenic toxicity impact. The normalised carcinogenic toxicity impacts for CSP electrolysis, Solar PV electrolysis, and wind electrolysis were 0.0206, 0.0428 and 0.053, respectively. These normalised scores mean that the production of 48.5, 23.3, or 18.6 kg of green hydrogen powered by CSP, solar PV or wind, respectively, would equate to the annual human carcinogenic toxicity impact of one person from the global population. For the rest of the impact assessment categories, the normalised impact scores ranged from 0.00009 to 0.006 for all five production scenarios.

*4.2.6. Comparing electrolysis powered by various renewable energy technologies.*

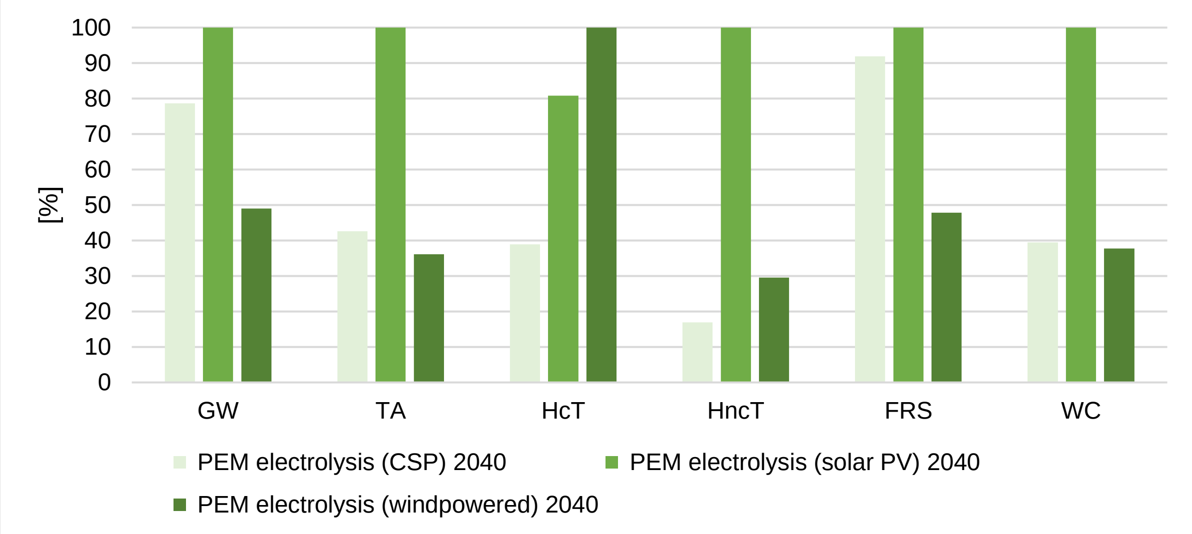


*Figure 4. 9: The environmental impacts of producing 1 kg of hydrogen via PEM electrolysis using three renewable energy sources*

Figure 4.9 compares the environmental impacts of renewable energy powered water electrolysis to produce 1 kg of hydrogen. This Figure is a zoomed-in version of Figure 4.7 focused only on the renewable hydrogen production options. Solar PV powered electrolysis resulted in the highest environmental impacts across all the impact categories except for human carcinogenic toxicity. The global warming impact of solar PV powered electrolysis was 3.68 kg$CO_2$ eq. The coal-based electricity and heat inputs for the manufacture of photovoltaic cells are the leading cause of the high global warming impact. The terrestrial acidification impact for solar PV electrolysis was 0.0255 kg $CO_2$ eq., caused by the copper production and copper mines operation. The fossil resource scarcity impact was 0.000946 kg$CO_2$ eq., caused by the operation of copper mines and coal preparation.

Solar PV powered electrolysis had a water consumption of 0.0689 $m^3$ because of the water consumption associated with the production of solar grade silicon used to produce photovoltaic panels. The environmental impacts of the updated solar PV electricity process used to model solar PV powered electrolysis, particularly water consumption and global warming, were significantly lower compared to the impacts of the solar PV electricity process found on ecoinvent; however, compared to the other renewable energy sources, solar PV is still the most environmentally impactful.

Wind-powered electrolysis had the highest human carcinogenic toxicity impact at 8.05 1.4-DCB. The toxicity is caused by the slag from the production of steel. Steel is one of the construction materials for wind turbines. This toxicity is concerning as it potentially increases the risk of cancer to human beings. Besides the high human carcinogenic toxicity impact, wind-powered electrolysis was the least environmentally impactful renewable hydrogen production scenario across the remaining five impact categories.

The absolute environmental impacts for these production scenarios could be overstated because some of the material and energy inputs for the electricity processes used to model the production scenarios represent current and not future technologies. However, a potential update to model a full 2040 scenario for all the technologies would lead to minimal changes to the current results.

### 4.2.7. Comparing electrolysis technologies

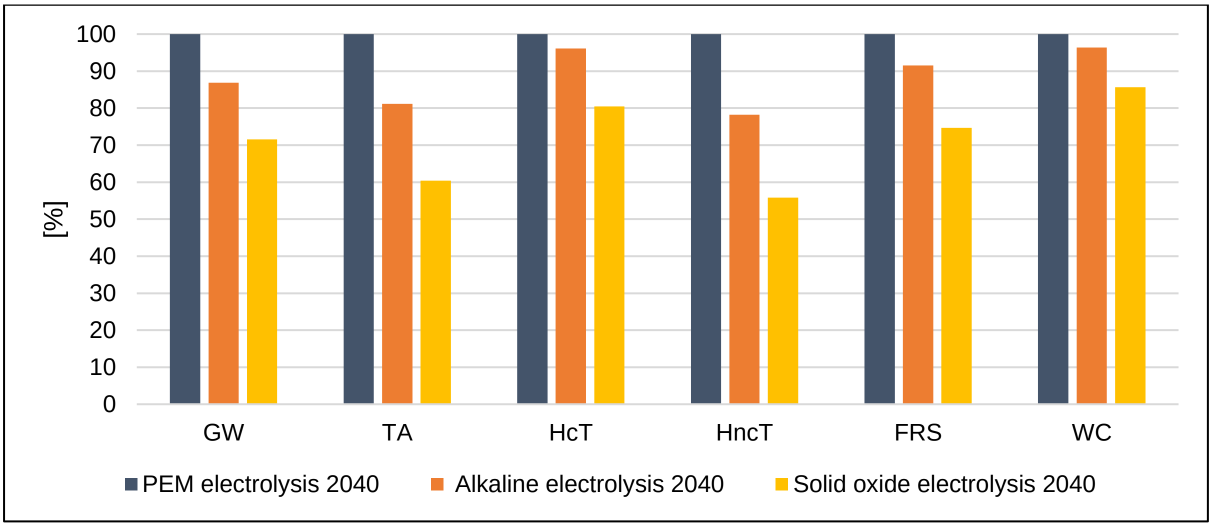


*Figure 4. 10: The environmental impacts of producing 1 kg of hydrogen from PEM, Alkaline and Solid oxide electrolysis powered by the same renewable energy source - wind*

Figure 4.10 above compares the environmental impacts of producing 1 kg of hydrogen from the three available electrolysis technologies, namely PEM, alkaline, and solid oxide electrolysis. PEM electrolysis had the highest environmental impact across all impact categories. This high impact is caused by the high electricity requirement for PEM electrolysis compared to the other technologies. The current electricity requirements to produce 1 kg of hydrogen for PEM, alkaline, and solid oxide electrolysis are 67, 64, and 50 kWh, respectively (IRENA, 2020). For future scenarios, they are expected to decrease proportionally. Solid oxide electrolysis is, therefore, the least environmentally impactful technology. While solid oxide electrolysis has excellent potential, it is currently at a lab-scale (IRENA, 2020). It requires further research and development before it can be implemented to reach a commercial scale, like PEM and alkaline electrolysis.

### 4.2.8. Combined wind and solar PV powered electrolysis

While wind-powered electrolysis was found to be the least environmentally impactful hydrogen production route, wind power cannot be used as a standalone electricity source because of its low-capacity factor. Wind and solar PV energy should be combined to power green hydrogen production to maximise the use of electrolysers throughout the year. This combination will reduce the electrolyser portion required to produce 1 kg of hydrogen. The current South African solar and wind capacity factors are 26.4% and 35.2%, respectively (Calitz and Wright, 2021). Based on a solar and wind aggregation study for South Africa done by Bofinger et al. (2016), A combined solar PV and wind electricity scenario of 75% wind and 25% solar PV was modelled on SimaPro to achieve a combined capacity factor of 61.6%. This capacity factor was based on the assumption that the two renewable energy sources would operate complementarily, hence, it is an addition of the individual capacity factors.

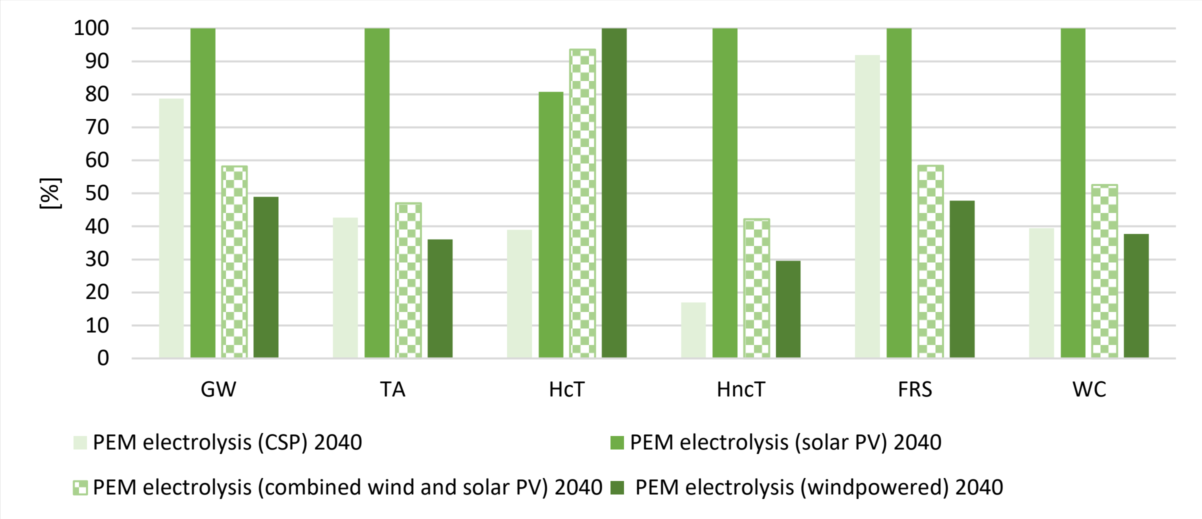


*Figure 4. 11: The environmental impact comparison of producing 1 kg of hydrogen with renewable energy powered electrolysis, including combined renewable energy powered electrolysis*

Figure 4.11 shows the environmental impacts of producing 1 kg of hydrogen via water electrolysis powered by individual and combined renewable energy sources. The environmental impacts of combined solar and wind electrolysis were between the solar PV and wind-powered electrolysis impacts across all impact categories. The environmental impacts of combined solar PV and wind-powered electrolysis were closer to the impacts of wind-powered electrolysis, which is expected given that the combined solar PV and wind electricity mix consists of 75% wind. Electrolysis powered by combined solar and wind electricity was, therefore, the second least environmentally impactful hydrogen production scenario and realistically the most suitable and sensible route to produce green hydrogen.

#### *4.2.9. Sensitivity Analysis of the Normalised results*

A sensitivity analysis was conducted for the normalised environmental impact results illustrated in Figure 4.8. This analysis aims to test the sensitivity of the normalised impact assessment results to the impact assessment method used. Two normalisation sets from the ILCD method were used for this analysis. These sets are the EU27 (2010) and the PROSUITE. The EU27(2010) considers the 2010 population of 27 European countries and normalises the results against the average yearly impact of one European person. The PROSUITE normalisation method considers the 2010 global population. It normalises the results against the average annual impact of one person from the global population, similarly to the ReCiPe method normalisation set.

Firstly, the ReCiPe 2016 normalised results shown in Figure 4.8 are compared to the ILCD PROSUITE results shown in Figure 4.12, thus comparing the normalised results of two methods that are both based on a global population. Secondly, the ILCD PROSUITE results are compared to the ILCD EU27 (2010), thus comparing the normalised results of the same impact assessment method based on a global and a European population. The ILCD midpoint+ impact assessment method is explained in more detail in (European Commission Joint Research Centre, 2012). The impact categories chosen from the ILCD method for this analysis are as close as possible to the impact categories used from the ReCiPe 2016 midpoint method. These impact categories are shown in Table 4.7 below.

*Table 4. 7: The ILCD impact categories chosen for the assessment of the sensitivity to the choice of normalisation*

| **Impact category** | **Unit** |
|---|---|
| Climate change | kg $CO_2$ eq. |
| Human toxicity, cancer | CTUh- Comparative Toxic unit for humans |
| Human toxicity, non-cancer | CTUh- Comparative Toxic unit for humans |
| Acidification | Molecule H+ eq. |
| Mineral, fossil, and renewable resource depletion | kg Sb (antimony) eq. |
| Water resource depletion | $m^3$ water eq. |

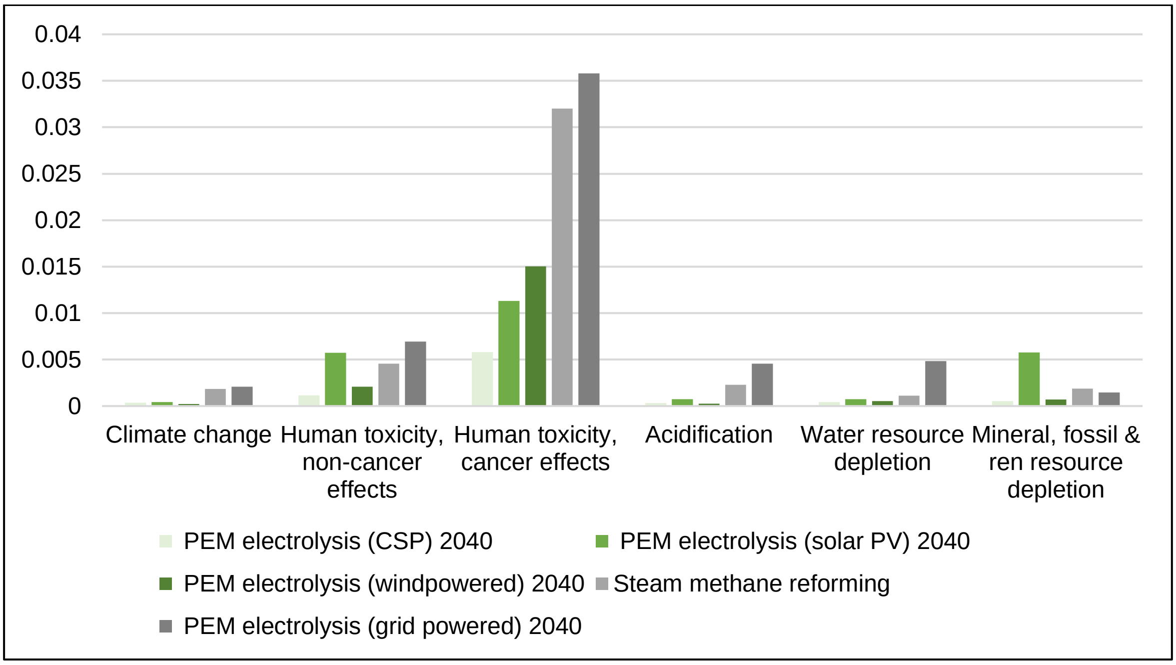


*Figure 4. 12: The normalised environmental impacts of producing 1 kg of hydrogen from five production scenarios (method- ILCD-PROSUITE)*

Figure 4.12 shows the ILCD normalised impact results for producing hydrogen from the different production scenarios for the PROSUITE normalisation set. The normalised impact scores for ReCiPe 2016 and ILCD PROSUITE are expected to be similar, given that their normalisation sets consider the global population. Human carcinogenic toxicity is the dominant impact category for both normalisation sets; however, the magnitudes of the normalised scores differ. The ReCiPe 2016 normalised impact scores are larger than the ILCD PROSUITE impact scores, with the highest normalised score (human toxicity with cancer effects for grid-powered electrolysis) for the two sets being 3.6 times higher for the ReCiPe 2016 normalised results. Even though the human carcinogenic toxicity is dominant for both impact assessment methods, the dominance is quite extreme for the ReCiPe 2016 normalisation results, with the other impact categories barely showing up in Figure 4.8.

For wind-powered electrolysis, the human toxicity with cancer effects is 3.5 times higher for the ReCiPe 2016 normalised results. The toxicity of wind-powered electrolysis is caused by the supply chains of wind turbines. The next dominating impact category is human toxicity with non-cancer effects. However, this impact category barely shows up in Figure 4.8 due to the extreme dominance of the human carcinogenic toxicity impact.

It is important to note that the units of measure for the human toxicity impacts are different for these methods. The toxicity impact unit is kg eq. of 1.4-DCB for ReCiPe 2016 and CTUh (comparative toxicity unit for humans) for ILCD. This difference in units might also contribute to the unexpected observations when comparing the normalised results for these two methods. The difference in the magnitudes of the normalised scores for Figures 4.8 and 4.12 also shows that the two methods use different normalisation techniques and evaluate each impact category differently. Climate change, acidification and water resource depletion have the lowest normalised impact scores for all the production scenarios.

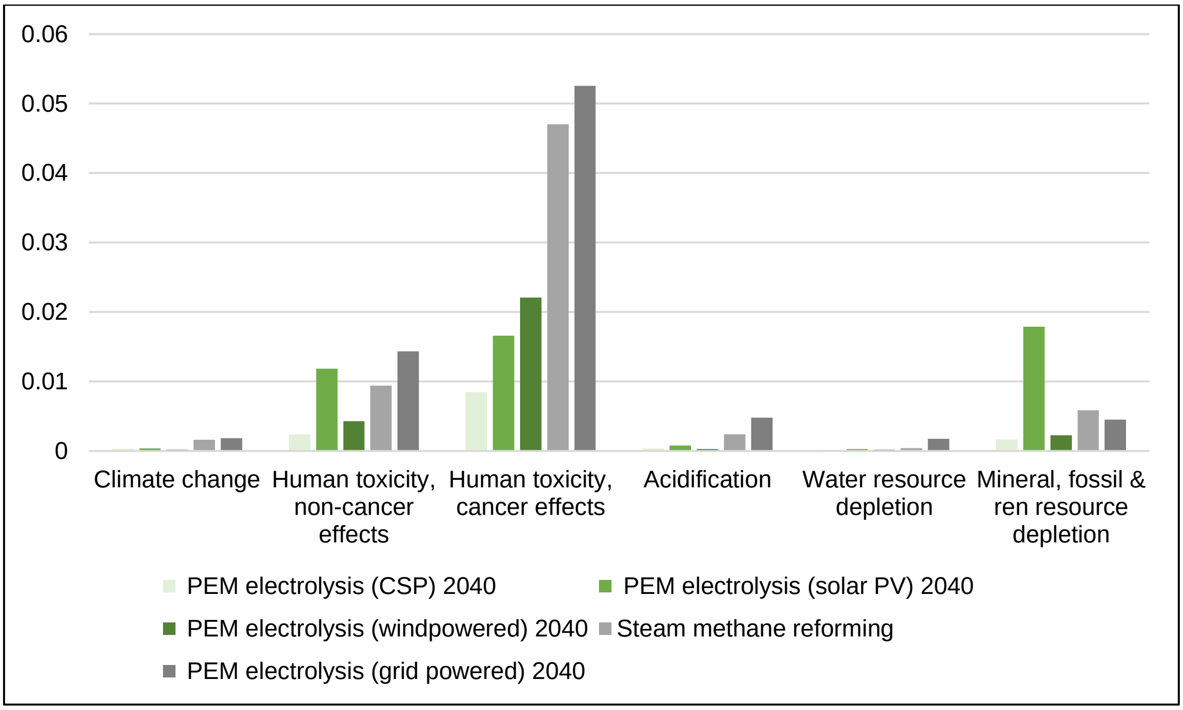


*Figure 4. 13: The normalised environmental impacts of producing 1 kg of hydrogen with five production scenarios (ILCD-EU27 2010)*

Figure 4.13 compares the normalised environmental impacts of producing 1 kg of hydrogen from five different hydrogen production scenarios. The graph displays similar results to Figure 4.12, with human toxicity with cancer effects having the highest normalised impact scores for the production scenarios. Given that this normalisation set considers a European population, the normalised scores were expected to be larger than the normalised impact scores for the normalisation set focused on the global population, as the European population makes up about 10% of the global population. When comparing Figure 4.12 and this figure, this expectation is observed for some impact categories.

