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Faculteit Bedrijfseconomische Wetenschappen

master handelsingenieur

Masterthesis

Environmental techno-economic assessment of an electrocatalytic conversion process of carbon dioxide into ethylene: towards more sustainable chemistry

Ignace Koopmansch

Scriptie ingediend tot het behalen van de graad van master handelsingenieur, afstudeerrichting technologie in business

PROMOTOR :

Prof. dr. Sebastien LIZIN

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This master thesis was written during the COVID-19 crisis in 2020-2021. This global health crisis might have had an impact on the (writing) process, the research activities and the research results that are at the basis of this thesis.

Preface

As a second year master student in business engineering with specialization 'Technology in Business', a final master's dissertation was in place. As I have always been interested in innovations and assessing the viability of alternative technologies, this subject of combining the economic viability to the environmental analysis felt like a perfect fit. This master's dissertation was written as a continuation of the results found during my internship at VITO earlier in the academic year.

This work will focus on sustainable ethylene production in order to help mediate the growing climate change issues. A techno economic and life cycle assessment will make it possible to determine the economic and environmental viability of alternative ethylene production compared to traditional production methods like the cracking of naphtha. The chosen alternative approach is an electrocatalytic conversion of H₂O and captured CO₂. Through different scenarios, a wide scope of analysis will be provided.

I would like to thank my promotor prof. dr. Sebastien Lizin and my colleagues at VITO, with in particular dr. Miet Van Dael for their guidance throughout this project. Their insights and critical feedback have been an essential part to completing this master's dissertation.

As tweedejaars masterstudent handelsingenieur met afstudeerrichting 'Technologie in Business' dient een finale, afsluitende masterthesis geschreven te worden. Aangezien ik altijd al geïnteresseerd ben geweest in innovaties en het onderzoeken van de haalbaarheid van nieuwe technieken, leek het combineren van de economische haalbaarheid met de ecologische haalbaarheid van een alternatieve technologie een perfecte keuze. Deze masterthesis werd geschreven als verderzetting op de gevonden resultaten tijdens het bedrijfsproject bij VITO eerder in het academiejaar.

Deze thesis focust op het duurzamer produceren van ethyleen teneinde de welbekende klimaatproblematiek te mediëren. Een techno economische en levenscyclus analyse laten toe de economische en ecologische haalbaarheid van alternatieve ethyleenproductie te vergelijken met de traditionele productiemethode doormiddel van het kraken van nafta. De gekozen alternatieve technologie is het elektrokatalytisch omzetten van H₂O en opgevangen CO₂. Doormiddel van verschillende scenario's wordt een zo ruim mogelijke scope gecreëerd en een zo volledig mogelijke analyse.

Ik zou graag mijn promotor prof. Dr. Sebastien Lizin willen bedanken, alsook mijn collega's op VITO, met in het bijzonder dr. Miet Van Dael voor hun begeleiding doorheen dit project. Hun kennis, inzichten en kritische feedback waren essentieel bij het uitvoeren van deze masterthesis.

Abstract

In order to mediate climate change due to CO₂ emissions, alternative technologies should be looked at across sectors. One such sector is the chemical industry in which 30% of all end products have ethylene (C₂H₄) as an intermediary. Therefore, the traditional cracking of naphtha will be reevaluated and more sustainable processes based on CCU can be suggested. Through the execution of an 'Environmental Techno Economic Assessment' (ETEA), the alternative process of producing C₂H₄ via electrocatalysis will be evaluated on both the economic and environmental aspects. These analysis showed a base case negative NPV of - €188 million, with different scenarios showing values between - 316.8 and -91.3 million euros. Main contributors to this NPV are the selectivity level (FE), electricity price and the applied potential. A business currently importing ethylene could however benefit from this technology, providing import cost savings and pushing the NPV up towards in the most optimistic scenario € 167 million. The environmental aspect showed that, when green electricity can be used, lower carbon emissions of 1 tonne CO₂ per tonne C₂H₄ can be achieved by using electrocatalysis as a production method. However, water consumption will be higher, causing the overall environmental impact score to be worse. It will be important to increase technological development on both the economic and environmental aspects and to search for sustainable sources for both electricity and water in order to make electrocatalysis for ethylene a viable route.

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1. Introduction

The chemical industry contributes to approximately 8% of the global GDP, making it an important sector on an international level (CEFIC, 2019). With ethylene being an intermediary product for 30% of all chemical end products, it is seen as one of the most important chemical substances and the primary chemical building block (Alshammari et al., 2016; ARGKG, 2018; Ghanta et al., 2014; United Nations, 2019). Uses of ethylene vary from fertilizers in for the agricultural sector to a wide range of plastics.

The chemical industry however is also a large contributor to the environmental impact. This happens in multiple ways, a first is by the use of raw materials which are detrimental for the environment, such as natural gas or naphtha (OECD, 2001; Ghanta et al., 2013). A second way is through the energy use, approximately 18% of energy consumption in OECD countries can be attributed to the chemical industry. Of that percentage, 60% of the consumed energy comes from petrochemical sources (IEA, 2016; OECD, 2001). Traditional methods of producing ethylene are mainly forms of cracking such as steam cracking or fluid catalytic cracking. Another approach is dehydrogenation of light alkanes (Alshammari et al., 2016; ECI, 2017). All these processes operate at high temperatures and have a high environmental impact because of the feedstocks such as crude oil that are used (Ghanta et al., 2014; Chuapet et al., 2016).

Climate change has become a pressing issue in the past couple of years as CO₂ concentrations have been increasing since the pre-industrial era from approximately 250ppm to 410ppm in 2014. This increase can be attributed for a large part to the use of fossil fuels which are also the main source of emissions when producing ethylene (IPCC, 2014). As per the Paris Agreement, Europe has committed to reduce emissions by at least 40% compared to 1990 by 2030. By 2050, they want to take it even further with the 'European Green Deal' by aiming for carbon neutrality in this timeframe (European Commission, 2018). Ways envisioned to achieve this are the transition towards renewable energy, but also Power to X processes, alternative business models and reuse of certain streams (European Commission, 2018; Jenck et al., 2004). Power to X can be seen as using surplus electricity to produce a wide range of products like chemicals, fuels or gas. This surplus electricity can be generated through sustainable conversions such as photovoltaic panels or windmills (Rego de Vasconcelos and Lavoie, 2019). Transitions should be looked at, not only at the production stage, but also further down the line. This means investigating the possibilities of closed loop systems and cradle-to-cradle processes (Federchima, 2013).