For mineral, fossil and renewable resource depletion, acidification, human toxicity with cancer effects, and human toxicity with non-cancer impacts, the normalised scores for the EU27 (2010) normalisation set are 3, 0.9, 1.5, and 2.07 times larger than the normalised scores for the PROSUITE normalisation set, respectively. The highest normalised score, which is the human toxicity with cancer effects for grid electricity-powered electrolysis, is 0.052 for the EU27 (2010) normalisation set and 0.036 for the PROSUITE normalisation set. The PROSUITE normalised scores for water resource depletion and climate change are 2.7 and 1.1 times larger, respectively.

The next dominating impact category is human toxicity with non-cancer effects for both the EU27 (2010) and PROSUITE normalisation set. The production route with the highest score in this impact category is grid powered electrolysis, followed by solar PV powered electrolysis. The opposite result is observed for the ReCiPe 2016 results, with solar PV powered electrolysis causing the highest human toxicity with non-cancer effects among all the production routes. This toxicity impact is caused by the supply chains of solar PV panels.

The EU27 (2010) results also show significant dominance for the mineral, fossil and renewable resource depletion impact of solar PV powered electrolysis, which is not observed for the PROSUITE results shown in Figure 4.12. The cause for the high score is the production of zinc concentrate, silver, and tantalum, which are all used to manufacture solar PV panels. So, the high impact is mostly concentrated on mineral resource depletion and not necessarily fossil or renewable resource depletion.

The comparison for Figure 4.12 and 4.13 shows that the impacts do not only depend on population size, but they also depend on the known impacts of a certain population, so even if the European population makes up 10% of the global population, the impacts of the European population could be larger or smaller relative to the impacts of the global population based on the consumption behaviour of Europeans and use of relatively cleaner or “dirtier” technology.

This sensitivity analysis, to some extent, validates the result from Figure 4.8, but also cautions against too forceful an interpretation. It confirms that human carcinogenic toxicity is a concerning impact related to hydrogen production, especially non-renewable hydrogen production. This analysis also reveals certain levels of impact assessment method sensitivity associated with the normalised impact results as different methods have different normalisation sets and evaluate the normalised impacts differently. Following human carcinogenic toxicity, the next concerning impact categories for green hydrogen are the human non-carcinogenic toxicity impact, and mineral resource depletion of solar PV powered electrolysis, resulting from the supply chains of solar PV electricity.

## 4.3. Interpretation

The interpretation phase of the LCA assesses the significant issues identified in the lifecycle inventory analysis and impact assessment and evaluates the uncertainty associated with the impact assessment results.

### *4.3.1. Identification of significant uncertainty issues*

Data and input uncertainty

Various data sources, particularly peer-reviewed journal articles and publications, were used to collect the inputs required for the LCI. All the inputs thus have a level of uncertainty.

The Zhao et al. (2020) study was used to collect the materials of construction data for electrolysers. In some instances, the materials used for constructing the electrolysers were not available on ecoinvent, in which case, a similar process was chosen as a representative. Given the negligible impact contribution of the electrolyser construction materials, these substitutes would not compromise the quality of the results.

The electricity data source used for the generation and storage mix for current and future grid electricity was the 2020 CSIR Meridian Economics technical report (Wright and Calitz, 2020). Given that electricity was the dominant driver of environmental impacts for water electrolysis, the source chosen for the electricity data and the scenario used from this source was quite significant and caused uncertainty, as a different choice of source would significantly change the outcomes of the LCA. The 2030 and 2040 electricity mixes are based on projections and therefore aren't entirely accurate, thus contributing to temporal uncertainty.

The Cetinkaya et al. (2012) and Mehmeti et al. (2018) studies were used to collect inventory data for the steam methane reforming product system. The Mehmeti et al. (2018) study was the most significant source for the natural gas input required to produce the functional unit. The Cetinkaya et al. (2012) study was a bit dated and therefore contributes to the temporal uncertainty of the inputs. However, it was only used for plant construction materials data which had an insignificant contribution to the final impacts of the steam methane reforming product system.

The actual construction process for the plant equipment was omitted for both product systems. This is due to a lack of data for the construction processes. The omission of this part was also seen in similar LCA studies found in the literature such as studies conducted by Patterson et al. (2014), and Zhao et al. (2020). Given that construction materials already have a small contribution to the final environmental impacts of hydrogen production, it was assumed that the construction process contribution would be insignificant. This missing data contributes some uncertainty to the inputs; however, it was not expected to affect the assessment outcomes significantly.

The product stages were modelled as much as possible for the South African region. However, the data used from the ecoinvent database has a level of geospatial uncertainty. The reason for this uncertainty is that the lifecycle processes of each input contain processes such as water or electricity from other regions, and some of the input materials making up these processes were produced in other regions. Furthermore, some data values were averaged for the entire South African region but did not necessarily represent individual South African regions.

Method uncertainty

Firstly, the process-based model used to conduct this LCA presents some uncertainty as it assumes that the process accurately represents the lifecycles as they are, which is not the case. Secondly, the software used to conduct the LCA (SimaPro) presents some uncertainty. Other software tools such as openLCA and GaBi could have been used to perform this LCA, each with different calculation procedures that would lead to different results, hence the uncertainty. SimaPro was used because it was the only lifecycle assessment software available at the University of Cape Town. The database used to model the LCI is the ecoinvent database, as it was the same database used in similar LCAs in literature and readily available on SimaPro. The impact assessment methods used are the Recipe 2016 H midpoint method and the ILCD 2011 method. The ILCD 2011 midpoint method was used to conduct sensitivity analyses for some of the impact assessment and uncertainty results generated from the ReCiPe 2016 midpoint method.

#### *4.3.2. Data completeness check*

The significant issue identified in the previous section regarding hydrogen production was the energy input to power the different hydrogen processes. For green hydrogen, the electricity input is a significant factor. Natural gas used as a feedstock and fuel to power the steam methane reforming process was a significant factor. The renewable electricity processes used to model green hydrogen production were found on the ecoinvent database. The electricity mix used to model a prospective grid electricity-powered electrolysis scenario was sourced from a reputable paper in partnership with the CSIR, as mentioned in the lifecycle inventory analysis. The data was enough to fulfil the goal of the lifecycle assessment and to model the processes mentioned as significant issues contributing to the uncertainty of the results.

### *4.3.3. Results uncertainty and Monte Carlo uncertainty analysis*

The data and methods uncertainty make up the uncertainty associated with the results. Single and comparative uncertainty analyses were conducted for the impact assessment results of producing hydrogen via combined solar and wind-powered PEM electrolysis and producing hydrogen via steam methane reforming to evaluate the uncertainty associated with the results quantitatively. SimaPro uses the Monte Carlo statistical method to conduct uncertainty analyses. The Monte Carlo analysis runs 1000 random samples for the impact assessment results and produces a range of uncertainty for the calculated results (Goedkoop et al., 2016).

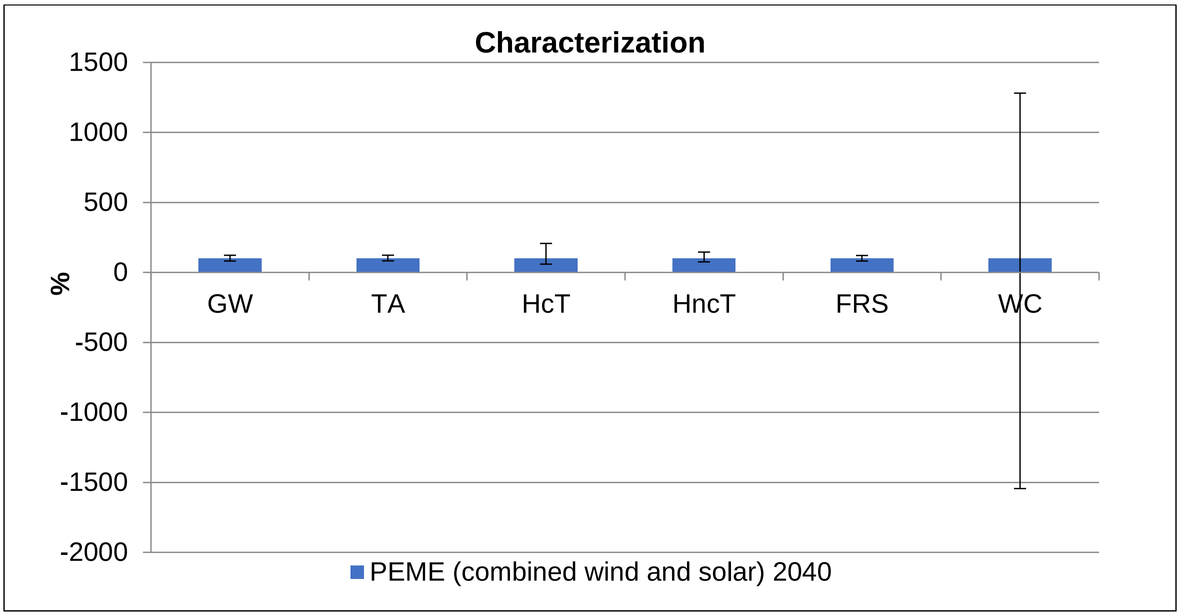


*Figure 4. 14: Monte Carlo analysis for the environmental impacts of producing hydrogen via PEM electrolysis powered by combined solar and wind electricity (impact assessment method: ReCiPe 2016 midpoint method, confidence interval: 95%)*

Figure 4.14 shows the Monte Carlo analysis for the impact assessment results of producing 1kg of hydrogen from PEM electrolysis powered by combined wind and solar PV. The vertical bars show the uncertainty range for each impact category for a 95% confidence interval. Water consumption had quite an extensive uncertainty range of -1644% to 1181%. This range indicates the uncertainty related to the inventory material and energy flows contributing to the water consumption for PEM electrolysis. Referring to the impact assessment, the significant contributor to high water consumption for renewable energy powered PEM electrolysis was the manufacture of photovoltaic panels, which involves solar grade silicon production and silicon wafer production. Therefore, the data inputs making up the supply chain of photovoltaic panels cause water consumption uncertainty. The second highest uncertainty range was associated with human carcinogenic toxicity (40% to 107%). Wind-powered electrolysis had the highest human carcinogenic toxicity caused by the supply chain of wind turbines. There is also some uncertainty associated with the data inputs for manufacturing wind turbines.

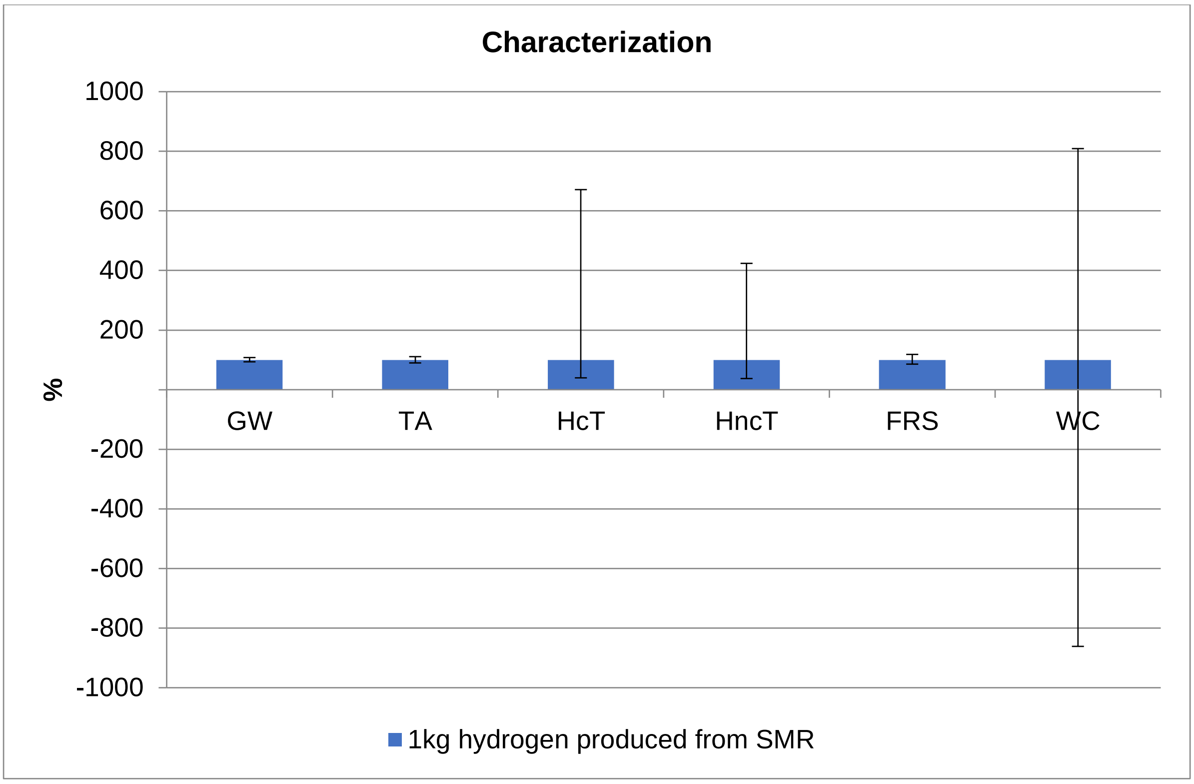


*Figure 4. 15: Monte Carlo analysis for the environmental impacts of producing hydrogen via Steam Methane Reforming (impact assessment method: ReCiPe 2016 midpoint method, confidence interval: 95%)*

Figure 4.15 is the Monte Carlo analysis to produce hydrogen via steam methane reforming. Similarly to the water electrolysis Monte Carlo analysis, water consumption has the most extensive range of uncertainty. The natural gas input was the most significant contributor to water consumption for the steam methane reforming system. The natural gas material process from the ecoinvent database used to model hydrogen production from steam methane reforming had a few non-geographic input processes that could have caused the large uncertainty range for water consumption. The next impact categories with large uncertainty ranges are human carcinogenic and non-carcinogenic toxicity. The significant contributor to the toxicity impacts of steam methane reforming is coal ash and spoils treatment from coal mining. Coal was a feed required to produce natural gas. The reason for the high uncertainty range of the human toxicity impacts could be the aggregated inputs making up the treatment processes, such as material residual landfill, which had no specificity.

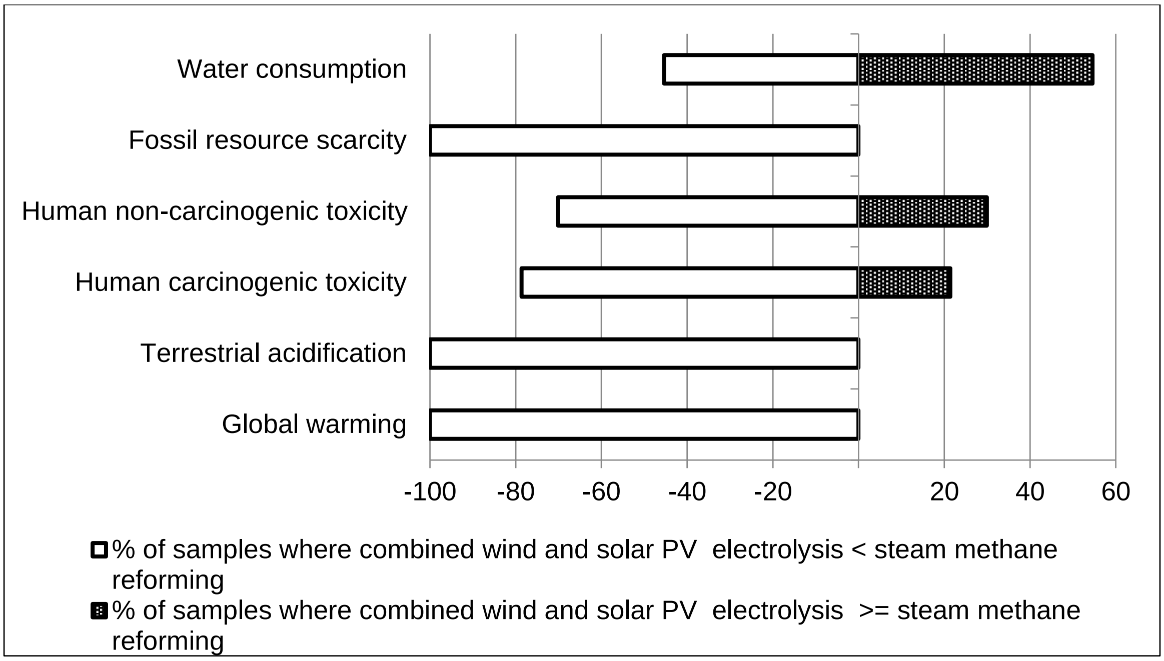


*Figure 4. 16: The Monte Carlo comparative analysis for producing hydrogen via steam methane reforming and renewable energy powered electrolysis (method: ReCiPe 2016)*

The bulk of this lifecycle assessment compares the quantitative environmental impacts of grey and green hydrogen production scenarios. Figure 4.16 is the comparative Monte Carlo analysis for the potential environmental impacts of producing hydrogen from steam methane reforming and producing hydrogen from PEM electrolysis or, rather, grey and green hydrogen production. There is a 100 % certainty that grey hydrogen production is more environmentally impactful than green hydrogen production for fossil resource scarcity, terrestrial acidification, and global warming. Grey hydrogen production is still more impactful for the human toxicity impacts, with an uncertainty ranging from 23% to 30%. Green hydrogen production is more water-intensive, with a 47% uncertainty. There is almost a 50% chance that either green or grey hydrogen production could be more water consumptive. The uncertainty distributions for this diagram can be seen in appendix 8.3.

## 4.4. Summary of the production lifecycle assessment

The hydrogen production LCA was conducted following the four phases of the lifecycle assessment framework: the goal and scope, the lifecycle inventory analysis, the lifecycle impact assessment, and the Interpretation. An attributional lifecycle inventory modelling method was followed where all emissions were attributed to the main product produced, hydrogen. The ReCiPe 2016 midpoint method was used in conducting the impact assessment. Wind-powered electrolysis was the least environmentally impactful hydrogen production scenario. However, combined wind and solar PV powered electrolysis was realistically the best option when considering the combined capacity factor and thus the operation of electrolysers throughout the year.

The different contributors to the uncertainty of the impact assessment were discussed in the interpretation phase. The Monte Carlo analysis assessed the certainty with which green hydrogen production is less impactful than grey hydrogen production across the six impact categories. As discussed in the interpretation phase, the uncertainty analysis proved that green hydrogen production is less impactful with significant certainty. Hydrogen produced via solar PV and wind-powered electrolysis was used as an input for the hydrogen utilisation lifecycle assessment to assess the best way to use the green hydrogen in South Africa.

# 5. HYDROGEN UTILISATION INVENTORY AND IMPACT ASSESSMENT

## 5.1. Inventory Analysis

### *5.1.1. Planning and collecting the data*

The inventory data was collected using various literature sources on previous lifecycle studies for hydrogen utilisation in transport and transport unit processes on the ecoinvent database. Following a unit process on ecoinvent for conventional truck transportation, the main processes making it up are the fuel input, the truck assembly, road construction, and road maintenance. The transport unit processes were used to guide the LCI modelling of the transport scenarios in this assessment. The models excluded road construction and maintenance, which would have had the same impacts for all the scenarios.

### *5.1.2. Hydrogen fuel input*

The main material process making up the transport unit process is the hydrogen fuel input. The hydrogen material process was taken from the previous LCA, which was carried out to determine the best hydrogen production route. The hydrogen process used was the hydrogen produced from polymer electrolytic membrane (PEM) electrolysis, powered by wind and solar electricity. Combined solar PV and wind electricity was the best option because it had a capacity factor of 65% and above (Bofinger et al., 2016), which is significantly higher compared to the individual capacity factors of solar PV and wind electricity; 26.4 % and 35.2% respectively (Calitz and Wright, 2021). The hydrogen fuel consumption for a heavy-duty hydrogen fuel cell electric vehicle (FCEV) is 0.088 kg/km (NACFE, 2020). Considering an average load of 20 tons for a heavy-duty truck, the amount of hydrogen required for one tkm truck transport activity was calculated to be 0.0044 kg.

### *5.1.3. Hydrogen used to fuel heavy-duty truck transport in South Africa*

A compressed hydrogen material process was created on SimaPro using the combined solar and wind-powered hydrogen process and the electricity required to compress hydrogen from 20 bar, the output pressure from the electrolyser to a refuelling pressure of 440 bar. The electricity required was 2.23 kWh/kg of hydrogen compressed (Gardiner and Satyapal, 2009). The compression stage was assumed to be carried out at the same location as the hydrogen production plant, so the renewable electricity source used to produce the hydrogen would be the same source for fulfilling the compression electricity requirement. Given that 70 kt would need to be compressed for a functional unit of 16 tkm, A total of 156 GWh of renewable electricity would be required for the compression.

### *5.1.4. Hydrogen (exported as ammonia) used to fuel heavy-duty truck transport in Germany*

A material unit process for hydrogen exported to Germany as ammonia was created on SimaPro. The process included the conversion of hydrogen to ammonia, ammonia shipping, reconversion and compression of hydrogen, and the utilisation of hydrogen to fuel heavy-duty trucks in Germany. The total energy required to synthesise green ammonia, including hydrogen production, nitrogen separation from the air, and feedstock compression to the Haber-Bosch reactor pressure, is 10-12 kWh/kg of ammonia produced (Giddey et al., 2017). Excluding the energy used to produce the hydrogen via electrolysis, the energy requirement for ammonia synthesis becomes 3 kWh/kg of ammonia produced.

The ammonia was assumed to be shipped from Saldanha Bay to the port of Rotterdam, which is 13 430 km away (Ports.com, 2021). Upon arrival, the ammonia would be reconverted to hydrogen via ammonia cracking, resulting in a 15% loss of hydrogen (Giddey et al., 2017). Thereafter, the hydrogen would be compressed from atmospheric pressure to 20 bar and from 20 bar to a refuelling pressure of 440 bar (Giddey et al., 2017). The total energy requirement for the compression was 3.28 kWh/kg of hydrogen, and it would be supplied by German grid electricity. A net-zero scenario for Germany's energy sector compatible with a carbon budget of 1.5°C was used for the 2030 electricity mix (Simon et al., 2022). The 2030 German electricity mix is shown in Table 5.1. The technologies with minimal shares on the grid mix, such as hydrogen, were not included when modelling this electricity mix on SimaPro. The import potion was also not included as there was no further information about where the electricity would be imported from and what technology it would fall under. Figure 5.1 shows the process description for the hydrogen shipped as ammonia.

*Table 5. 1: 2030 Net-zero budget scenario electricity mix (Simon et al., 2022)*

| **Gross power production in 2030 (%)** | |
|---|---|
| hard coal | 1.33E-06 |
| lignite | 1.33E-07 |
| oil | 0.00219 |
| natural gas | 12.1 |
| synthetic gas (CH4, H2) | 0.490 |
| hydrogen (conventional) | 1.93E-08 |
| hydrogen (RE) | 1.13E-07 |
| non-biogenic waste | 3.05 |
| biomass | 8.89 |
| hydro | 2.84 |
| photovoltaic | 18.8 |
| wind | 53.8 |
| geothermal | 0.0265 |
| Import (net, conventional) | 0.243 |
| Import (net, RE) | -0.284 |
| sum | 100 |

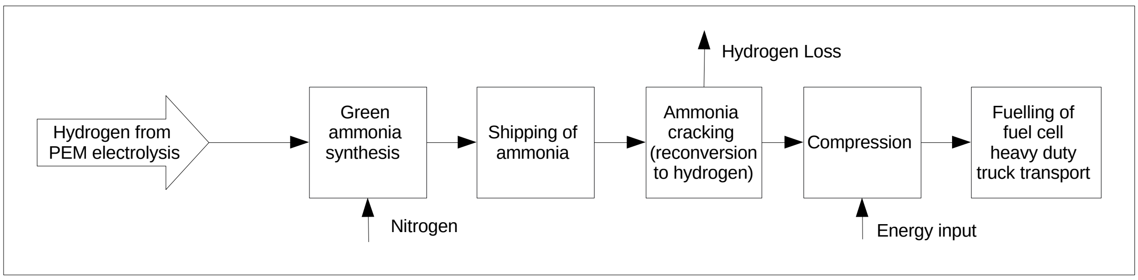


*Figure 5. 1: Block flow diagram of the process of hydrogen exported via ammonia to be used to fuel heavy-duty truck transport in Germany*

### *5.1.5. Hydrogen (exported as liquefied hydrogen) used to fuel heavy-duty truck transport in Germany*

The hydrogen gas would be liquefied by cooling it to its critical temperature of -240°C and condensing it at atmospheric pressure (Bossel and Eliasson, n.d.). Liquefied hydrogen would then be stored in vessels at a temperature of -253°C at 1 atm. The liquefaction process is an energy-intensive process that requires about 10 kWh/kg of hydrogen liquefied (Gardiner and Satyapal, 2009). The liquefied hydrogen would be transported by sea from Saldanha Bay to the port of Rotterdam in large tankers of about 10 000 $m^3$. At arrival, it would be regasified to hydrogen gas. (Aziz, 2021). The long-distance transportation of liquefied hydrogen leads to a 10% hydrogen loss (Roos, 2021). Figure 5.2 illustrates the process description.

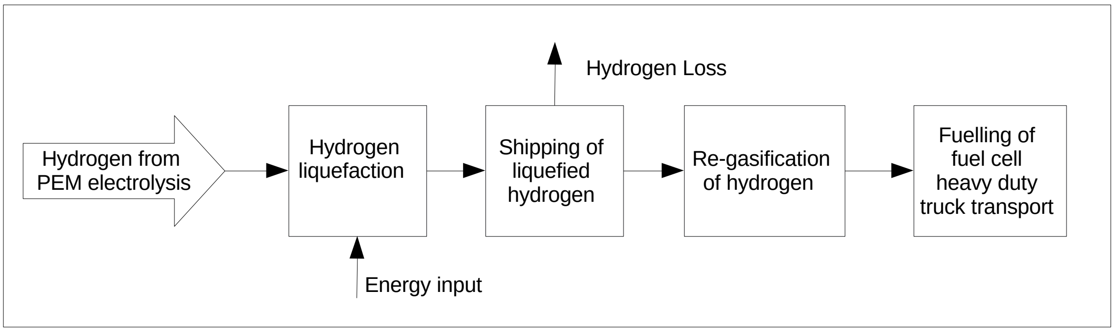


*Figure 5. 2: Block flow diagram of the process of hydrogen exported as liquefied hydrogen to be used to fuel heavy-duty truck transport in Germany*

### *5.1.6. The heavy-duty hydrogen fuel cell electric vehicle (FCEV)*

The hydrogen fuel cell electric vehicle was created using heavy-duty vehicle inventory data from peer-reviewed journal articles. The unit process is made up of a PEM fuel cell stack, an electric motor, a battery, glider components, and the energy and heat required to assemble the vehicle. A PEM fuel cell stack process on ecoinvent was used for the model and scaled up for a heavy-duty truck. The mass of the fuel cell stack on SimaPro is 110 kg (Patterson et al., 2014), and the mass required for two 114 kW fuel cell stacks for a Toyota Mirai heavy-duty truck is 114 kg (Yoshida and Kojima, 2015). Therefore, a ratio of 1.04 for the fuel cell stack input for the FCEV assembly was used. The required battery and electric motor masses are 130 kg and 145 kg, respectively (Marcinkoski et al., 2016). The glider components of a heavy-duty truck amount to 5092 kg, with an energy and heat requirement of 1977 kWh and 2974 MJ, respectively, for vehicle assembling (Wolff et al., 2020). Table 5.2 summarises the heavy-duty FCEV vehicle assembly.

*Table 5. 2: Heavy-duty hydrogen fuel electric vehicle assembly*

| **Processes used to build the FCEV assembly** | **Amount** | **Unit** | **Source** |
|---|---|---|---|
| Fuel cell stack | 1.04 | p | (Patterson et al., 2014), (Yoshida and Kojima, 2015) |
| Electric motor | 145 | kg | (Marcinkoski et al., 2016) |
| Battery | 130 | kg | (Marcinkoski et al., 2016) |
| Glider components | 5092 | kg | (Wolff et al., 2020) |
| Electricity | 1977 | kWh | (Wolff et al., 2020) |
| Heat | 2974 | MJ | (Wolff et al., 2020) |

### 5.1.7. *Diesel used to fuel heavy-duty truck transport in South Africa*

In South Africa, diesel is produced by Sasol via the Fischer-Tropsch (FT) process using coal as the primary feedstock. Diesel is also imported from other countries where it is produced in oil refineries. On the ecoinvent database, only euro 2 South African transport processes exist; however, to model a 2030 scenario, a euro 5 South African heavy-duty truck transport process was created. The European emission standards (euro standards) were set to provide strict limits for exhaust emission pollutants (AA, 2017). A euro 5 Europe heavy-duty truck transport process was adapted by replacing the Europe inputs with South African inputs. The transport process was created using low sulphur coal-based diesel. Coal-based diesel was used because it makes up part of the diesel market mix for South Africa, but the actual market mix was unknown. Therefore, coal-based diesel was used to quantify how much decarbonisation can be achieved by replacing coal-based diesel with hydrogen. The diesel consumption for heavy-duty truck transport processes on the ecoinvent database is 0.0192 kg/tkm.

### 5.1.8. *Diesel used to fuel heavy-duty truck transport in Germany*

In Germany, diesel is produced in refineries using crude oil as the primary feedstock. It was assumed that in 2030, Germany would have reached euro 7 standards for internal combustion engine trucks powered by diesel. However, A euro 6 diesel heavy-duty truck transport process on Ecoinvent was used, as it was the highest euro standard available for truck transport processes. The diesel consumption for the euro 6 heavy-duty truck transport process is also 0.0192 kg/tkm.

## 5.2. Lifecycle Impact assessment

The lifecycle impact assessment for hydrogen utilisation in heavy-duty trucks is conducted. Individual environmental impact comparisons for the two cases of hydrogen utilisation were carried out. The potential impacts of local hydrogen utilisation are compared with those of diesel utilisation for heavy-duty truck transportation, as diesel is one of the conventional fuels for heavy-duty trucks. The potential impacts of exported hydrogen utilisation in Germany are also compared with those of diesel utilisation in Germany to fuel heavy-duty trucks. In South Africa, part of the diesel is produced via the Fischer-Tropsch process, which uses coal as raw material, and in Germany, diesel is made from crude oil.

After the individual comparisons of using diesel or hydrogen fuel in South Africa and Germany, a system expansion is conducted to compare the potential impacts of using hydrogen locally and exporting hydrogen for usage in Germany. The two systems are expanded to create comparable systems with equal functional units. The process is explained in detail in Section 5.2.3.

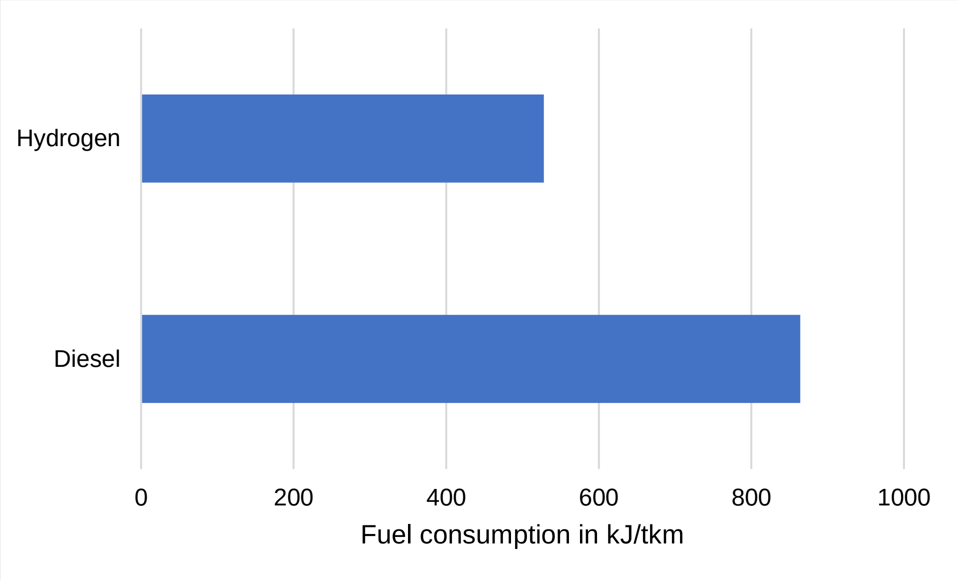


*Figure 5. 3: fuel consumption of hydrogen and diesel-fuelled heavy-duty trucks*

Figure 5.3 shows the different fuel consumption of trucks per tkm of transport activity. According to the lifecycle inventory, the diesel and hydrogen mass consumption rates for trucks are 0.0192 and 0.0044 kg/tkm, respectively. The diesel mass consumption is more than four times larger than the hydrogen consumption for trucks. However, when considering the lower heating values of diesel and hydrogen, the energy consumption rates for diesel and hydrogen-fuelled trucks are 864 KJ/tkm and 528 KJ/tkm, respectively. This comparison shows that internal combustion engine vehicles are less fuel-efficient than hydrogen fuel cell electric vehicles.

### *5.2.1. Individual environmental impact comparisons*

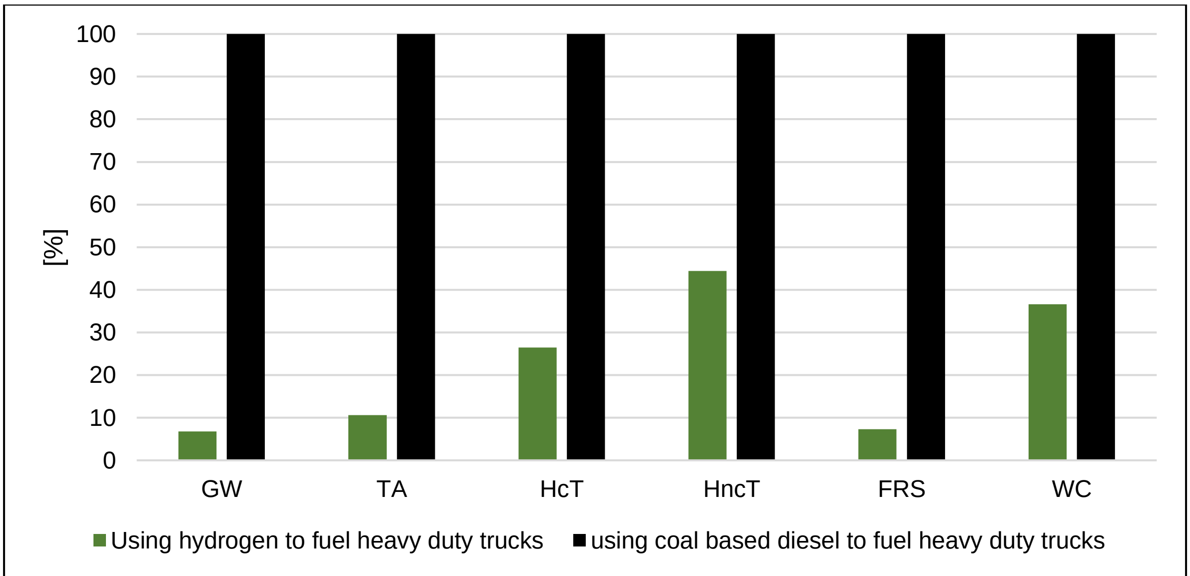


*Figure 5. 4: Comparing the environmental impacts of using hydrogen locally to replace diesel in heavy-duty trucks*

*Table 5. 3: Environmental impacts of using hydrogen and diesel to fuel 16 billion tkm truck transport activity*

| Impact category | Unit | Using hydrogen to fuel heavy-duty trucks | Using coal-based diesel to fuel heavy-duty trucks |
|---|---|---|---|
| Global warming | kg $CO_2$ eq. | 216 000 000 | 3 190 000 000 |
| Terrestrial acidification | kg $SO_2$ eq. | 1 280 000 | 12 100 000 |
| Human carcinogenic toxicity | kg 1,4-DCB | 47 500 000 | 180 000 000 |
| Human non-carcinogenic toxicity | kg 1,4-DCB | 1 610 000 000 | 3 630 000 000 |
| Fossil resource scarcity | kg oil eq. | 55 000 000 | 752 000 000 |
| Water consumption | $m^3$ | 3 240 000 | 8 860 000 |

Figure 5.4 compares the environmental impacts of using hydrogen and diesel to fuel heavy-duty trucks to fulfil the functional unit of 16 billion tkm truck transport activity. Diesel was significantly more environmentally impactful than hydrogen across all impact categories, especially global warming, terrestrial acidification, and fossil resource scarcity. For global warming, using hydrogen fuel is 93% less impactful than diesel fuel. The absolute global warming impacts for diesel consumption during truck transport activity of 16 billion tkm resulted in 3.19 billion kg $CO_2$ eq., and hydrogen fuel consumption resulted in 216 million kg $CO_2$ eq. The main contributors to the high global warming impact of coal-based diesel are the diesel Fischer-Tropsch production process and the emissions from the truck transportation, with contributions of 62% and 38%, respectively.

For terrestrial acidification, hydrogen fuel was 89% less impactful than diesel. Hydrogen fuel consumption was 93% less impactful than diesel consumption for fossil resource scarcity. Hydrogen fuel made up 26% and 44% of diesel fuel-related human carcinogenic and non-carcinogenic toxicity impacts, respectively. The contributors to the human toxicity impact of the diesel-fuelled trucks are the treatment of hard coal ash and the spoils from hard coal mining since the diesel is coal-based.

Lastly, using hydrogen fuel consumed 63% less water than using diesel fuel. Similarly to the global warming impact, the high water consumption for diesel fuel originates from the Fischer-Tropsch process of producing diesel from coal. Table 5.3 shows the absolute values for the environmental impacts of 16 billion tkm transport fuelled by diesel and hydrogen. The high impacts related to the usage of diesel fuel were expected because of the carbon-intensive and fossil fuel dependent process of producing diesel. Additionally, as shown in Figure 5.3, the fuel efficiency of internal combustion engine trucks is lower than the fuel efficiency of hydrogen fuel cell electric vehicles. This difference in efficiency is an additional reason for the high environmental impact of diesel-fuelled truck transport relative to the environmental impacts of hydrogen-fuelled truck transport.