One possibility of creating more closed systems is by using emissions from other sectors. General trends for environmental impact reduction are using that same approach and are evolving towards limiting the emission of CO₂. Carbon capture technologies as a consequence are becoming more interesting (Tcvetcov et al., 2019). In these cases, CO₂ gets captured either at the point of generation or directly from the atmosphere (Bui et al., 2018; Pires et al., 2011). A first possibility of carbon capture is to store the captured carbon dioxide, compress it into a supercritical fluid which can then be sequestered. This approach is called 'Carbon Capture and Storage' (CCS) and Bui et al

(2018) investigated the environmental benefits of this approach and found CCS to be environmentally more beneficial compared to the use of wind energy. It is a very important technical alternative, as it allows production processes to remain as they are while still minimizing the effect of CO₂ emissions on climate change (Bui et al., 2018; Pires et al., 2011). An extension of the CCS approach is 'Carbon Capture and Utilisation' (CCU). In that case, the captured CO₂ will be used as an input stream for the production of selected end-products such as ethylene. Applying CCU technologies, the total greenhouse gas (GHG) emissions can be significantly reduced and can substitute the conventional production technologies for basic chemicals, fine chemicals and even polymers (Kätelhön et al., 2019; Thonemann and Pizzol, 2019).

Combining the scale of the chemical industry and ethylene in particular with the goals set to mediate environmental impacts, an important step can be made in reducing the environmental impact by transitioning towards more sustainable processes for ethylene (Ghanta et al., 2013). One possible approach is to perform electrocatalytic conversion of CO₂, which is possible as ethylene is a hydrocarbon (Rego de Vasconcelos and Lavoie, 2019). After comparing the different types of installations, the electrocatalytic conversion will be performed by an alkaline electrolyzer in this work. This approach for conversion is a variation of 'Power to X' which has up until now mainly been investigated for the production of H₂, but has not yet been commercialized for the production of ethylene. Experimental units, such as from Li et al (2019), have however been investigated already to produce other substances such as methanol or ethylene through electrocatalysis.

Not a lot of research has been performed regarding the economic and environmental viability of the technology for ethylene. This work will attempt to verify the sustainability of the electrocatalytic conversion process compared to the traditional production method. It will also try to assess the economic viability of this electrocatalytic conversion process in an elaborate way, as these two aspects are also necessary in order to decide whether or not to undertake a project. The technical feasibility, economic and environmental results ideally all provide promising numbers in order for a new sustainable technology to be able to thrive (Thomassen et al., 2018).

2. Methodology

2.1 ETEA

By integrating the technical, economic and environmental aspects into one framework, a more coherent decision can be made. Trade-offs and synergies can be identified, allowing for accurate decisions to be made based on results in all aspects. That is what an 'Environmental Techno Economic Assessment' (ETEA) enables by extending the 'Techno Economic Assessment' (TEA) with the environmental dimension in the form of a 'Life Cycle Analysis' (LCA) (Thomassen et al., 2019). Based on results on all of these aspects, recommendations for the technology can be made. This approach has been selected as it is possible for a technology to be technologically feasible, but economically and environmentally unrealistic. In order for a new technology to actually thrive, it is necessary to perform well in all three dimensions and the ETEA framework will allow for all these dimensions to be analyzed simultaneously. A specific set of steps will be followed in order to acquire the necessary numbers in every dimension.

2.1.1 Market study and literature review

In the first step, a market study is performed which will allow for the ethylene market to be researched and opportunities to be found. This analysis will allow for certain technical parameters to be identified such as energy requirements, minimum potential and more. It will also make it possible to select or eliminate certain technologies to be used in the following steps. Prices of all required parameters will also be investigated in this step in order to achieve a complete economic and technical integration in the following steps. This initial study will also make it possible to define the goal and scope of the project for the environmental analysis, which will be elaborated in more detail in the case description (Thomassen et al., 2018).

2.1.2 Mass and energy balance

The second step will take all findings from the market study and literature review and combine them into a mass and energy balance with a corresponding visual representation in the form of a process flow diagram (PFD). By balancing the required inputs to the final outputs and linking every step in between, an automated model can be created and every parameter can be quantified (Thomassen et al., 2018; Thomassen et al., 2019). This mass and energy balance will serve as the key technical starting point for the rest of the case.

2.1.3 Economic dimension

In the third step, economic parameters will get linked to the mass and energy balance, enabling an economic analysis. The main evaluation criterium used to assess the case, will be the 'Net Present Value' (NPV). Based on this criterium, different recommendations will be made in the interpretation step regarding the economic viability of the project. It will also enable the identification of main contributors to this viability in the interpretation step. Whenever insufficient data was available, a regression analysis is performed in order to get accurate data on the investment (Thomassen et al., 2018).

Results of TEA studies will allow decision makers to direct their research and development towards certain specific aspects (Kuppens et al., 2015). By being able to identify the factors with the most influence on the end results, decisions in the right directions can be made (Van Dael et al., 2013). The entire process and analysis is modeled and linked in Excel, meaning that changes in specific variables automatically recalculate the dependent variables, showing the updated results. Because of this integration, a sensitivity and uncertainty analysis can be performed in order to get a broad view on the possible outcomes of the project (Thomassen et al., 2018).

2.1.4 Environmental dimension

The fourth step will add the environmental dimension to the traditional TEA framework by performing an LCA. According to ISO 14040 and 14044, an LCA can be defined as "A compilation and evaluation of the inputs, outputs and potential environmental impacts of a product system throughout its life cycle." (ISO, 2006a; ISO, 2006b). After the mass and energy balance has been set up, just like economic parameters can be linked, environmental parameters can be as well. In databases such as EcoInvent in SimaPro, data of environmental impacts of inputs and waste streams are collected. In order to evaluate the environmental impacts, the ReCiPe (2016) method will be used, which can be applied on a global scale. For temporal scope for this case, the 'hierarchist' viewpoint will be taken as it encompasses 100 years, which is the standard viewpoint for an LCA study. The individualistic and egalitarian viewpoints will not be used as they focus on the short term and long term respectively (Huijbregts et al., 2016).