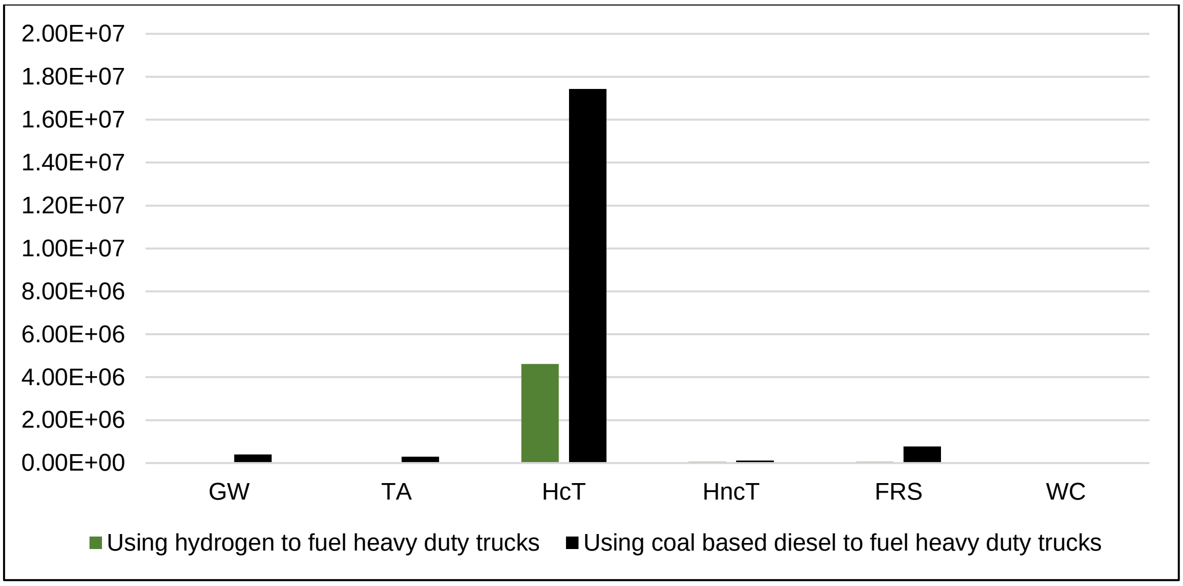


*Figure 5. 5: Comparing the normalised environmental impacts of using hydrogen locally to replace diesel in heavy-duty trucks*

Figure 5 .5 shows the normalised impacts of using hydrogen locally to fuel heavy-duty trucks and using diesel to fuel heavy-duty trucks. From these normalised results, Human carcinogenic toxicity was extremely dominant compared to other impact categories. The human carcinogenic toxicity impact is concentrated on the hydrogen input. The dominance of this impact category tracks back to the hydrogen production lifecycle assessment. As mentioned in the hydrogen production impact assessment, the human carcinogenic toxicity impact of hydrogen production primarily originates from caused by the supply chains of wind turbines.

### *5.2.2. Exporting hydrogen*

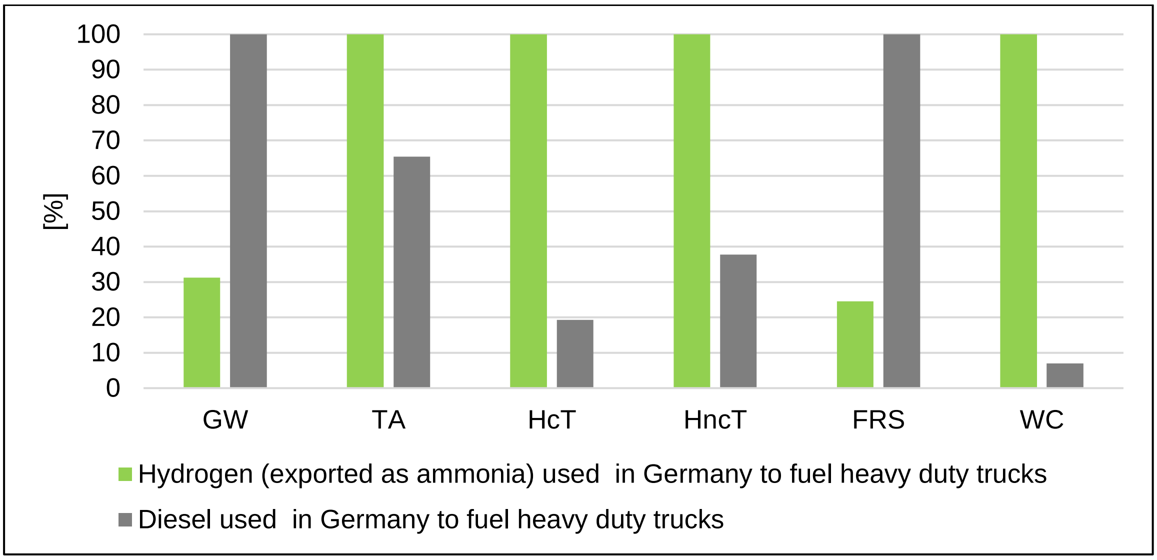


*Figure 5. 6: Environmental impact comparison using hydrogen (exported as ammonia) to replace diesel fuel in heavy duty trucks in Germany*

*Table 5. 4: The environmental impacts of using hydrogen and diesel to fuel heavy-duty truck transportation in Germany*

| Impact category | Unit | Hydrogen (exported as $NH_3$) used in Germany to fuel heavy-duty trucks | Diesel used in Germany to fuel heavy-duty trucks |
|---|---|---|---|
| Global warming | kg $CO_2$ eq. | 303 000 000 | 968 000 000 |
| Terrestrial acidification | kg $SO_2$ eq. | 2 260 000 | 1 480 000 |
| Human carcinogenic toxicity | kg 1,4-DCB | 57 600 000 | 11 100 000 |
| Human non-carcinogenic toxicity | kg 1,4-DCB | 1 760 000 000 | 663 000 000 |
| Fossil resource scarcity | kg oil eq. | 80 000 000 | 326 000 000 |
| Water consumption | $m^3$ | 6 720 000 | 473 000 |

Figure 5.6 shows the environmental impact comparison for using hydrogen exported from South Africa to Germany to fuel heavy-duty trucks and diesel to fuel heavy-duty trucks in Germany. Table 5.4 shows absolute values for potential environmental impacts. The functional unit for this comparison is 13.5 billion tkm. This functional unit is less than 16 billion tkm because it accounts for the losses of hydrogen that occur throughout the conversion processes and shipping of the hydrogen. Using diesel fuel to fuel heavy-duty trucks was more environmentally impactful for global warming and fossil resource scarcity. The global warming impact of using hydrogen fuel to fulfil the functional unit was 303 million kg $CO_2$ eq. which was 69% less than the global warming impact of using diesel fuel which was 968 million kg $CO_2$ eq.

Using exported hydrogen was more environmentally impactful for terrestrial acidification, human toxicity, and water consumption. Using hydrogen fuel was 75% less impactful for terrestrial acidification than diesel fuel. The main contributors to terrestrial acidification for the utilisation of exported hydrogen were the shipping of ammonia and hydrogen production. Particularly for hydrogen production, acidification is caused by the extraction and processing of platinum used to manufacture PEM electrolysers. It is also caused by copper production processes as copper is one of the materials used to manufacture wind turbines. For the human toxicity impacts, using diesel fuel was 81% and 62% less impactful for human carcinogenic and non-carcinogenic toxicity, respectively. The hydrogen input contributed 72% and 56% of the human carcinogenic and non-carcinogenic toxicity impacts of hydrogen-fuelled trucks. The main contributors to the human toxicity impacts are the supply chains of electrolysers and solar PV installations required for green hydrogen production.

Using diesel fuel consumed 7% of the water consumption related to using hydrogen fuel. The contributors of water consumption related to using hydrogen fuel are the hydrogen input and the production of green ammonia. For the hydrogen input, the high water consumption is caused by the production of solar grade silicon which is part of the supply chain of photovoltaic panels. Exporting hydrogen to Germany increases the initial impacts for hydrogen fuel utilisation hence the dominance of hydrogen utilisation in some of the impact categories.

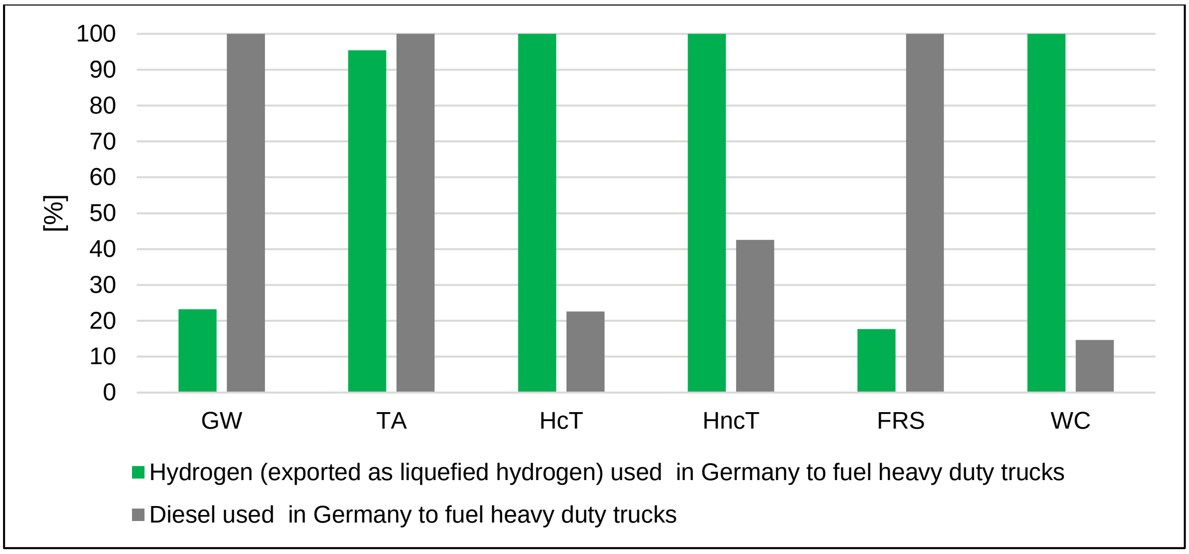


*Figure 5. 7: Environmental impact comparison using hydrogen (exported as liquefied hydrogen) to replace diesel fuel in heavy-duty trucks in Germany*

Figure 5.7 above compares the environmental impacts of using hydrogen exported as liquefied hydrogen to fuel heavy-duty trucks and diesel to fuel heavy-duty trucks in Germany. The exported hydrogen utilisation option includes the liquefaction of hydrogen, shipping to Germany, and reconversion to gaseous hydrogen. The functional unit for this comparison is 14.3 billion tkm, as it also accounts for hydrogen losses throughout the exporting and converting of hydrogen.

Like the previous comparison for the case of exporting hydrogen as ammonia, hydrogen fuel was less impactful for the global warming and fossil resource scarcity impacts. It was more impactful for the other impact categories. The global warming impact of using hydrogen fuel made up 23% of the global warming impact of using diesel fuel. For terrestrial acidification, the environmental impacts of the two options were not far off from each other, with the impact of hydrogen being 5% smaller than the impact of diesel. For the human carcinogenic and non-carcinogenic toxicity impacts, using diesel fuel was 77% and 57% less impactful than using hydrogen fuel, respectively. For fossil resource scarcity, using hydrogen fuel was 82% less impactful than diesel fuel. Using diesel fuel consumed 75% less water than using hydrogen fuel.

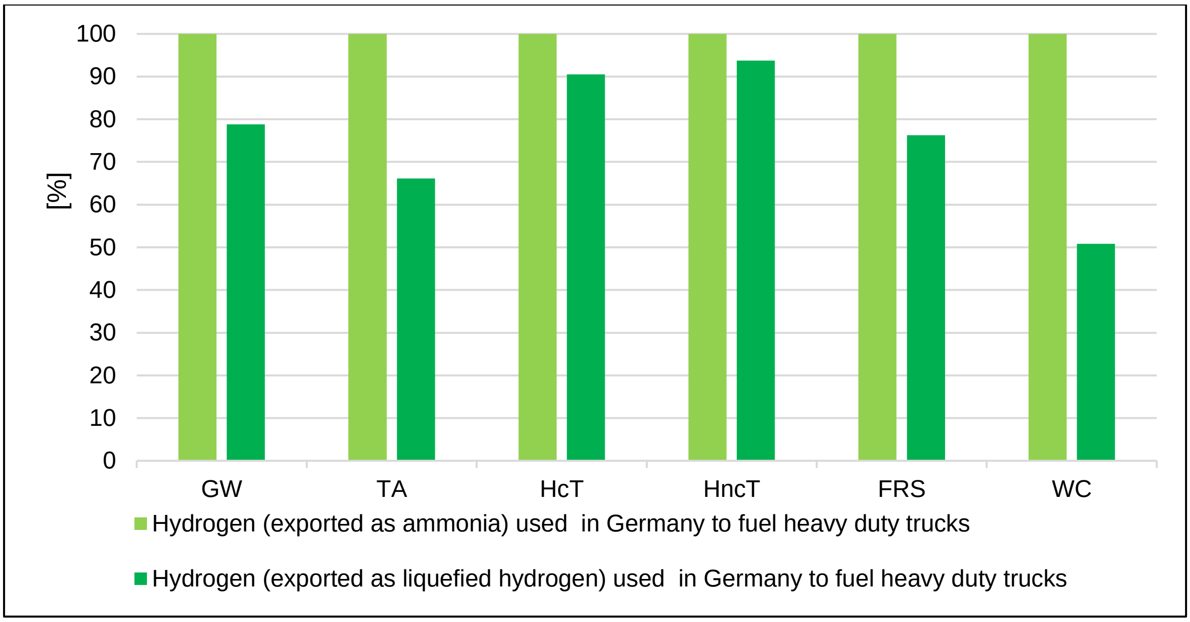


*Figure 5. 8: Comparing the environmental impacts of exporting hydrogen as ammonia and exporting hydrogen as liquefied hydrogen*

Figure 5.8 shows the environmental impact comparison results for hydrogen exported as liquefied hydrogen and hydrogen exported as liquid ammonia to be used as fuel for heavy-duty truck transportation in Germany. The truck transport activity fulfilled by hydrogen exported as ammonia and liquefied hydrogen is 13.5 and 14.3 billion tkm, respectively. This difference in fulfilled functional units is caused by the different amounts of hydrogen loss occurring during the conversion and export processes of the two options. According to the lifecycle inventory analysis, the hydrogen losses for the ammonia export route and liquefied export route were 15% and 10%, respectively. The environmental impacts of the ammonia case were higher across all impact categories.

The global warming impact of using hydrogen exported as liquefied hydrogen was 21% smaller than the impact of using hydrogen exported as ammonia. Likewise, with terrestrial acidification, the impact of using hydrogen exported as liquefied ammonia was 34% smaller. The human toxicity impacts are not too different for the two cases. The human carcinogenic and non-carcinogenic toxicity impact of using hydrogen exported as liquefied hydrogen is 9 and 6% less impactful, respectively. For fossil resource scarcity, using hydrogen exported as liquefied hydrogen was 24% less impactful, and for water consumption, it consumed 49% less water.

The ammonia export case resulted in higher environmental impacts because of the energy requirement of ammonia synthesis, which is higher than the energy requirement of hydrogen liquefaction per kg of hydrogen converted. Secondly, more volume is shipped for the ammonia case because there is about 0.2 kg of hydrogen in a kg of ammonia. While ammonia may be currently the cheapest way to export hydrogen over long distances (Engie Impact, 2021), it seems to be the more environmentally harmful option for hydrogen export. The infrastructure for large-scale hydrogen liquefaction and long-distance transportation of the liquefied hydrogen is currently unavailable (Giddey et al., 2017); however, that could change in the future.

### *5.2.3. Process of system expansion*

The two hydrogen utilisation systems were expanded to compare the level of decarbonisation that could be achieved for these two cases of either using hydrogen locally or exporting for usage in another country. Diesel was chosen as an alternative fuel for heavy-duty trucks, so it was used to expand the systems. The local hydrogen utilisation system was expanded by adding the amount of tkm that would be achieved should hydrogen be exported to be used in Germany for heavy-duty trucks. That amount was assumed to be fulfilled by diesel in Germany. The additional functional unit for this expansion was 13.5 billion tkm, as shown under the grey block in Figure 5.9.

The hydrogen export case was expanded in the same way by adding the tkm that could be achieved should hydrogen not be exported and instead used locally. That tkm amount was then modelled to be fulfilled by diesel in South Africa. The additional functional unit for this expanded system was 16 tkm. The hydrogen export case used in this system expansion was exporting it as ammonia. As shown in Figure 5.9, after this expansion, the functional units of the expanded systems became equal; thus, a like for like comparison could be conducted to compare the extent of decarbonisation that can be achieved from the two hydrogen utilisation cases. Figure 5.9 illustrates the process followed for the system expansion. Further calculations for the system expansion can be found in appendix 8.2.

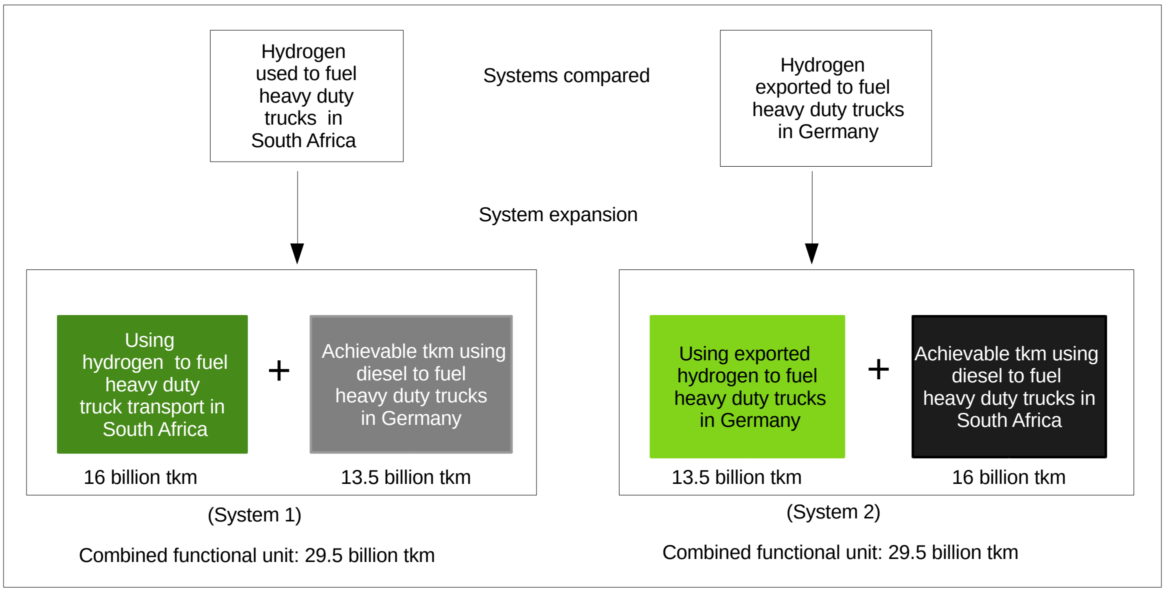


*Figure 5. 9: Process of system expansion*

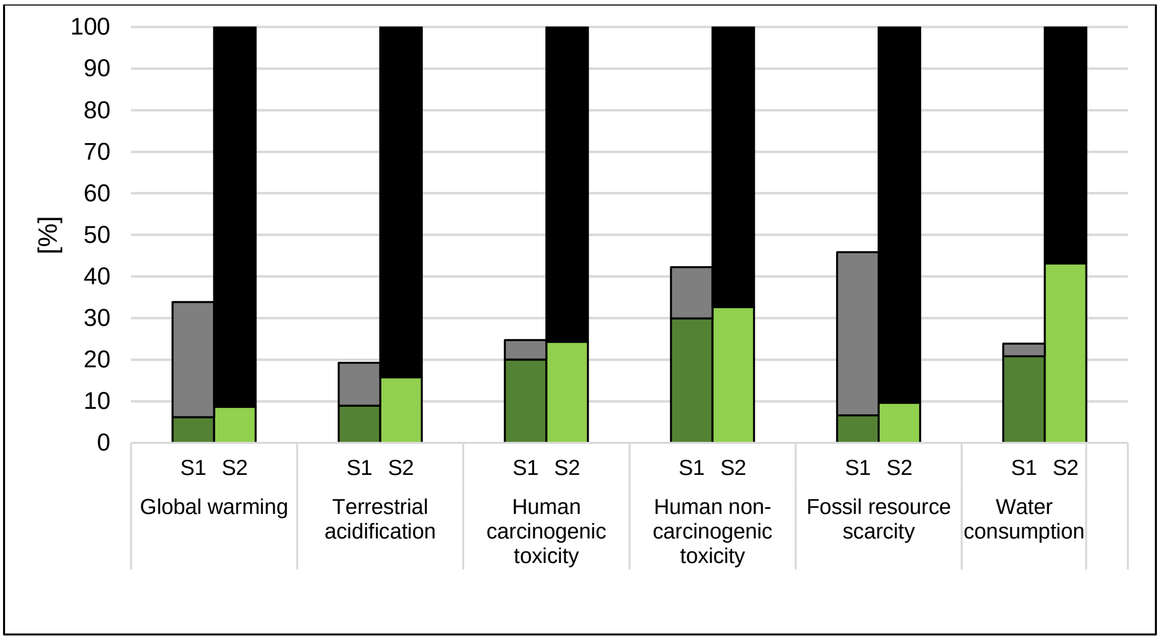


*Figure 5. 10: Environmental impact comparisons of expanded systems 1 and 2*

*Table 5. 5: Environmental impacts of expanded system 1 and 2 for a functional unit of 29.5 billion tkm*

| Impact category | Unit | Hydrogen utilisation in SA-expanded system 1 | Hydrogen utilisation in Germany-expanded system 2 |
|---|---|---|---|
| Global warming | kg $CO_2$ eq. | 1 180 000 000 | 3 500 000 000 |
| Terrestrial acidification | kg $SO_2$ eq. | 2 760 000 | 14 300 000 |
| Human carcinogenic toxicity | kg 1,4-DCB | 58 600 000 | 237 000 000 |
| Human non-carcinogenic toxicity | kg 1,4-DCB | 2 280 000 000 | 5 390 000 000 |
| Fossil resource scarcity | kg oil eq. | 381 000 000 | 832 000 000 |
| Water consumption | $m^3$ | 3 720 000 | 15 600 000 |

Figure 5.10 and Table 5.5 show the environmental impacts of the two expanded systems of hydrogen utilisation. As seen in Figure 5.10, The environmental impacts of the expanded system of exporting hydrogen to be used in Germany far outweigh the environmental impacts of the expanded system of using hydrogen locally across all impact categories. The global warming impact of the expanded system of using hydrogen in South Africa was 1.18 billion kg $CO_2$ eq., which was 33% of the global warming impact of the expanded system of exporting hydrogen to Germany. The terrestrial acidification of using hydrogen locally was 2. 76 million kg $SO_2$ eq. making up 19% of the acidification caused by using hydrogen in Germany.

For human carcinogenic and non-carcinogenic toxicity, the impact of using hydrogen locally was 25% and 42% of the impact of exporting hydrogen to Germany. For fossil resource scarcity, the impacts of using hydrogen made up 46% of the impacts for the case of exporting the hydrogen. Lastly, the expanded system of using hydrogen locally made up 24% of the water consumption of the expanded system of exporting the hydrogen. Terrestrial acidification had the largest difference in impacts for the two expanded systems, followed by water consumption and human carcinogenic toxicity.

The environmental impacts across all categories were dominated by the black bar, which represents diesel used to fuel heavy-duty trucks in South Africa. Diesel produced in South Africa is the “dirtier” fuel compared to diesel produced in Germany because it is coal-based. Therefore, the coal heightens the impacts across all the impact categories. For the human toxicity impacts and the water consumption of expanded system 2, the hydrogen utilisation portion, represented by the light green bar, significantly contributed to the total impacts. Exporting hydrogen to Germany resulted in added environmental impacts due to the hydrogen conversion, shipping, and reconversion before fuelling heavy-duty trucks.

When analysing expanded system 1, German diesel was a dominant contributor only to global warming and fossil resource scarcity. For the rest of the impact categories, the impacts are dominated by the portion of using hydrogen fuel. Hydrogen fuel is more impactful for human carcinogenic and non-carcinogenic toxicity than diesel produced in Germany. Hydrogen is also more water consumptive than using diesel in Germany. Diesel produced in Germany is of a higher quality standard compared to diesel to diesel produced in South Africa, and it is also based on a less environmentally impactful feedstock.

The main observation from the comparative analysis of these two expanded systems is that using hydrogen to decarbonise heavy-duty trucks locally is less environmentally impactful and more beneficial as the hydrogen would be decarbonising the most environmentally harmful fuel.

## 5.3. Interpretation

The interpretation phase is the last phase of the lifecycle assessment. It aims to evaluate the uncertainty associated with the lifecycle inventory analysis and lifecycle impact results. The result of the interpretation phase is supposed to be substantial conclusions and recommendations related to the goal and scope of the lifecycle assessment. However, Chapter 6 will cover this aspect. This interpretation section is broken down into three parts: data completeness check, significant issues contributing to uncertainty and lastly, a quantitative uncertainty analysis of major findings from the impact assessment.

### *5.3.1. Significant Issues contributing to uncertainty*

Fuel input is the most significant factor contributing to the environmental impacts of the two hydrogen utilisation systems compared. These fuel inputs were hydrogen and diesel. The hydrogen process used to model hydrogen utilisation in heavy-duty trucks was taken from the hydrogen production lifecycle assessment. The hydrogen produced from PEM electrolysis powered by combined solar PV and wind was used as it was the best option. The diesel processes used were found on the ecoinvent database. The diesel process for Germany found on ecoinvent was diesel produced in crude oil refineries. Due to the market mix of South African diesel being unavailable, the diesel process used for the impact assessment was the coal-based diesel produced from the Fischer-Tropsch process.

Fuel consumption is another significant issue because different consumption values would significantly change the inventory analysis and impact assessment results. The diesel consumption value for heavy-duty trucks (0.0192 kg/tkm) was found on the ecoinvent database for diesel truck transport processes. The hydrogen consumption for hydrogen fuel cell electric trucks was sourced from literature as stated in the lifecycle inventory analysis.

*5.3.2. Data completeness check*

The purpose of this check was to evaluate the completeness of the data used for all the processes and inputs which were identified as significant issues (Hauschild, Rosenbaum and Olsen, 2018). For both the fuel inputs and the fuel consumption, the available data used for modelling was enough to meet the goal and scope of the lifecycle assessment. The missing data for the inventory analysis were the South African transport processes for internal combustion engine heavy-duty trucks with updated EURO standards. The European processes were used and adapted to the South African context as much as possible. Given that the euro standards for the internal combustion engine trucks caused minimal impacts relative to the fuel input, these missing data do not significantly affect the results of this lifecycle assessment.

*5.3.3. Monte Carlo uncertainty analysis*

The Monte Carlo analysis was conducted on SimaPro to assess the uncertainty associated with the results. A comparative uncertainty analysis was conducted for the environmental impact comparison of local hydrogen utilisation and hydrogen exportation, shown in Figure 5.11.

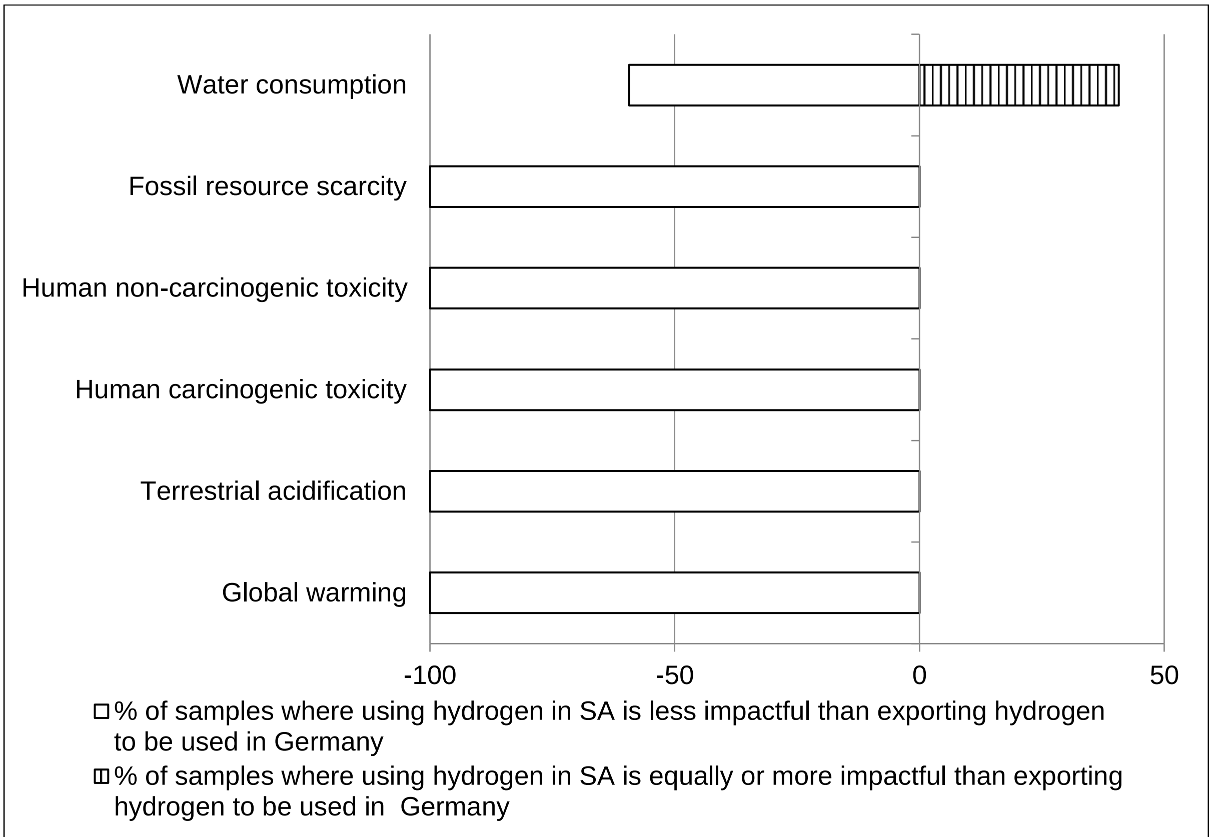


*Figure 5. 11: Comparative uncertainty analysis of the expanded systems of using hydrogen locally and exporting hydrogen (method: ReCiPe 2016, confidence interval: 95%)*

Figure 5:11 shows the uncertainty analysis comparing the two expanded hydrogen utilisation systems. According to the analysis conducted, there is a 100% certainty that using hydrogen locally is less impactful than exporting hydrogen to be used in Germany across five of the impact categories, excluding water consumption. There is a 59% certainty that the expanded system of exporting hydrogen is more environmentally impactful. This uncertainty analysis validates that the expanded system of using hydrogen locally is less environmentally impactful and results in a greater extent of decarbonisation in heavy-duty truck transportation. The uncertainty distributions for this comparison can be seen in appendix 8.4.

## 5.4. Summary of hydrogen utilisation lifecycle assessment

A comparative hydrogen utilisation lifecycle assessment was conducted. The assessment focused on two cases; local hydrogen utilisation to fuel heavy-duty trucks and exporting the hydrogen to Germany also to fuel heavy duty trucks. The main objective was to determine the highest amount of decarbonisation that could be achieved using the limited green hydrogen resource that would be produced in South Africa. The ReCiPe 2016 method was used to conduct the impact assessment, and six impact categories were considered.

Firstly, Individual environmental impact comparisons were conducted for hydrogen-fuelled trucks and conventional diesel-fuelled trucks locally and in Germany. The environmental impact reductions for these comparisons were discussed. Secondly, a system expansion of the two cases was carried out to make the systems comparable with equal functional units. It was found that the environmental impacts of exporting hydrogen far outweigh the impacts of using hydrogen locally. Using the hydrogen locally to decarbonise heavy-duty truck transportation results in the highest environmental benefit because hydrogen would be replacing the “dirtier” fuel, South African diesel produced from coal. The Monte Carlo analysis confirmed this result with a 100% certainty for five of the six impact categories assessed.

# 6. CONCLUSION AND RECOMMENDATIONS

This is the concluding chapter of the dissertation. The objectives stated in Chapter 1, which were to conduct a thorough literature review, a hydrogen production lifecycle assessment, and a hydrogen utilisation lifecycle assessment, were carried out in Chapters 2, 4 and 5. Conclusions are drawn from the two lifecycle assessments conducted. The hypotheses stated in Chapter 3 are validated, and the key questions accompanying each hypothesis are answered in this chapter. Lastly, comprehensive recommendations are made for industrial practices and for further research from the conclusions drawn.

## 6.1. Conclusion for the hydrogen production LCA

A hydrogen production lifecycle assessment was conducted for a cradle to gate system. The Recipe 2016 midpoint method was used to conduct the lifecycle impact assessment. Upon analysing the potential environmental impacts of hydrogen production, the most significant contributor to the environmental impacts is the energy required to power the production processes. For green hydrogen production, the energy required is the electricity input for water electrolysis. For grey hydrogen production, the energy requirement is fulfilled mainly by natural gas. The energy requirement for green hydrogen production causes 85 to 95% of the environmental impacts, and for grey hydrogen production, natural gas causes 90 to 99.9% of the environmental impacts.

The potential environmental impacts of renewable and non-renewable hydrogen production were quantified. When comparing the environmental impacts, the impacts of non-renewable hydrogen production far outweigh the impacts of renewable hydrogen production across most impact categories. Specifically for global warming, the potential environmental impact of producing 1 kg of hydrogen from renewable energy powered PEM electrolysis is 3.68 kg $CO_2$ eq. In comparison, the potential global warming impact of steam methane reforming and grid electricity powered electrolysis are 15.2 and 17.1 kg $CO_2$ eq. respectively. Grid electricity-powered electrolysis has the largest potential environmental impacts for all the impact categories except for human non-carcinogenic toxicity, where solar PV powered electrolysis has a slightly higher potential human carcinogenic toxicity impact; 27.2 kg eq. (compared to 25.9 kg eq.) of 1.4 DCB. This high non-carcinogenic toxicity impact is caused by the supply chains of solar PV panels.

The normalised impact results for comparing the production scenarios displayed that human carcinogenic toxicity is an environmental hotspot. It had the highest normalised impact scores among all the impact categories. A sensitivity analysis was conducted for the normalised results using two normalisation sets from the ILCD 2011 midpoint + impact assessment method. In magnitude, the normalised scores were different from the ReCiPe 2016 normalised scores; however, the analysis confirmed the result of human carcinogenic toxicity being an environmental hotspot for hydrogen production.

Among the renewable hydrogen production options, wind-powered electrolysis has the least potential environmental impacts for all the impact categories except human carcinogenic toxicity. Here, wind-powered electrolysis has the highest potential human carcinogenic toxicity impact, at 0.546 kg eq. of 1.4 DCB, though this is less than half the value of non-renewable hydrogen production (1.35 kg eq. of 1.4 DCB). This toxicity is caused by the supply chains of wind turbines. Therefore, wind-powered electrolysis might be the least impactful production route, but it could pose a risk of cancer to humans because of the carcinogens. Due to the low capacity factors of individual renewable energy sources, the combination of solar PV and wind energy was explored. Powering electrolysis with combined solar and wind power is the best option due to the increased capacity factor that can be achieved and, therefore, the increased use of electrolysers throughout the year.

The potential environmental impacts of PEM, alkaline, and solid oxide electrolysis were compared. PEM electrolysis is the worst environmentally performing technology across all impact categories. PEM electrolysis has the lowest system efficiency in comparison to alkaline and solid oxide electrolysis, leading to a higher electricity requirement. PEM electrolysis also entails the use of platinum as a construction material for electrolysers, which is an environmentally impactful material. However, the potential impacts related to the electricity input far outweigh the impact of the materials used to manufacture electrolysers. Solid oxide electrolysis is the best performing technology across all impact categories; however, it is reportedly underdeveloped compared to PEM and alkaline electrolysis (Zhao et al., 2020). The PEM and alkaline electrolysis technologies are thus more preferred due to their maturity and advantages, which have been discussed in the literature review.

An uncertainty analysis was done to compare the environmental impacts of combined solar PV and wind-powered water electrolysis and steam methane reforming or green hydrogen and grey hydrogen production. The Monte Carlo uncertainty analysis tool on SimaPro was used. There is a 100% certainty that green hydrogen production is potentially less impactful than grey hydrogen production for the fossil resource scarcity, terrestrial acidification, and global warming impacts. Green hydrogen production was less impactful for the human toxicity impacts with a 23 to 30% range of uncertainty. Green hydrogen production is more water consumptive with a 55% certainty, meaning that there us almost a 50/50 chance that either green or grey hydrogen production has a higher water footprint.

## 6.2. Conclusion for the hydrogen utilisation LCA

A lifecycle assessment was conducted for two cases of hydrogen utilisation. The hydrogen used to model hydrogen utilisation was assumed to be produced from combined solar PV and wind-powered PEM electrolysis. The two cases of hydrogen utilisation considered were local use and exportation to be used in Germany, both to fuel heavy-duty truck transportation. Hydrogen utilisation was first individually compared with using conventional fuel for both cases. For local utilisation, the potential environmental impacts of using hydrogen to fuel heavy-duty trucks are lower than using diesel fuel across all impact categories. For the exportation case, using hydrogen is less impactful for global warming and fossil resource scarcity; however, it is more impactful for water consumption, human toxicity, and terrestrial acidification. The added impacts of exporting hydrogen to Germany explain the higher impacts of hydrogen fuel for the export case.

To compare these two cases, the systems were expanded. The system expansion is explained in detail in Chapter 5, Section 5.2.3. The functional unit for the expanded system was 29.5 billion tkm, made up of 16 billion t.km in South Africa and 13.5 billion t.km in Germany. The potential environmental impacts of the expanded system of exporting hydrogen outweigh the environmental impacts of using hydrogen locally to fuel heavy-duty trucks. For the global warming potential, the impact of the local hydrogen utilisation system amounts to 1.18 billion kg $CO_2$ eq., which is 33% of the impact of the hydrogen export case, 3.5 billion kg $CO_2$ eq. The impacts of local hydrogen utilisation are also lower for the rest of the impact categories. Local hydrogen utilisation thus leads to the best environmental benefit. This is because using hydrogen locally would mean replacing the most environmentally impactful fuel, South African coal-based diesel, to fuel heavy-duty trucks. Diesel produced in Germany is made from more sophisticated processes and a less impactful feedstock compared to diesel produced in South Africa. The results of the system expansion confirm that when allocating a low impact limited resource, it is best to use it to replace the most harmful fuel.

The fuel consumption for diesel-fuelled trucks and hydrogen-fuelled trucks was compared. Diesel fuel consumption is 1.6 times higher than hydrogen fuel consumption. This poor fuel efficiency for diesel-fuelled vehicles significantly contributes to the high potential environmental impacts of diesel-fuelled trucks.

A comparative uncertainty analysis was conducted for the expanded systems using the Monte Carlo uncertainty analysis tool on SimaPro. There is a 100% certainty that local hydrogen utilisation to decarbonise heavy-duty trucks is beneficial in all the impact categories except for water consumption. For water consumption, there is a 50/50 chance that either local hydrogen utilisation or hydrogen exportation is the most water consumptive.

## 6.3. Validation of Hypotheses

Two hypotheses were formulated in Chapter 3 for hydrogen production and hydrogen utilisation

The first hypothesis is as follows:

- The environmental impacts of the energy required to produce hydrogen far outweigh the environmental impacts associated with the infrastructure and equipment used to produce the hydrogen for all production routes.

The energy source currently used in South Africa to produce hydrogen is natural gas; however, solar PV and wind power are most likely to be used for prospective green hydrogen production. South African Solar PV and wind electricity processes were available on the ecoinvent database for LCA modelling. They were representative of current technologies for solar PV and wind electricity production; however, they were still sufficient to be used to model 2040 hydrogen production scenarios. The electrolyser technology likely used for hydrogen production is PEM electrolysis due to the current developments of hydrogen technologies in South Africa, as stated in chapter 1. The results have proven that energy input is the highest contributor to the environmental impacts of hydrogen production, causing 85-95% of the impacts of green hydrogen; this hypothesis is thus confirmed. The energy requirement should thus be a primary factor when deciding on which hydrogen production route to use.