18 midpoint categories will be categorized and evaluated in this framework. Afterwards, these midpoint categories can be aggregated into three endpoint indicators (figure 1). These endpoint indicators will represent the different damage categories 'Human health', 'Ecosystem quality' and 'Resource scarcity'. Finally those endpoint categories can once again be aggregated into one single indicator (Huijbregts et al., 2016). For each of the different levels of detail, separate analysis and conclusions can be made. Midpoint indicators will give a wide overview of all possible environmental impact sources that can be attributed to a certain production process. Aggregating those into the endpoint indicators will make it possible to identify hotspots for each production process. This makes it possible to pinpoint which damage category is most critical and needs attention the most. Finally aggregating everything into a single indicator will make it possible to clearly communicate which of the selected processes is more sustainable. The scientific validity of these results will decrease as less values get reported, however it will become easier to communicate these values, therefore the entire spectrum will be reported below.



Figure 1: Aggregation of midpoint towards endpoint categories (based on Huijbregts et al (2016))

2.1.5 Interpretation

The fifth and final step will consist of interpreting the results from previous steps and performing a sensitivity analysis. The technical and economic parameters with the largest influence on the end result can be identified by performing Monte Carlo simulations using the Oracle software package 'Crystal ball'. A triangular distribution of $\pm 10\%$ will be used for all parameters (Thomassen et al., 2018; Lee et al., 2017; Kuppens et al., 2018; Van der Spek et al., 2020). After these hotspots have been identified, a local sensitivity analysis will give an even clearer view of the scale of these impacts on the NPV and thus the profitability of the project. Throughout this study, different assumptions had to be made, the most significant ones are seen as separate scenarios which will be discussed in this step as well. Four different scenarios have been defined based on the assumptions that can be made concerning the electrocatalytic production of ethylene. These assumptions cannot be seen as certain, which is why they will be treated below in an uncertainty analysis.

Collecting and assessing the environmental impacts of different steps in the production process will allow for specific recommendations with regards to sustainability. By linking the environmental impacts to the mass and energy balance, the goal and scope of the project can be defined in accordance with each other, which will be done in the case description below.

2.2 PEM vs Alkaline

2.2.1 Type selection

When considering an alternative pathway, different alternatives were put against each other in order to make an accurate decision concerning the technology to utilize for the specific case study. There are three main types of electrolyzer, a first is the alkaline electrolyzer, second is the proton exchange membrane electrolyzer (PEM) and finally there is also the solid oxide electrolyzer (SOE). The SOE technology will not be considered in this work as the operating temperatures are a lot higher compared to the other two alternatives. Also, SOE installations are currently not stable and will therefore not be taken into the analysis (Sapountzi et al., 2017).

The two other technologies were investigated and based on results from literature, a technology was picked as a base case (table 1). Since alkaline electrolyzers have been commercialized for longer than PEM electrolyzers, the TRL level for that technology is higher already and higher capacities can be achieved. Where an alkaline electrolyzer is capable of sizes deep into the MW range, this is harder to achieve with a PEM electrolyzer (Carmo et al., 2013; Zorica et al., 2014). It will become clear later in this paper why the size plays an important role specifically with ethylene production.

Table 1: Alkaline vs PEM (based on Zorica et al (2014) and Carmo et al (2013))

ALKALINE	PEM
Well established technology	More compact design
Stacks in the MW range	Higher current density
Long-term stability	Higher partial load range
Non-noble catalysts (less expensive)	Higher pressure

Another aspect why alkaline is better suited for large scale installations and global integration, is because of the catalysts that are used. In a PEM installation, noble materials or platinum group metals (PGM) are needed. These are not only expensive, but also scarce, making large scale application hard (Marini et al., 2012; Mayyas et al., 2019). The use of these materials in a large scale installation could affect the prices of these materials and indirectly affect the mobile phone market and other sectors where PGM's are used (Carmo et al., 2013). Another factor to take into account, is the lifetime of an electrolyzer. Currently, an alkaline electrolyzer will last approximately 20 years compared to 10 years for a PEM installation. Combining the lifetime and overall lower cost of an alkaline installation, in terms of capital expenditures, the alkaline electrolyzer is less demanding (Mayyas et al., 2019; Zorica et al., 2014).

For an alkaline installation, costs average at around € 930/kW, whereas prices for PEM installations amount to € 1,570/kW on average (Ruth et al., 2017). Because of this and a lower complexity in configuration of the stack, an alkaline electrolyzer seems most suited for this ethylene case. Prices of alkaline and PEM installations are expected to get closer to each other in the future as the TRL of PEM installations increases (Schmidt et al., 2017; Wei et al., 2014). This means that in the future, with developments taken into account, PEM could become the more dominant technology. According

to the case study of Schmidt et al (2017), most experts identify PEM as the technology that will be most dominant in 2030 for hydrogen production with other end products possible as well. Alkaline installations are already seen as a mature technology, making cost improvements on a technological aspect harder (Saba et al., 2018).

On the other hand, an alkaline installation will not be as compact as a PEM installation, meaning that a larger surface area would be occupied because of the bulky stack configuration. Some other disadvantages of alkaline compared to PEM, is the lower current density which can be applied, determining the rate of conversion and the possibility of cross diffusion (Carmo et al., 2013; Mayyas et al., 2019). The latter causes for products at the anode and cathode to get mixed slightly, resulting in lower purity of the desired end product (ethylene in this case) which means that possibly extra steps might be required in order to get the desired product. Finally there is also the lower pressure at which an alkaline installation operates. A higher pressure is preferred as the output stream can be condensed further making transport easier, but also making the gaseous separation easier according to Fick's law (Carmo et al., 2013). Possible developments towards a hybrid system combining the advantages of both described technologies, is a solid alkaline system. Since not enough detailed information could be found, this option has not been investigated further, but will be left open for further research in the future (Sapountzi et al., 2017).