The second hypothesis is as follows:

- The most environmentally beneficial way to utilise the hydrogen produced in South Africa, which would initially be a scarce resource, would be to use it to decarbonise the most environmentally harmful fuel in heavy-duty truck transportation.

Multiple utilisation options are considered for renewable hydrogen ranging from mobility mining to industrial processes. However, the scope of the second LCA was narrowed to only focus on hydrogen used to fuel heavy-duty trucks- this can be considered as a case study. The conventional fuels used to fuel trucks in South Africa are diesel and petrol. These are the fuels that can potentially be replaced by hydrogen. The master's thesis by Melamu (2008) was used as a guide to expand the two cases of hydrogen utilisation considered for the second LCA. The system expansion is detailed in chapter 5. The second hypothesis is confirmed as the results prove that local hydrogen utilisation is less impactful and more beneficial in all impact categories studied, with the exception of water consumption, where significant uncertainty could not be resolved. The best environmental benefit is achieved by replacing South African coal-based diesel, the "dirtiest fuel".

## 6.4. Recommendations for further research

The conclusions above from the lifecycle assessments cannot be stated with equally high levels of confidence for all the impact categories studied due to a limitation caused by the uncertainties associated with the results. The uncertainty analysis in the hydrogen production lifecycle showed a high range of uncertainty associated with water consumption. The range is high for both renewable energy powered electrolysis and steam methane reforming. This high water consumption uncertainty was also observed for hydrogen utilisation. Therefore, it is recommended that further research be conducted to investigate the water footprints associated with these hydrogen production processes, particularly the water footprint of renewable electricity production in the case of electrolysis powered by solar PV, and natural gas production in the case of steam methane reforming.

Hydrogen utilisation for the second lifecycle assessment was narrowed to heavy-duty truck transportation. As discussed in Chapter 1, renewable hydrogen can be used to decarbonise multiple other sectors such as aviation, mining, steel, and the chemicals industry. It is recommended that an investigation be conducted to determine the emissions reduction that can be achieved using hydrogen in these sectors. Local hydrogen utilisation has been proven to potentially lead to the highest environmental benefit compared to hydrogen exportation; however, it is possible that within the local region, other sectors outside of road transport could benefit more from renewable hydrogen.

A cradle to gate system boundary was considered for the first lifecycle assessment. The second lifecycle assessment considered the utilisation phase for hydrogen, which was the operation of trucks. It is recommended that a hydrogen LCA focused on the end-of-life phase be carried out. There may be significant impacts in the end-of-life phase of renewable energy infrastructure which need to be identified and addressed.

It is recommended that a social lifecycle assessment and lifecycle costing be carried out for renewable hydrogen to consider the non-environmental impacts and benefits associated with renewable hydrogen. For the social assessment, impact categories such as job creation could be assessed, in particular to investigate the often-cited preference of PEM electrolysers in the South African context. For the costing, indicators such as hydrogen cost/kg and profitability indicators such as return on investment and payback period could be considered.

## 6.5. Recommendations for industrial practice

Green hydrogen was found to be indeed “greener” than grey hydrogen, and from an environmental perspective it is thus recommended that South African policy-makers and investors build on the continuously generating momentum for green hydrogen. That noted, there are some findings which have potential implications for technology choice, as detailed below.

Solid oxide electrolysis was shown to have the least potential environmental impacts compared to PEM and alkaline electrolysis: however, it is the least developed. It is recommended that the developers of hydrogen projects pay attention to the further development of solid oxide electrolysis. As stated in the conclusion, wind power has the highest potential human carcinogenic toxicity impact compared to other renewable energy sources. It is recommended that more attention be given to the supply chains of wind turbines. Wind turbine manufacturers should pay more attention to the construction materials used to manufacture the wind turbines and the toxicity impact these materials may cause. The manufacturers could explore less impactful alternatives to manufacture wind turbines.

Solar PV powered electrolysis was found to have the highest potential human non-carcinogenic toxicity impact. It is recommended that solar PV panel manufacturers improve the supply chains of solar PV panels and the technologies used to produce solar PV electricity. To power water electrolysis, it is recommended to use a combination of solar and wind electricity to maximise the capacity factor that can be achieved and consequently maximise the usage of electrolysers for hydrogen production throughout the year.

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# 8. APPENDICES

## 8.1. Network diagrams – ReCiPe 2016 characterisation results for global warming

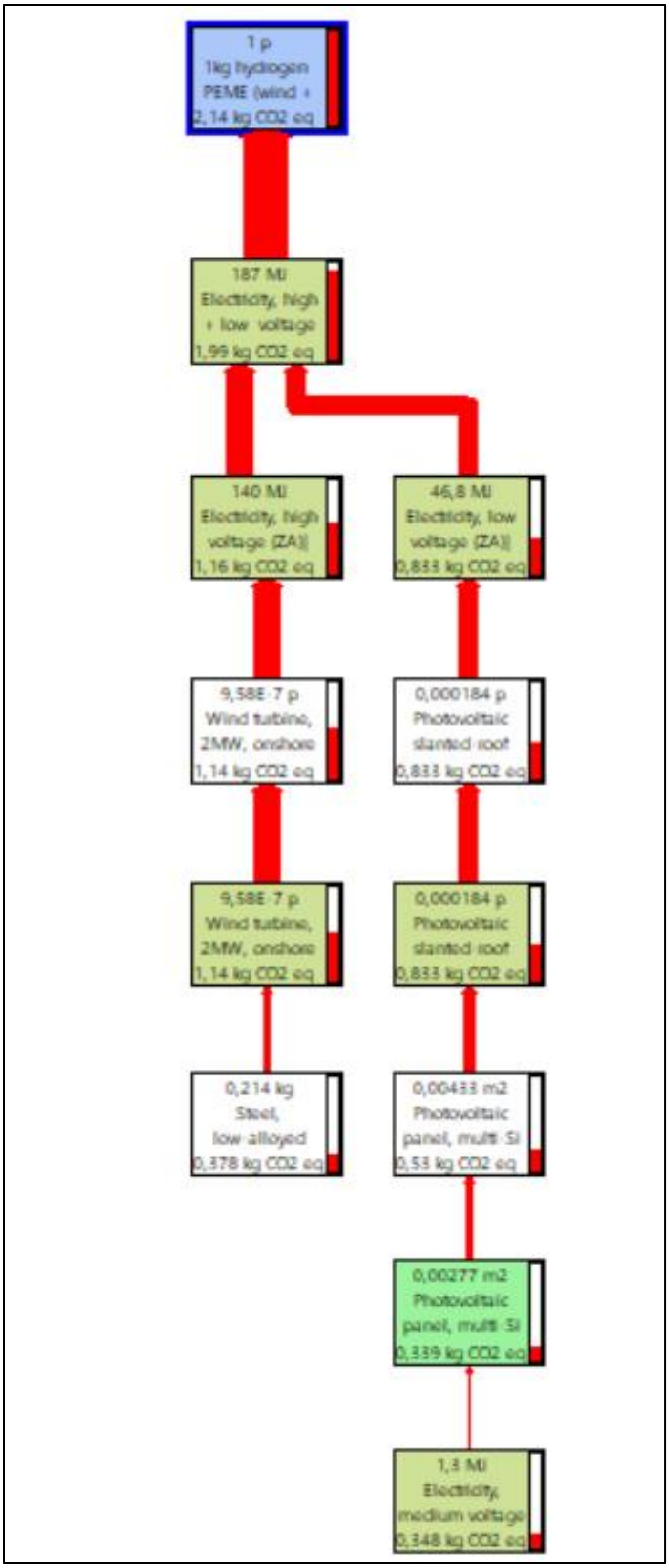


*Figure 8. 1: Assembly for 1 kg of hydrogen produced from wind and solar powered PEM electrolysis*

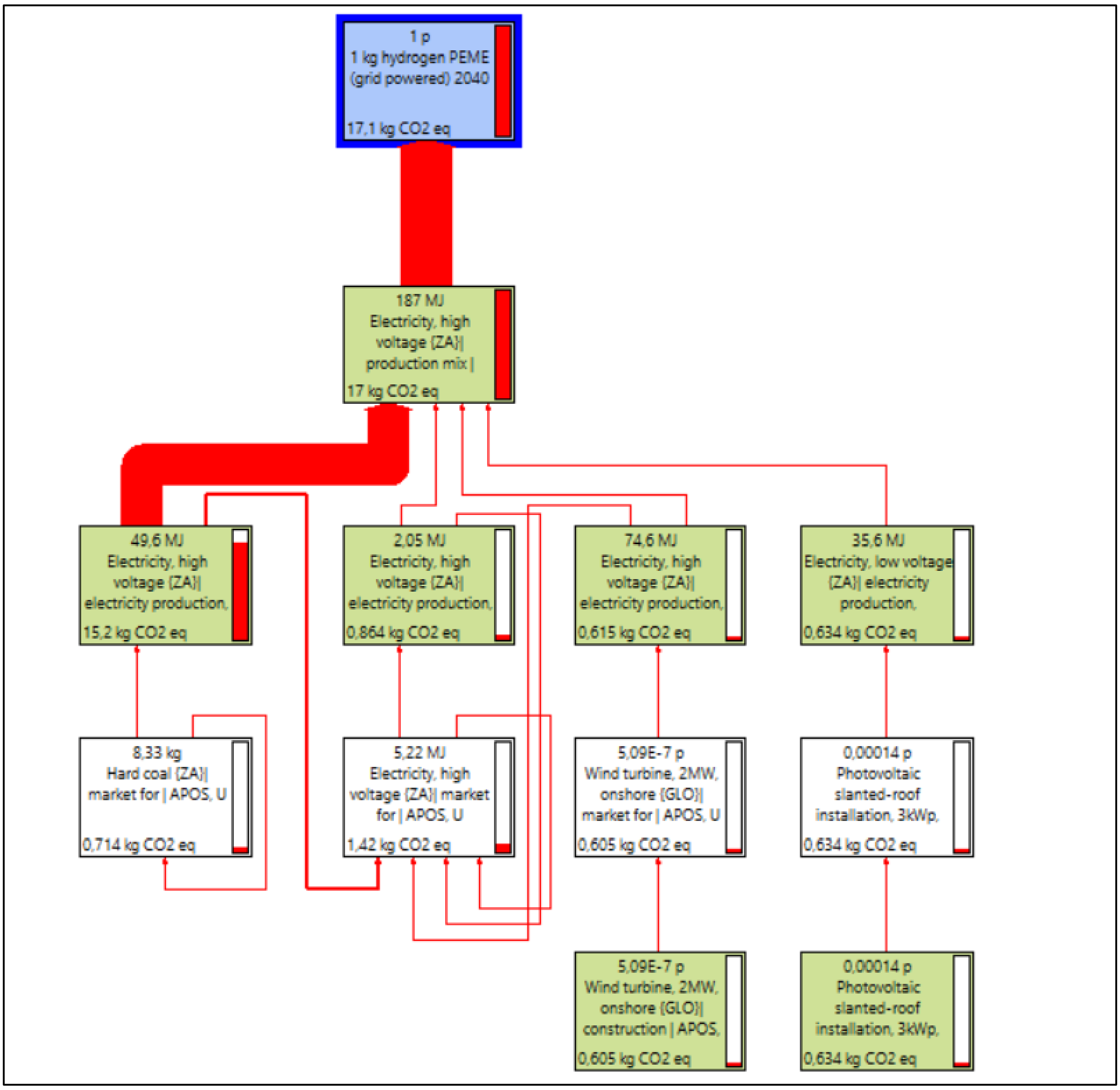


*Figure 8. 2: Assembly for 1 kg hydrogen produced from PEM electrolysis powered by a 2040 grid electrcity mix*

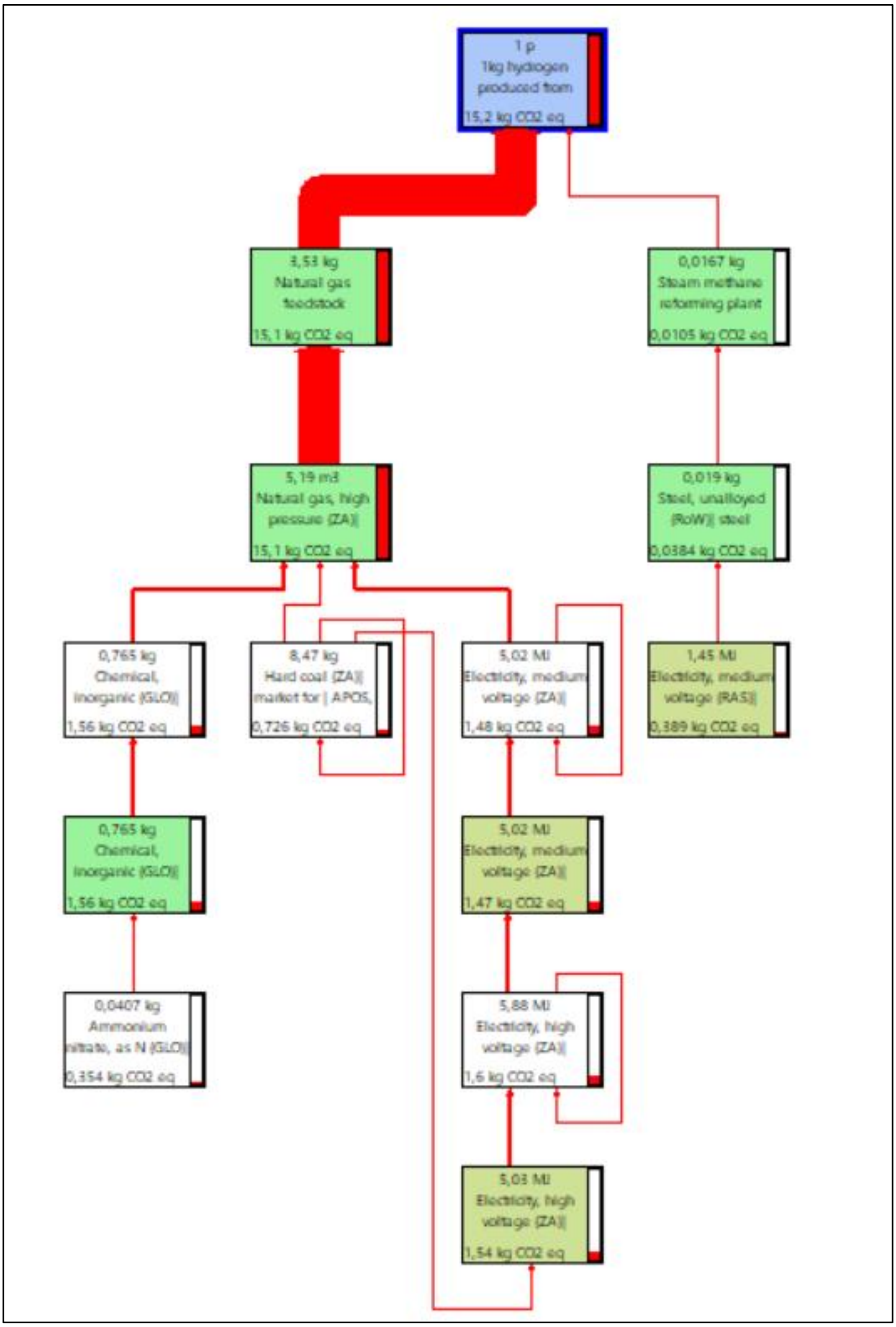


*Figure 8. 3: Assembly of hydrogen produced from steam methane reforming*

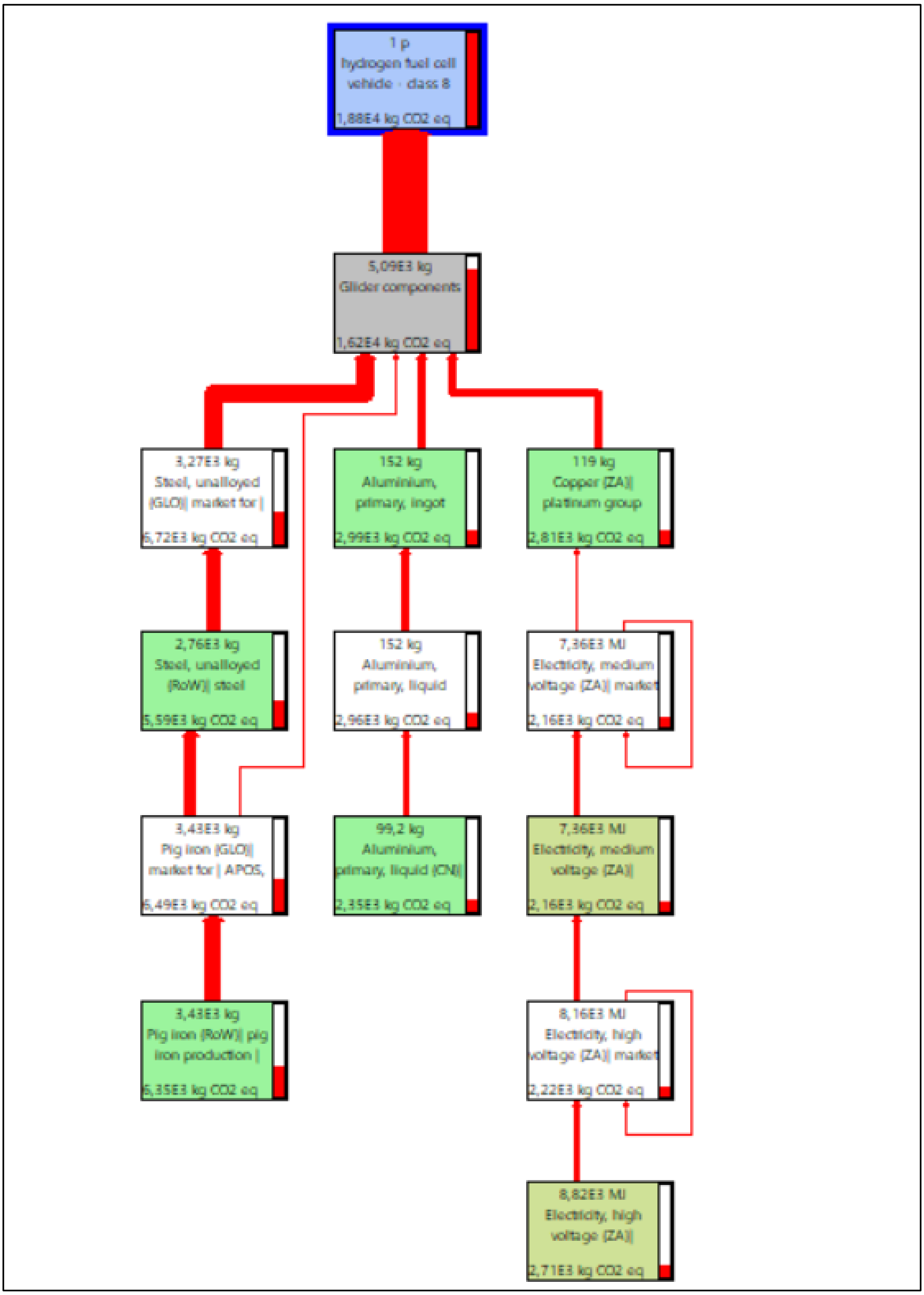


*Figure 8. 4: Assembly of a heavy-duty hydrogen fuel cell electric vehicle*

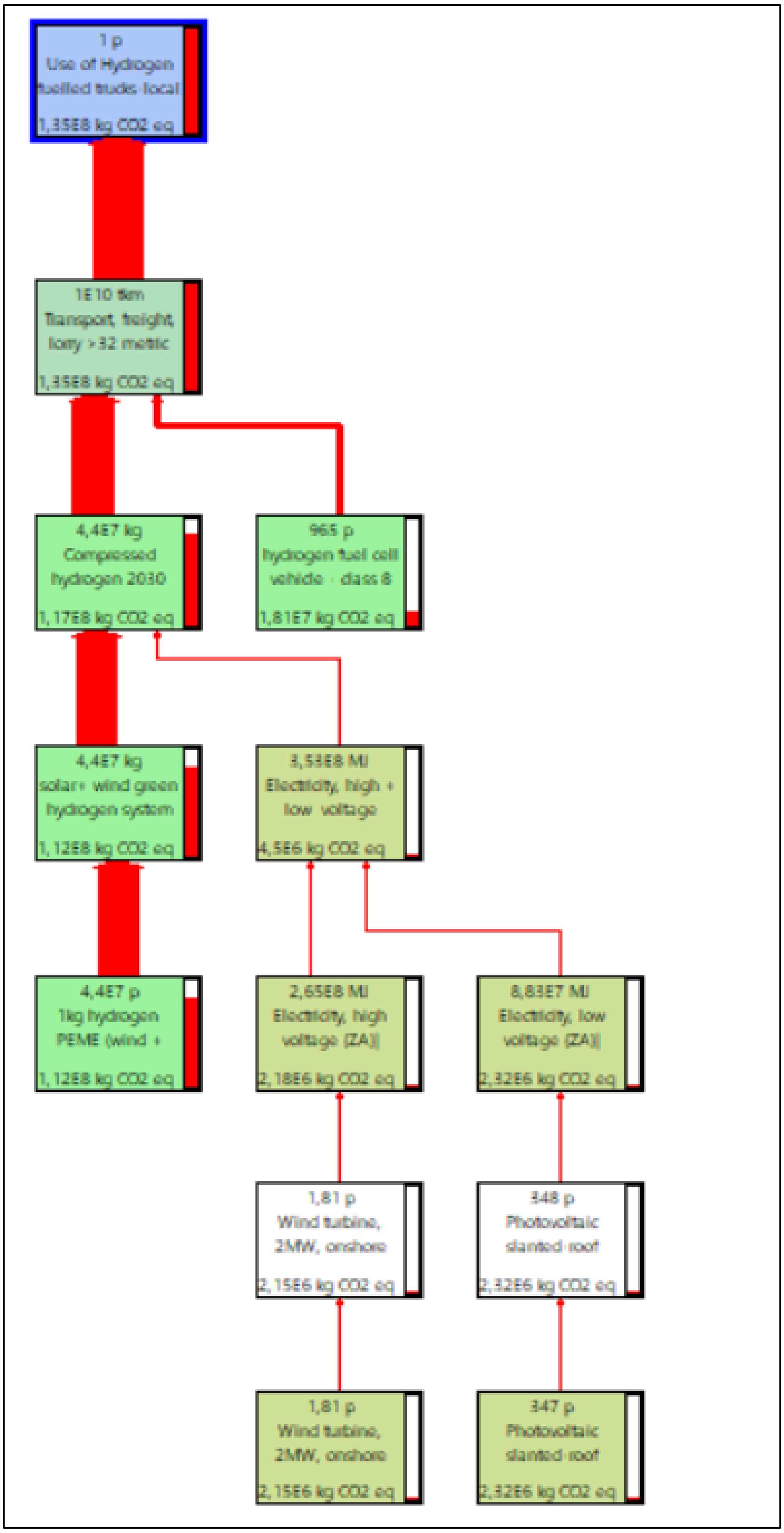


*Figure 8. 5: Network diagram for the local green hydrogen utilisation*

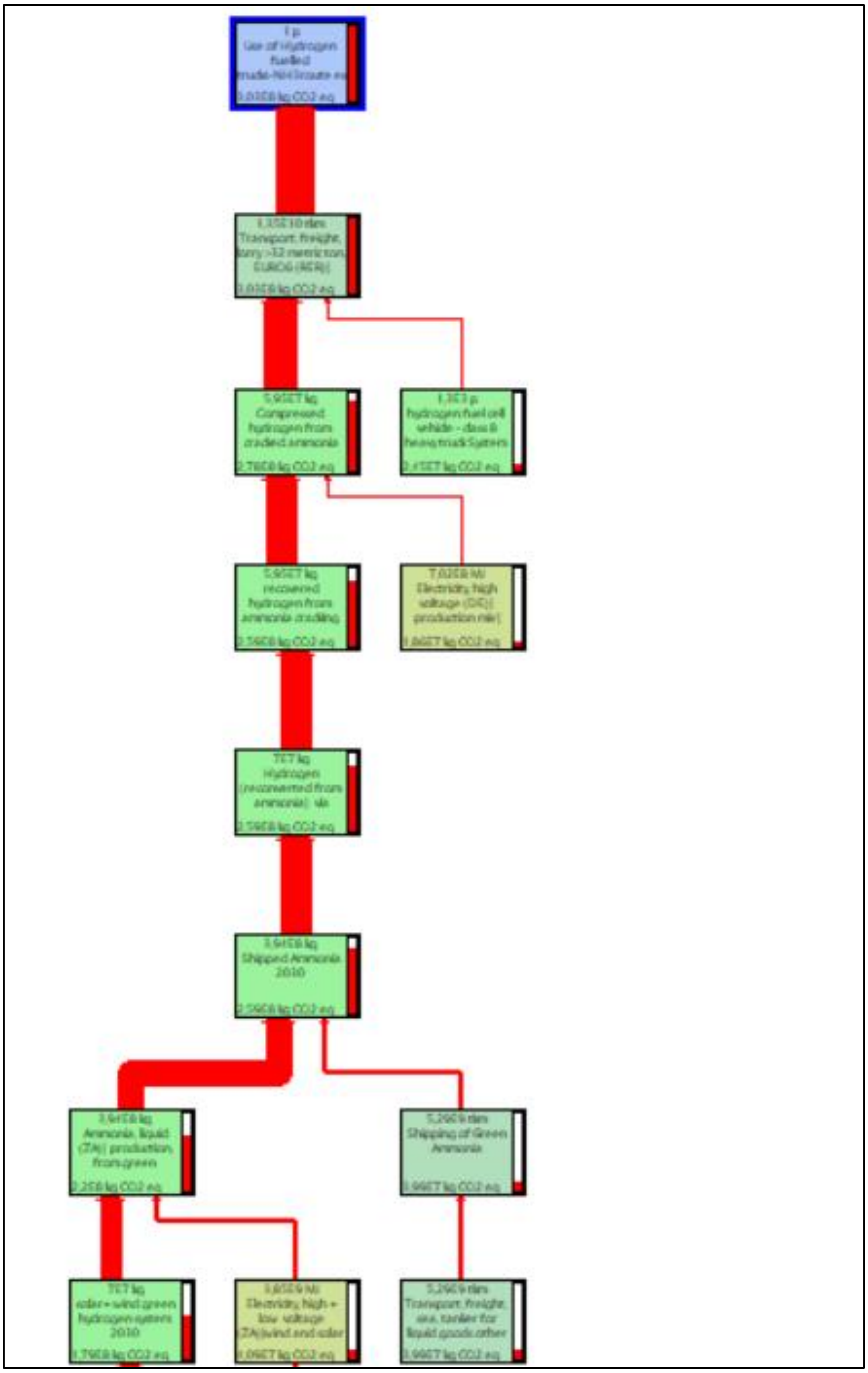

*Figure 8. 6: Network diagram for hydrogen exported as ammonia to Germany and used for heavy duty truck transportation*

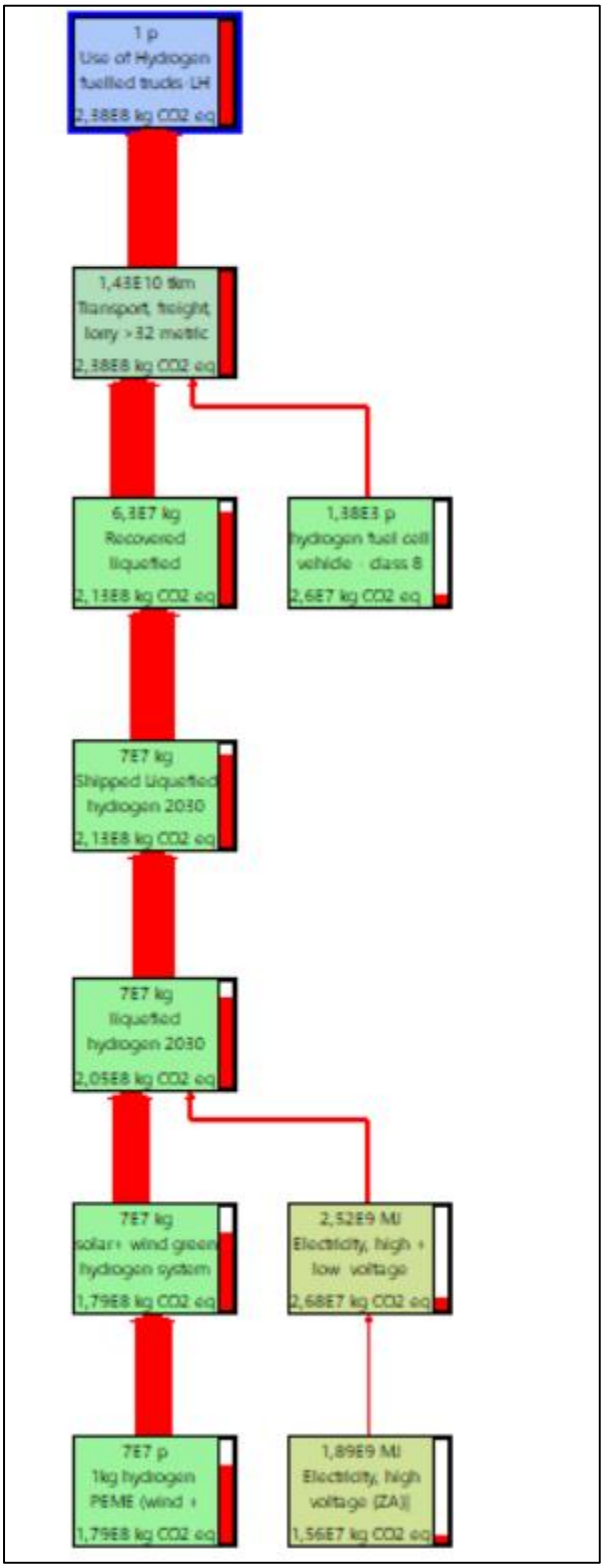


*Figure 8. 7: Hydrogen exported as liquefied hydrogen to Germany, and used for heavy duty truck transportation*

## 8.2. System Expansion Calculation

*Table 8. 1: System expansion of local green hydrogen utilisation case*

| | | | | |
|---|---|---|---|---|
| **hydrogen amount** | **70000** | **ton** | | |
| functional unit -amount of heavy-duty truck transport activity achieved with 70 kt of hydrogen | 16 | billion tkm | | |
| | 16000000000 | tkm | | |
| **Calculating tkm that would be achievable in Germany if the hydrogen was exported** | | | | |
| | Exported as ammonia | | Exported as liquefied hydrogen | |
| hydrogen loss | 15% | | 10% | |
| hydrogen amount after losses | 59500 | ton | 63000 | ton |
| hydrogen consumption | 0.0044 | kg/tkm | | |
| achievable tkm from the hydrogen | 13500000000 | tkm | 14300000000 | tkm |
| | 13.5 | billion tkm | 14.3 | billion tkm |
| **Diesel needed in heavy duty trucks in Germany to achieve the tkm** | | | | |
| | | | | |
| Diesel consumption in Euro 6 Germany trucks | 0.0192 | kg/tkm | 0.0192 | kg/tkm |
| | | | | |
| Amount of diesel required | 259000000 | kg | 275000000 | kg |
| | 259000 | ton | 275000 | ton |
| **Final functional unit** | **29.5** | **billion tkm** | **30.3** | **billion tkm** |

*Table 8. 2: System expansion of green hydrogen export case*

| | | | | |
|---|---|---|---|---|
| **Hydrogen amount exported to Germany** | **70000** | **ton** | | |
| | Exported as ammonia | | Exported as liquefied hydrogen | |
| | | | | |
| hydrogen loss during conversion and transportation | 10500 | ton | 7000 | ton |
| amount of hydrogen on arrival | 59500 | ton | 63000 | ton |
| | | | | |
| hydrogen consumption | 0.0044 | kg/tkm | 0.0044 | kg/tkm |
| tkm achieved in Germany | 13500000000 | tkm | 14300000000 | tkm |
| | **13.5** | **billion tkm** | **14.3** | **billion tkm** |
| **Calculating tkm that would be achievable in SA if the hydrogen was not exported** | | | | |
| hydrogen amount | 70000 | ton | | |
| tkm achievable in SA | 16000000000 | tkm | 16000000000 | tkm |
| | 16 | | 16 | |
| diesel consumption for heavy duty trucks | 0.0192 | kg/tkm | 0.0192 | kg/tkm |
| SA diesel required | 307200000 | kg | 307200000 | kg |
| | 307200 | t | 307200 | t |
| **Final functional unit** | **29.5** | | **30.5** | **billion tkm** |

## 8.3. Uncertainty distributions for comparison of wind and solar PV powered electrolysis (A) and steam methane reforming (B)