Because the case which will be discussed in this paper concerns the targeted conversion of captured CO_2 and H_2O into C_2H_4 , it is necessary to compare the capacity to convert these two molecules into the desired end-product. Wang et al (2018) found that PEM installations are naturally less reactive when it comes to converting the carbon dioxide. This means that further research will be needed in order to achieve a higher CO_2 conversion efficiency in these types of installations. This lower conversion efficiency can also be seen in the aggregation of other literature in table 2. In that table different cases concerning electrocatalytic ethylene production have been summarized. Based on the faradaic efficiency (FE) and stable operating hours, a ranking could be made between the different cases. Faradaic efficiency is the most commonly used metric for selectivity as it describes the yield throughout the entire catalytic region (Passard et al., 2016).

This ranking, combined with the above mentioned advantages and disadvantages of each installation type will allow for the selection of a case to base the rest of the research on. This selected case will serve as a base case and will not be seen as fixed. Throughout the analysis in this paper, different scenarios will be discussed in which specific parameters are varied.

The results from the literature in table 2 have been visualized in figure 2. There it is clear that Alkaline electrolyzers achieve higher FE and stable production hour combinations compared to PEM installations. There is however one PEM installation which gets close to the level of the best alkaline installation. Because of the low reactivity to CO_2 conversion, shorter lifespan, higher initial investment cost and size availability, a PEM installation did not get preference. It was thus opted to use an alkaline electrolyzer for the further analysis of electrocatalytic conversion of CO_2 into C_2H_4 .

Table 2: Literature overview: Elektrolyzer performance

SOURCE	TYPE ELEKTROLYZER	TYPE CATALYST	FARADAIC EFFICIENCY (FE)	STABLE OPERATING HOURS
BATURINA ET AL, 2014	PEM	Doped CU	max ca. 37%	/
DINH ET AL, 2018	Alkaline	Cu	70%	150 hours
GABARDO ET AL, 2019	Alkaline	Cu	50%	100 hours
GAO ET AL, 2017	Plasma	Cu(100)	45%	/
MERINO GARCIA ET AL, 2017	PEM	Cu	10%	100 minutes (=duration of experiment)
HOANG ET AL, 2018	PEM	CuAg	60%	/
KAS ET AL, 2015	PEM	Cu(100)	44%	/
LEE ET AL, 2018	Alkaline	Cu ₂ O/AN-Cu	40%	40 hours
LI ET AL, 2019	Alkaline	Cu	72%	190 hours
MA ET AL, 2016	Alkaline	Cu	69%	4 hours (=duration of experiment)
MA ET AL, 2016B	Alkaline	Cu-Cu ₂ O	69%	4 hours (=duration of experiment)
MA ET AL, 2020	Alkaline	Cu	65%	40 hours
MALKHANDI ET AL, 2019	PEM	Cu	70%	150 hours
MERINO GARCIA ET AL, 2017B	PEM	Cu ₂ S	92.8% 86.8%	45 minutes (=duration of experiment)
MERINO GARCIA ET AL, 2019	PEM	Cu	91.1%	/
NA ET AL, 2019	PEM	Cu	70%	/
PENG ET AL, 2017	PEM	CU	40%	8 hours (=duration of experiment)
REN ET AL, 2020	PEM	Cu-Cu ₂ O	51%	10 hours
SPURGEON AND KUMAR, 2018	PEM	Step 1: Ag Step 2: Cu	/	/
THEVENON ET AL, 2019	Alkaline	Cu (with 1-Br ₂)	45%	40 hours
ZHANG ET AL, 2020	Alkaline	Nanodefactive Cu nanosheet n-CuNS	83.20%	14 hours (=duration of experiment)
ZHU ET AL, 2019	SOE	Iron	48.40%	100 hours

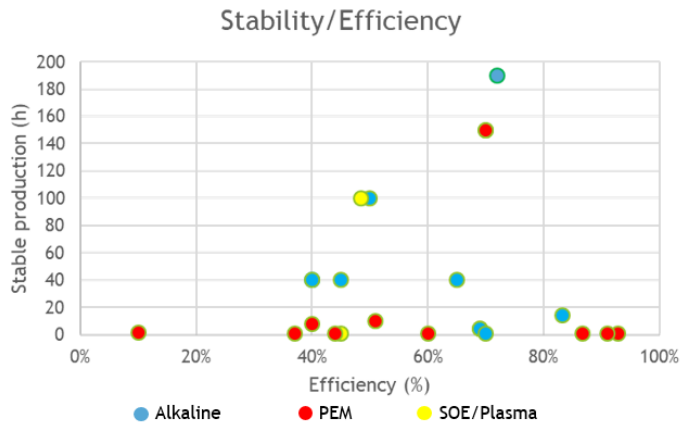


Figure 2: Performance overview ethylene formation

2.2.2 Working principles

The main working principles of an alkaline electrolyzer installation operate around the reactions taking place at the anode and cathode. Figure 3 gives a simplified representation of what the installation would look like with all of the reactions depicted. The reaction to form the target product ethylene will happen at the cathode side, using 12 electrons to convert the combination of CO₂ and H₂O inputs. The OH⁻ that also gets formed as a result will migrate through the membrane towards the anode side of the cell. As it is an alkaline membrane and OH⁻ will be transported, an anion membrane will be needed, in this case the 'Fumapem FAA-3-PK-130' will be used (Li et al., 2019). The membrane will serve as a separation between the reaction at the anode side (anolyte) and the cathode side (catholyte). It ensures that no unwanted side reactions can take place, while still allowing transfer the OH⁻ that needs to migrate from cathode to anode (Birdja et al., 2019). Since no full selectivity towards ethylene is possible, some side reactions will be taking place and side products will get formed as well (Li et al., 2019). On both the anode and cathode, a layer of catalyst is applied. This will help steer the reactions towards the desired end product. Here Cu(12) has been used, as it yielded the highest selectivity towards ethylene while still maintaining consistent stable production (table 2). Since this Cu(12) is a catalyst, it will not participate in the reactions, but will solely serve to facilitate them.

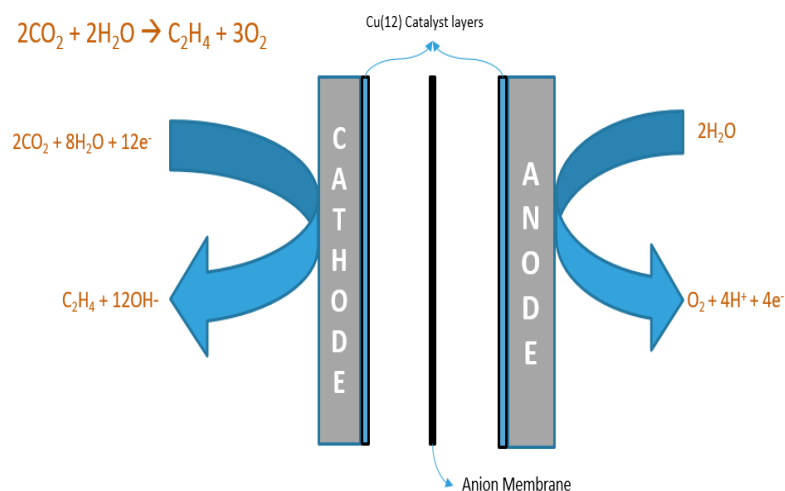
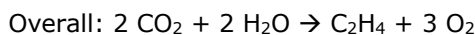
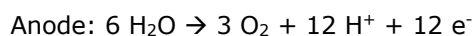
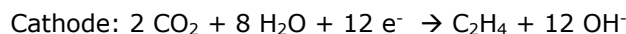


Figure 3: Alkaline electrolyzer schematic

Putting the chemical reactions happening at the cathode and anode, the overall reaction to form ethylene:



Looking at the larger picture of an alkaline electrolysis installation, some important components can be identified. First there is the stack where all the reactions will be taking place. A stack is composed of a set of cells which each have a certain capacity. Depending on the required power to get the desired output quantity, a different number of cells will be needed to build the stack. These cells will need to be held together by wires and other housing and protective materials, the balance of stack (De Silva and Middleton, 2017). This balance of stack is generally assumed to account for approximately 13% of the stack (Peters et al, 2003). The number of cells including the required active area in order to produce the necessary amounts will determine the overall installation size (Heremans et al., 2017). Finally, the thickness of the catalyst layer that is applied will help determine the conversion rate and will generally be in the range between 0.5 and 2 mg/cm² (Dinh et al., 2018; Merino Garcia et al., 2019; Zhang et al., 2020).

As will be demonstrated in later sections, ethylene requires a lot of energy to be produced electrocatalytically. With 12 electrons needed and a total gibbs free energy of 1331 kJ/mol, it is noticeable that it will be an energy intensive production process with high costs originating from that aspect.

2.3 Base case

2.3.1 Mass and energy balance

After performing the market study and literature review, the main technology has been selected. In the next step, all necessary parameters will be given values based on literature or calculations. A base case will make it possible to set up the mass and energy balance in order to be able to vary parameters in the next steps while still working with a correct balanced system. This base case will also serve as a first result for both the economic and environmental dimensions. Figure 4 provides a visual representation of the process.

There are three main inputs needed in order for the electrocatalytic conversion to be performed. The first is CO₂, which has arbitrarily been set at 50,000 tonnes per year. Taking into account the molar balance of a reaction, this means that 20,467 tonnes of H₂O will need to be added in order to balance the reaction. The final input needed is the electricity, which amounts to approximately 940,000 MWh/y. Considering an output of ethylene of 11,156 tonnes/y, this means an electricity consumption of 84 MWh per tonne C₂H₄ and productivity of only 12kg C₂H₄ per MWh of electricity. Main cause for this, is the need of 12 electrons in order to produce ethylene and the high Gibbs free energy of 1,331 kJ/mol as mentioned above already.

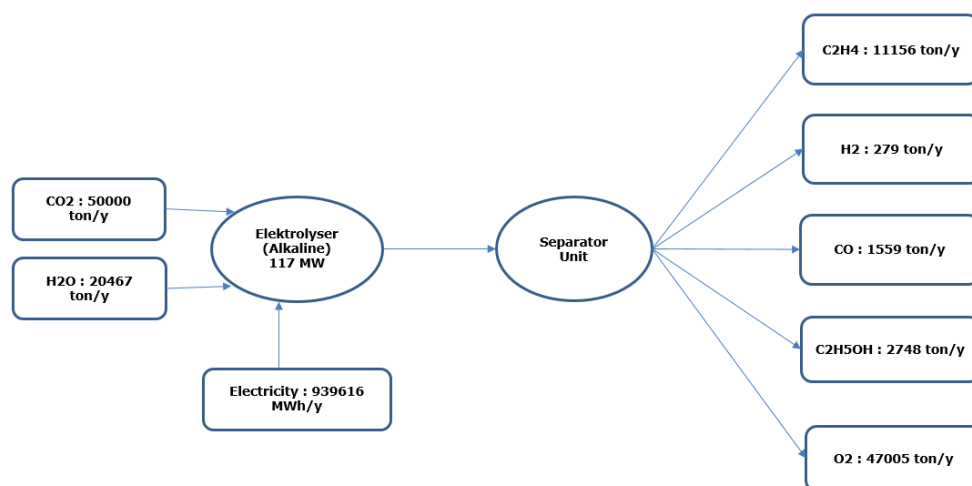


Figure 4: PFD electrocatalytic ethylene production

A separator unit has been placed after the elektrolyzer as well in order to be able to separate all outgoing products from each other and being able to deliver products with sufficient degrees of purity (Peters et al., 2003) (figure 4).

In this base case, a FE of 70% has been used, meaning that other reactions will still happen inside the elektrolyzer causing side products to be formed. These other reactions will have a selectivity of 4.9%, 7.3% and 10.5% for CO, H₂ and C₂H₅OH respectively. O₂ will get formed in each of the separate reactions (Table 3). Since there is a surplus of CO₂, there will also be 1,750 tonnes of CO₂ left at the end of the process. This CO₂ can be reused for the next cycle, closing the loop so no direct CO₂ gets emitted. The other remaining end products were of too low quantities to consider in this case, so they have been kept as 'others'. These 5,970 tonnes of other products needs to be experimentally determined in order to be able to decide what can be done with them.