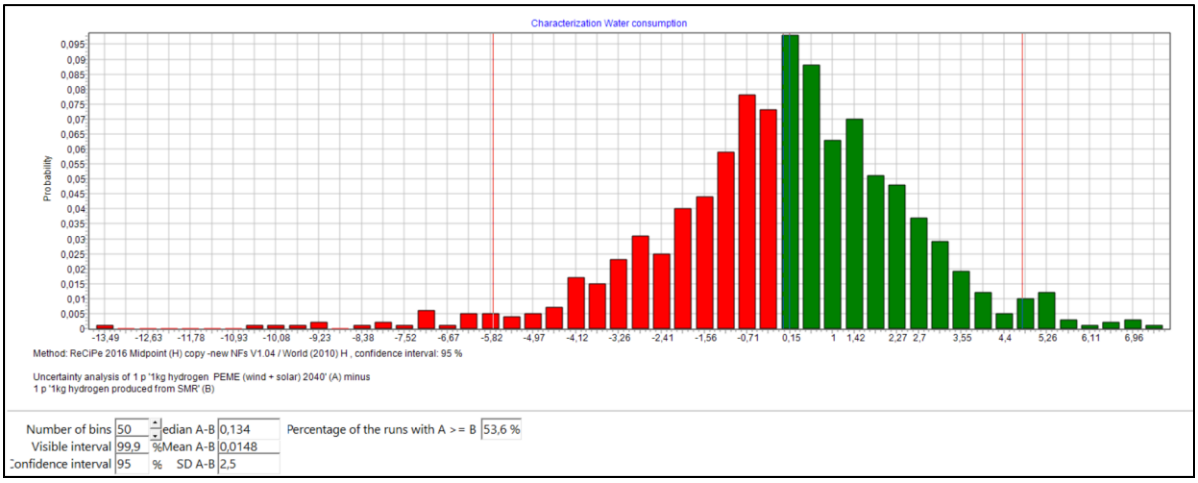


*Figure 8. 8: Uncertainty distribution for water consumption*

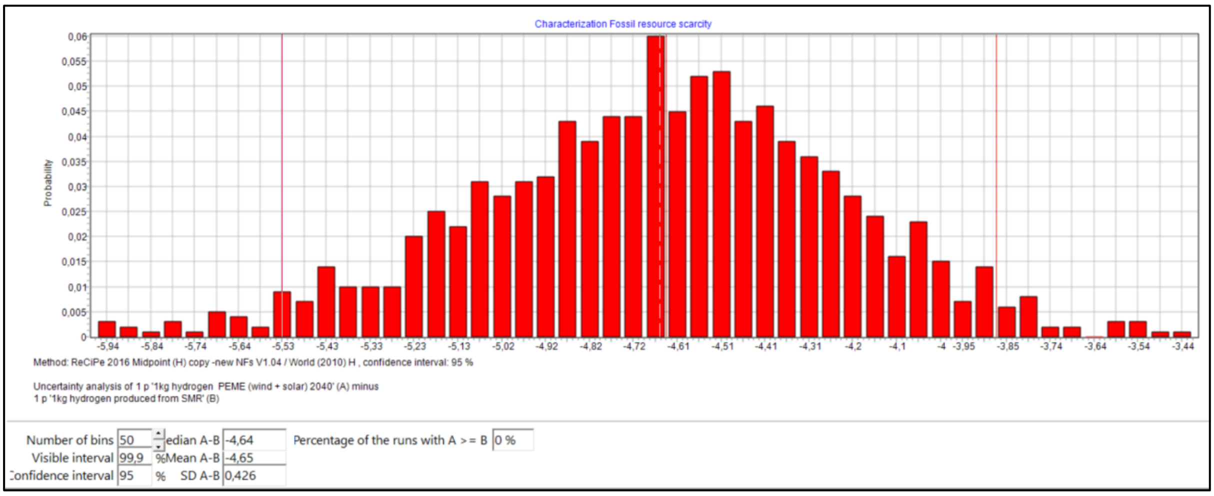


*Figure 8. 9: Uncertainty distribution for fossil resource scarcity*

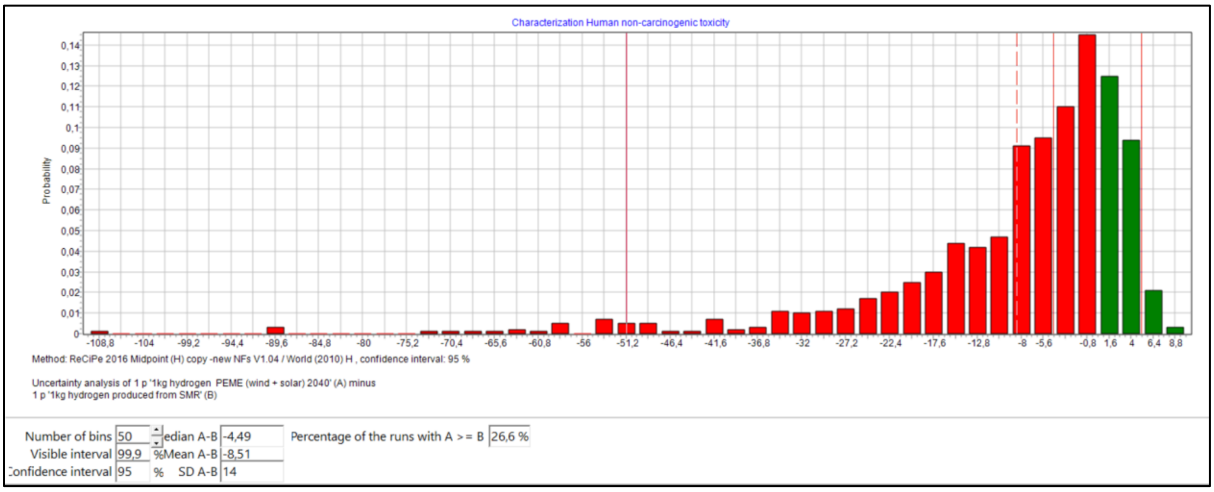


*Figure 8. 10: Uncertianty distribution for human non-carcinogenic toxicity*

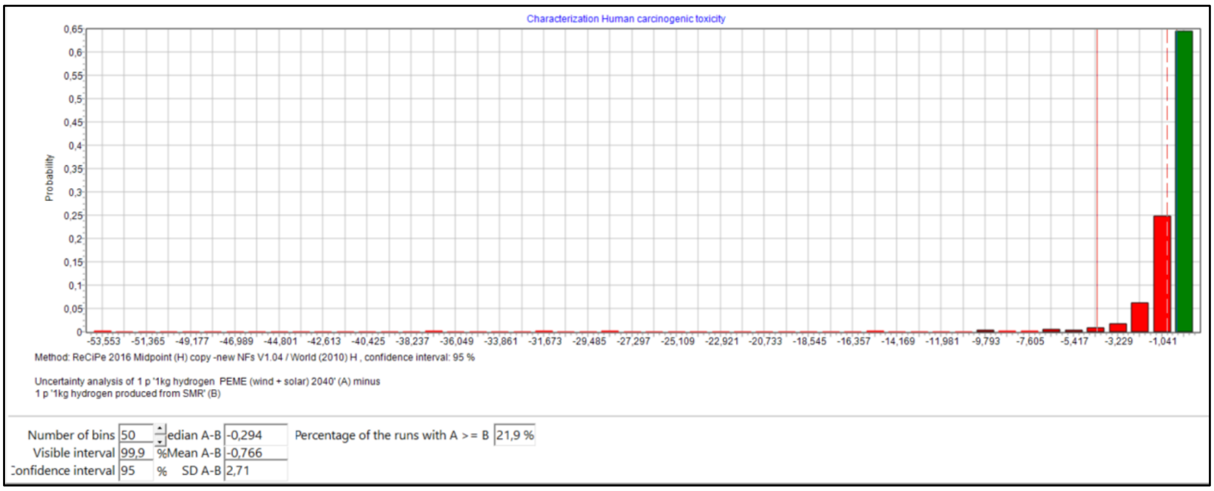


*Figure 8. 11: Uncertainty distribution for human carcinogenic toxicity*

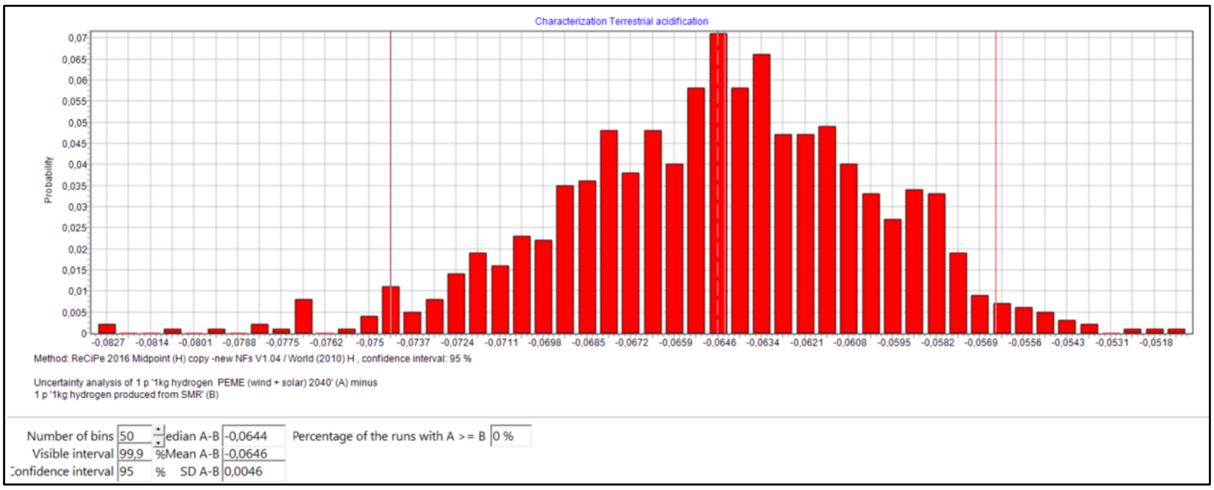


*Figure 8. 12: Uncertainty distribution for terrestrial acidification*

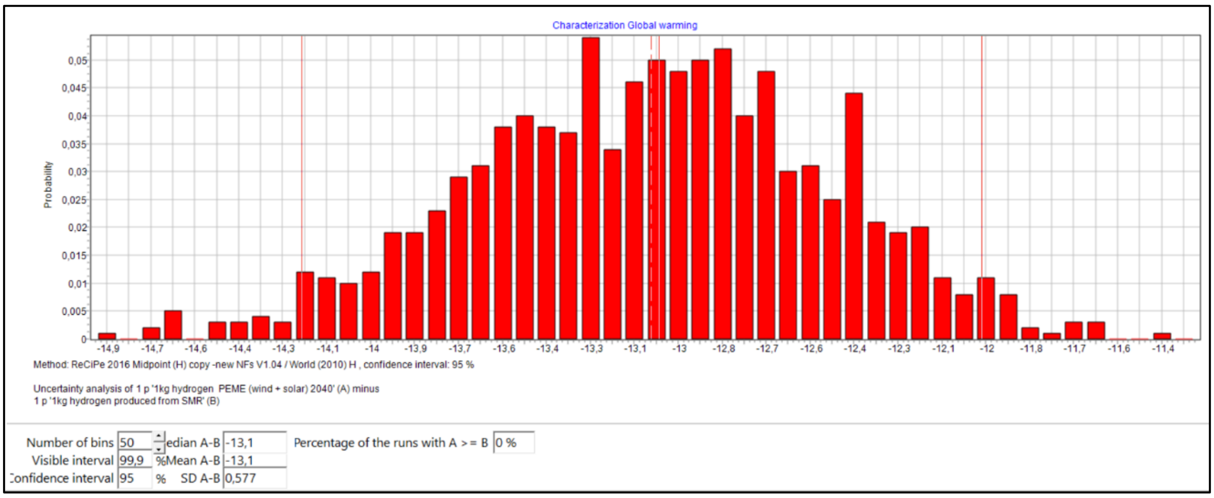


*Figure 8. 13: Uncertainty distribution for global warming*

## 8.4. Uncertainty distributions for comparison of local hydrogen utilisation (A) and hydrogen exportation for usage in Germany (B)

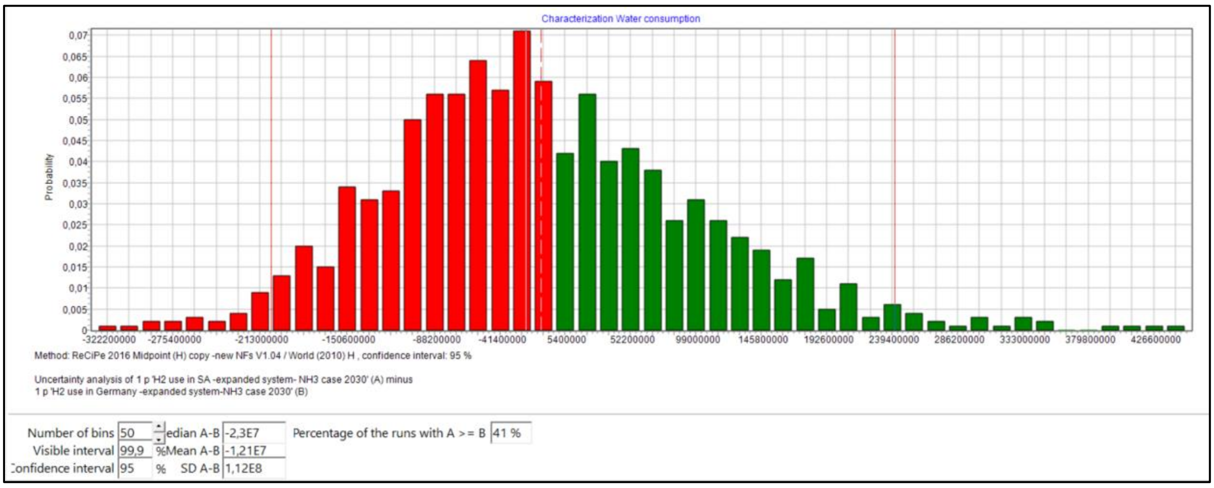


*Figure 8. 14: Uncertainty distribution for water consumption*

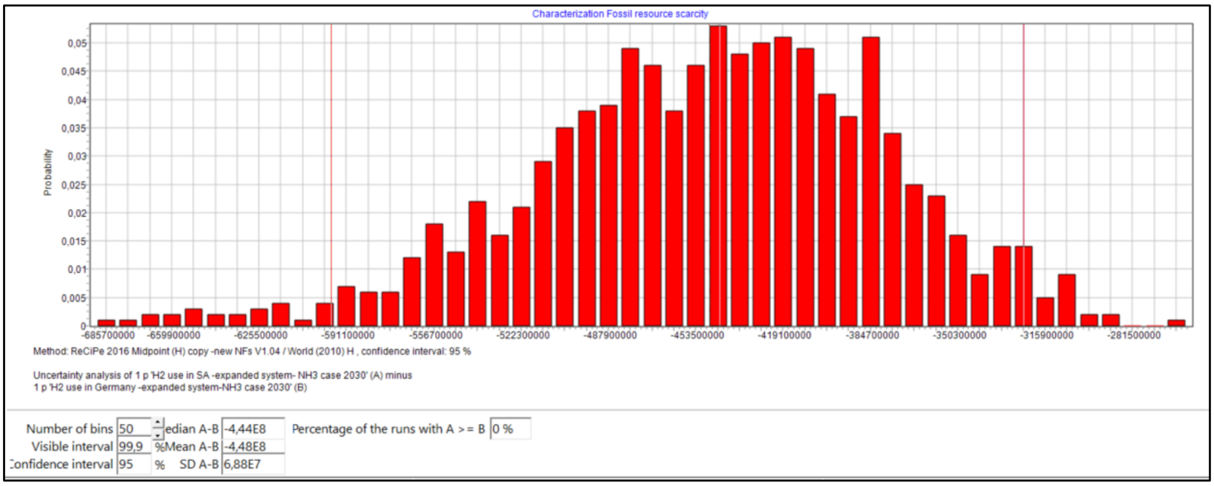


*Figure 8. 15: Uncertainty distributions for fossil resource scarcity*

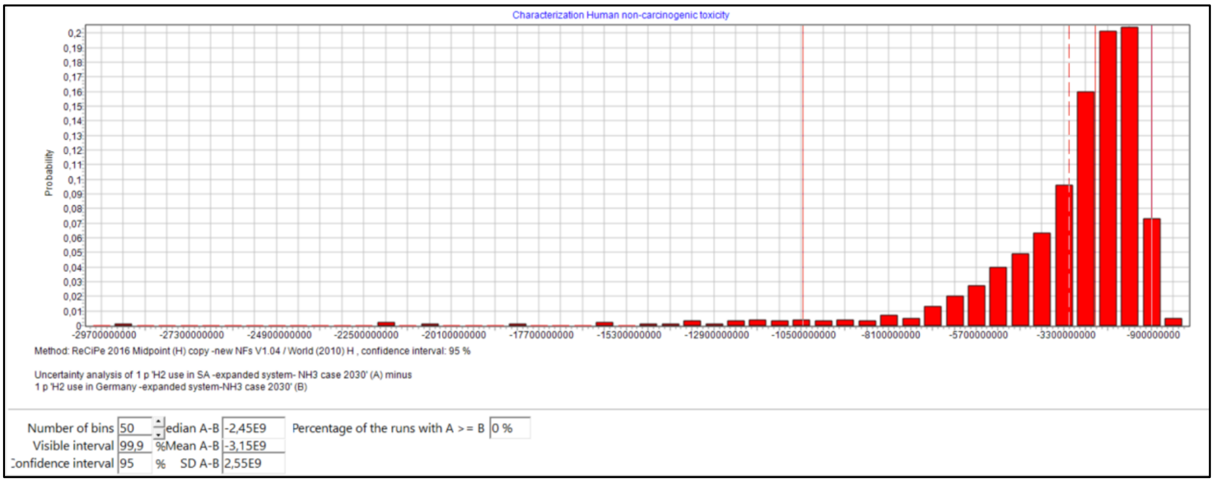


*Figure 8. 16: Uncertianty distribution of human non-carcinogenic toxicity*

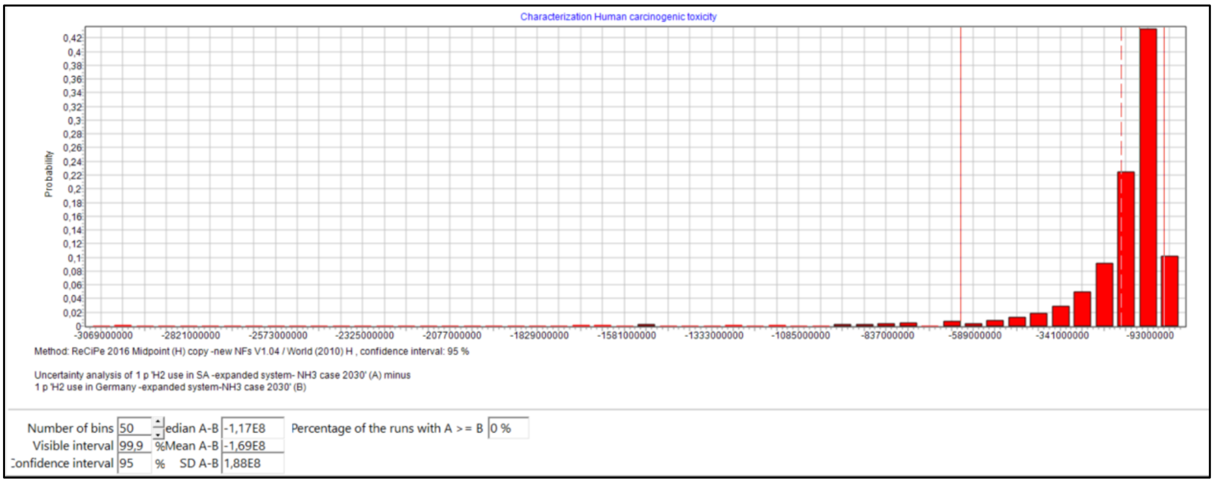


*Figure 8. 17: Uncertainty distribution of human carcinogenic toxicity*

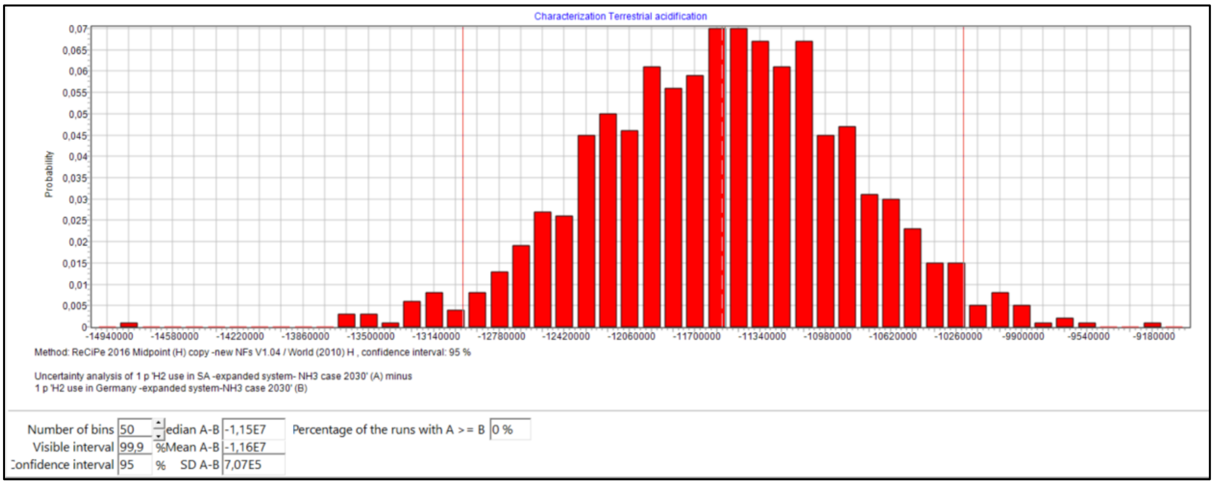


*Figure 8. 18: Uncertainty distribution of terrestrial acidification*

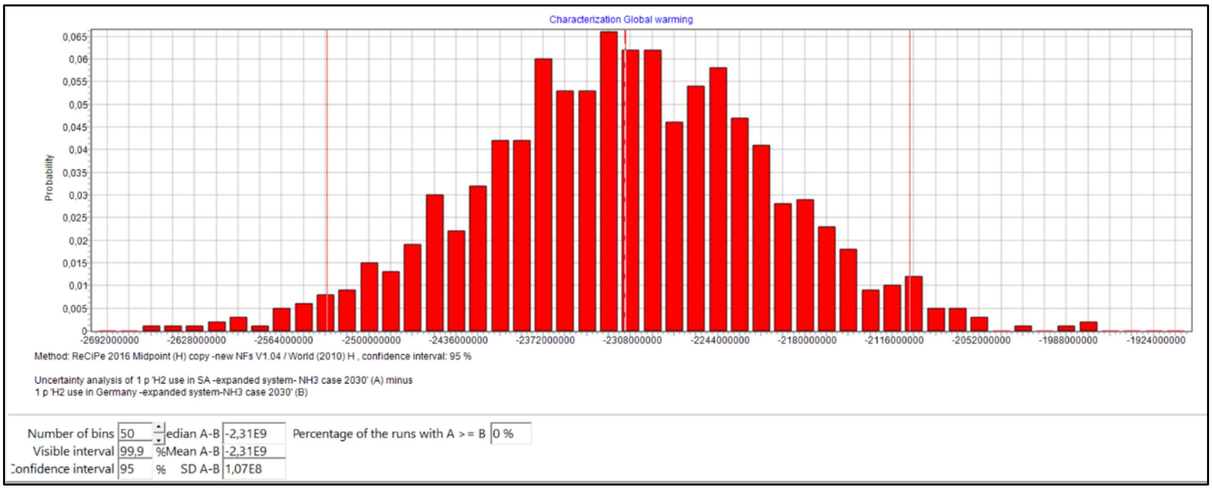


*Figure 8. 19: Uncertainty distribution for global warming*

## 8.5. Ethics Clearance Form

Application for Approval of Ethics in Research (EiR) Projects
Faculty of Engineering and the Built Environment, University of Cape Town

# APPLICATION FORM

**Please Note:**
Any person planning to undertake research in the Faculty of Engineering and the Built Environment (EBE) at the University of Cape Town is required to complete this form **before** collecting or analysing data. The objective of submitting this application *prior* to embarking on research is to ensure that the highest ethical standards in research, conducted under the auspices of the EBE Faculty, are met. Please ensure that you have read, and understood the **EBE Ethics in Research Handbook** (available from the UCT EBE, Research Ethics website) prior to completing this application form: http://www.ebe.uct.ac.za/ebe/research/ethics1

| APPLICANT'S DETAILS | | |
|---|---|---|
| Name of principal researcher, student or external applicant | | Ongezwa Mbaba |
| Department | | Chemical Engineering Department |
| Preferred email address of applicant: | | Mbbong001@myuct.ac.za |
| If Student | Your Degree: e.g., MSc, PhD, etc. | MSc |
| | Credit Value of Research: e.g., 60/120/180/360 etc. | 180 |
| | Name of Supervisor (if supervised): | Prof. Harro Von Blottnitz, Fadiel Ahjum |
| If this is a researchcontract, indicate the source of funding/sponsorship | | Inspired Evolution Investment Management, National Research Foundation |
| Project Title | | A comparative life cycle assessment of grey and green hydrogen in the South African context |

**I hereby undertake to carry out my research in such a way that:**

- there is no apparent legal objection to the nature or the method of research; and
- the research will not compromise staff or students or the other responsibilities of the University;
- the stated objective will be achieved, and the findings will have a high degree of validity;
- limitations and alternative interpretations will be considered;
- the findings could be subject to peer review and publicly available; and
- I will comply with the conventions of copyright and avoid any practice that would constitute plagiarism.

| APPLICATION BY | Full name | Signature | Date |
|---|---|---|---|
| **Principal Researcher/ Student/External applicant** | Ongezwa Mbaba | Signed by candidate | 02 Jun 2021 |
| **SUPPORTED BY** | **Full name** | **Signature** | **Date** |
| **Supervisor (where applicable)** | Click here to enter text. Prof. H. von Blottnitz | Signed by supervisor | 8 June 2021 Click here to enter a date. |
| **Supervisor (where applicable)** | Fadiel Ahjum | Signed by supervisor | Click here to enter a date. |

| APPROVED BY | Full name | Signature | Date |
|---|---|---|---|
| **HOD (or delegated nominee)** Final authority for all applicants who have answered NO to all questions in Section 1; and for all Undergraduate research (Including Honours). | Elaine Opitz Click here to enter text. | Signed by HOD | 06/07/2021 Click here to enter a date. |