Table 3: Overall reactions per end product including selectivity

Product	Selectivity	Reaction
C₂H₄ (Ethylene)	70%	$2 \text{ CO}_2 + 2 \text{ H}_2\text{O} \rightarrow \text{C}_2\text{H}_4 + 3 \text{ O}_2$
C₂H₅OH (Ethanol)	10.5%	$3 \text{ H}_2\text{O} + 2 \text{ H}_2\text{O} \rightarrow \text{C}_2\text{H}_5\text{OH} + 3 \text{ O}_2$
H₂ (Hydrogen)	7.3%	$2 \text{ H}_2\text{O} \rightarrow 2 \text{ H}_2 + \text{ O}_2$
CO (Carbon monoxide)	4.9%	$\text{H}_2\text{O} + \text{ CO}_2 \rightarrow \text{ CO} + \text{ O}_2 + \text{ H}_2$

In order to determine the size of the elektrolyzer, different parameters need to be determined. Literature shows an overpotential of around 1V, meaning that the theoretical potential of 1.15 needs to increase to about 2 V in order for the production to be possible. Recent developments however show promising results at a lower overpotential, with only 1.8V needing to be applied (Barco Burgos et al., 2020; Ma et al., 2020; Thevenon et al., 2019). This means the system would be operating at approximately 64% voltage efficiency. The applied current is dependent on the number of electrons which take part in the reaction as well as the amount of CO₂ input, leading to a total of over 65 million ampère. Since the elektrolyzer is an alkaline type, the actual applied current density will only be 200 mA/cm² (Li et al., 2019; Sapountzi et al., 2017; Garbado et al., 2019; Spurgeon et al.,

2018). This allows us to determine the size of the electrolyzer, as the minimal and effective power of 75MW and 117MW are calculated by multiplying the applied current with the theoretical and applied potential respectively. This shows the significant size of the electrolyzer which would be needed and explains why an alkaline electrolyzer was chosen over the PEM installation. This size of the electrolyzer also determines the extreme energy need of 939,616 MWh per year. The electrode area can be calculated based on the applied current and the current density. Based on findings from Mayyas et al (2019), the number of cells needed can be calculated based on this electrode area and the total cell area. With an active cell area of 91% taken into account and an average cell area of 500 cm², a total number of 652,512 cells will be needed (Mayyas et al., 2019; Barco Burgos et al., 2020). The land use had been calculated based on findings from Heremans et al (2017), by multiplying the cell land use with the total number of cells, a total land use of 4ha has been found. Based on a catalyst use of approximately 1.25 mg/cm² combined with earlier calculations of the electrode area, the total catalyst loading could be determined at 408 kg (Gabardo et al., 2019; Garcia et al., 2017; Ma et al., 2020). The catalyst that will be used throughout this work will remain the same as in this base case, Cu-12 (Li et al., 2019).

Operating hours were set at 8,000 hours per year, allowing for 760 hours of downtime for maintenance and unexpected issues (Bos et al., 2020). Personnel has been determined based on the total production hours and the scale of the installation. It was assumed that full time operation and monitoring was required, therefore work in 3 shifts will be applied at 260 working days per year with 8 hours per shift. This means that every employee works 2080 hours per year, bringing the minimum number of employees needed based on operating hours to 4.2.

Table 4: Mass and energy balance (base case scenario)

VARIABLE	VALUE	UNIT
CO₂ INPUT	50,000	ton/y
H₂O INPUT	20,467	ton/y
TOTAL INPUT	70,467	ton/y
ΔG	1,331	kJ/mol
CURRENT	65,251,128	A
ELECTRODE AREA	32,626	m ²
THEORETICAL POTENTIAL	1.15	V
MINIMAL REQUIRED POWER	75	MW
REACTOR (EFFECTIVE) POWER	117	MW
VOLTAGE EFFICIENCY	64%	%
ELECTRICITY USE	939,616	MWh/y
NUMBER OF CELLS	652,512	#
CATALYST LOADING	408	kg
LAND USE	4	ha
ETHYLENE OUTPUT	11,156	ton/y
O₂ OUTPUT	47,005	ton/y
H₂ OUTPUT	279	ton/y
CO OUTPUT	1,559	ton/y
ETHANOL OUTPUT	2,748	ton/y
REMAINING CO₂	1,750	ton/y
TOTAL OUTPUT	64,497	ton/y
OTHERS	5,970	ton/y

2.3.2 Economic approach

2.3.2.1 General

Economic parameters in the base case have been selected based on either literature or a regression analysis. First off, for the discount rate, a value of 12% has been chosen based on various factors described by Peters et al (2003). 10% is most commonly selected when a technology is used for an expansion or cost improvement in an existing market. A 15% discount rate is traditionally used for expansion of a conventional product or market. As this electrocatalytic conversion process is new to the market of ethylene, that percentage can be justified as well. Therefore, a value in between those two has been taken as the base value throughout this case. Higher discount rates will not be applicable in our case as they apply more to speculative ventures and will also be evaluated in a sensitivity analysis (Peters et al., 2003).

Learning effects for reinvestments of the elektrolyzer were set at 15% as technological developments allow for the installation to be optimized (Schoots et al., 2008; Thomassen et al., 2020). Even though a more sustainable production method is used, no price premium was applied in this base case in order to be able to assess the costs and revenues directly compared to the traditional method. Since the CO₂ used for this process will have been captured from a point source, a benefit can be gained when considering the 'Emission Trading Scheme' (ETS), which will provide a benefit of € 25/tonne CO₂ that is emitted less compared to the traditional production method (Galinato and Yoder, 2010; Business Insider, 2021). In this case, the carbon dioxide that does not get emitted in the electrolysis process compared to the traditional process, will become a benefit as they can possibly be sold to other manufacturers who do emit more. Exact values on the CO₂ emissions that are avoided are calculated in the environmental section.

Values for all the input and output values can be found in table 5. All side products are assumed to be of sufficient purity to be sold at their respective market values. CO₂ is assumed to be captured from a point source. The elektrolyzer investment cost regression has been performed based on 17 different cost estimates from existing elektrolyzers were used. This makes it possible to get an accurate estimate of the investment cost depending on the required size as the exact size is not readily available in literature (figure 5). Regression analysis led to a power function:

$$Y = 1494.5 * x^{-0.252}$$

In which y is the investment cost per kW and x indicates the actual size of the elektrolyzer.

Table 5: Input and output values

PRODUCT	VALUE	SOURCE
CO ₂	40 €/tonne	Dieterich et al., 2020
H ₂ O	3.7 €/m ³	VMM, 2019
C ₂ H ₄	1,000 €/tonne	De Luna et al., 2019
C ₂ H ₅ OH	400 €/ tonne	Business insider, 2020
H ₂	3,900 €/tonne	De Luna et al, 2019
CO	500 €/tonne	De Luna et al, 2019

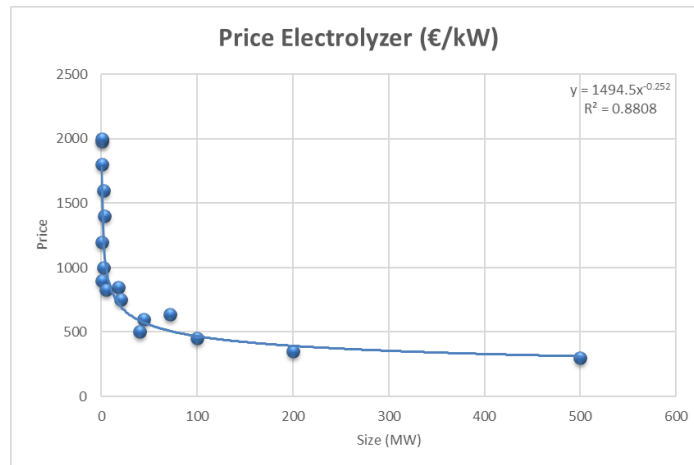


Figure 5: Elektrolyzer cost regression

Some other costs depend on the initial investment cost, the site preparation will for example amount to 10% of the initial investment. Insurance, repair and maintenance rates will amount to 0.5%, 1% and 3% of the initial investment respectively (Peters et al., 2003). Finally, 13% of stack is the so called balance of stack (stack housing, wires, manifolds, insulation material, ...).

2.3.2.2 Uncertainty assumptions

In order to assess an even wider spectrum of possible outcomes, the base case can be extended beyond a sensitivity analysis by adding uncertain assumptions. Based on these assumptions, different outcomes might be possible, the base case as described above being one possibility. Table 6 below describes the possible assumptions that will be used to further analyze the viability of the project by creating different scenarios based on a combination of these assumptions.

Elaborating on these assumptions, first of all it will be assumed that sufficient green electricity is available to sustain production. This might be through a combination of local production and import from another region as conditions for green electricity production are more ideal in other regions compared to Belgium. Still, a fixed price for electricity will be used per scenario. The value of CO₂ will mainly depend on the way it has been captured, with CO₂ via DAC being significantly more expensive compared to the point capture source. Next, as mentioned above, 4 hectares of land would be needed for this installation. It is assumed that whichever size is needed, the required land will be available.

A next assumption describes whether or not the produced side products can be sold on their own or not. If they can, prices as mentioned in table 5 will be used. Depending on the need for specific separation of the end products in order to guarantee the required purity levels, a separator unit will have to be added at a cost of 40% of the initial investment cost of the elektrolyzer (Peters et al., 2003). Learning effects will be able to vary between 0% and 20% to account for developments in the technological aspect, possibly making installations more cost effective in the future.

Another uncertain assumption depends on the viewpoint taken for the project. If it is considered from an end-product producing company which already uses ethylene in their processes, it is possible that their ethylene is imported. By then producing ethylene themselves, they are able to save on certain importing costs such as import duties and shipment costs. This means that next to producing their ethylene (partially) themselves, they can also benefit from not having to import that quantity from another region. It is also possible that more ethylene is needed than what can be produced locally, in that case benefits for only the produced quantity will be taken into account. According to S&P Global Platts (2020), the quantity imported is at 100,00 tonnes per year, making that the maximum quantity to take into account for this benefit. If the viewpoint changes to that of a company that solely produces ethylene already or a new company, this approach will no longer be valid and no import avoidance benefit will be counted.

The production scale will also be able to change, if a goal is set of producing ethylene in order to take up 1% of the market, another quantity will have to be calculated as opposed to when an arbitrary CO₂ quantity is taken as input or if the entire import wants to be offset with local production (PetroChemEurope, 2021; S&P Global Platts, 2020).

Next, it is possible to include a price premium or not as it is not certain that the market will actually be willing to pay a premium. The percentage of this price premium can be changed as well depending on how optimistic a scenario is estimated. Price premium will amount to approximately 15% to 30% above the current market value, meaning that ethylene would trade between 1150 and 1300 euros.

The total cost of the electrolyzer can be calculated in two different ways. A first possibility is to use cost estimates of existing separators with different capacities and calculate the regression through all these installations in order to find the generalizable formula to use in function of the needed size as mentioned above. The second possibility is to take into account all the components that are needed in an electrolyzer and build a system using those costs. The latter possibility is the hardest one to calculate, as all components need to be included. Finally, in the base case, the subsidy was assumed to be available, this value fluctuates depending on the market value of ETS rights (Business insider, 2021).

Table 6: Uncertain case assumptions

PARAMETER	POSSIBLE VALUES	ASSUMPTION	SOURCES
ELECTRICITY	10 – 60 €/kWh	Only green electricity will be used (photovoltaic)	(EuroStat, 2020) (Bellini E., 2021)
CO₂	0 – 90 €/tonne 222 – 268 €/tonne	Point capture Direct air capture	(Dieterich et al., 2020)
SIZE	/	Enough land available to build the required reactor size	/
SALE SIDE PRODUCTS	0/1	If purity high enough and clientele found, side products can be sold at market value	/
SEPARATOR	0/40% I ₀	If side products want to get sold and specific separation is needed	(Peters et al., 2003)

LEARNING EFFECTS	0-20%	Production and installations become less expensive throughout the years	(Schoots et al., 2008) (Thomassen et al., 2020)
IMPORT	0/1	The quantity C ₂ H ₄ produced is seen as benefit as it are saved expenses	/
SCALING	-Arbitrary CO ₂ input -1% market share -Enough to stop import	Multiple viewpoints depending on where you look from. Starting from CO ₂ input or ethylene need	(PetroChemEurope, 2021) (S&P Global Platts, 2020)
PRICE PREMIUM	0/1	A price premium can be asked for ethylene produced in a more sustainable way. Price can be elevated by 15 to 30%	(Iles and Martin, 2013)
ELEKTROLYZER INVESTMENT COST	0/1	Option 1: Building installation from scratch, components costs Option 2: Regression based on size and cost per kW	(De Luna et al., 2019) (Dieterich et al., 2020) See table 1
SUBSIDY	0-50 €/tonne	If ETS rights can be sold to other companies because less emissions are created, this will become a benefit. Rights will be sold at market value.	(Galinato and Yoder, 2010) (Business Insider, 2021)

Based on the assumptions described above (table 6), we can distinguish the following scenarios: A first scenario will be an optimistic one in which the avoided import is seen as a benefit, a price premium is asked and side products are sold. In this scenario a separator unit will consequently be needed as well. The benefit of ETS will also be included in this case and the above mentioned variables will be optimized. The cost of the elektrolyzer will also be lowered by 20% in order to incorporate both margins and learning effects in the scenario already. Next is a slimmed down version of the first scenario with the only change being that import avoidance is no longer seen as a benefit. The third scenario will be an intermediate scenario, with no import benefit, but still a price premium and side product sale. ETS benefits will still apply, but at a lower value compared to the first scenario. The other parameters will be set at the values assumed in the base case as well. The elektrolyzer benefits will also get moderated to only 10% reduction. Finally the fourth scenario will represent the most pessimistic approach where in addition to the second scenario no sale of the side products will occur and the price premium gets dropped. The ETS benefits will still remain in place as the process will still cause less CO₂ emissions compared to the traditional process like was mentioned in the environmental section above. Electricity price has been set to 2020 electricity mix prices in Belgium (EuroStat, 2020). Below, when discussing the results, these four scenarios will be compared to each other as well as to the base case.

2.3.3 Environmental approach

The goal of this work can be defined as assessing the environmental impact of electrocatalytic ethylene production opposed to the traditional production method by cracking naphtha. Figure 6 gives a visual representation of the system boundaries that will be used in this case. The reference flow of the LCA can be determined based on the production scale of the project. In this case, a reference flow of 1 tonne of ethylene was chosen. The selection of this reference flow will make it possible to compare the suggested electrocatalytic production pathway to the current production method by cracking naphtha. As can be seen in Figure 6, this case can be seen as a 'gate-to-gate'

system as the collection of resources is not included in the analysis. Collecting CO₂ through direct air capture or point source capture have not been included. The use phase of ethylene has also not been included, which means that only the environmental impact of the production process will be taken into account. The use and end-of-life phases of the production process do not need to be taken into account as they will remain the same for both the traditionally produced as well as the electrocatalytically produced ethylene (Muller et al., 2020; Nabil et al., 2021). The system boundary of the traditional process is represented in figure 7.

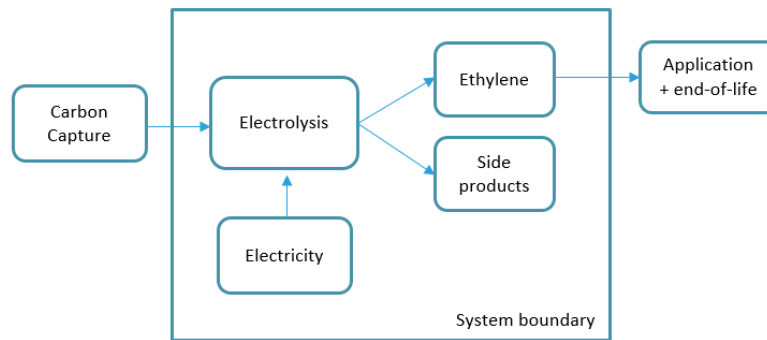


Figure 6: System boundaries ethylene production electrocatalytic

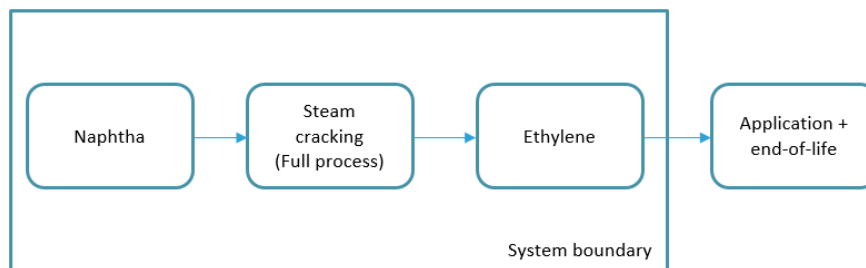


Figure 7: System boundaries ethylene production cracking naphtha

In the base case, the source of electricity has been chosen to be photovoltaic panels at 1kV-60kV in Belgium. Values for mid- and endpoint categories were taken from the EcoInvent database in SimaPro. As side products will be sold, they do not need to be taken into account for the environmental impact in this case. The main environmental impact will stem from the high energy demanded by the process. Individual impacts will be normalized in order to compare them directly to each other as per the normalization factors provided by Sala et al (2017). Below it will be shown in the results that normalizing these environmental impacts makes it possible to identify hotspots and compare the different categories to each other.

In the environmental part of the study, some separate scenarios will be defined as well. If the side products will not get sold, these will have to be treated as waste streams and will thus have an environmental impact as they will need to be disposed of. When these products are produced at high purity and ready to be sold, they can be treated in the same way as the produced ethylene. A second possible assumption to be made is the type of electricity that can be used. On the one hand there is the current Belgian electricity mix, on the other hand a full 100% green electricity source can be found. The four different compositions of these assumptions will be treated as separate scenarios and quantified in the results section below.

3. Results

3.1 Economic

3.1.1 Base case

The base case described earlier yields an NPV of - €188,517,782. This negative value implies that that specific scenario would not be profitable over the course of the next 30 years. When analyzing the operational expenditures (OPEX) opposed to the revenues, it can be noticed that a yearly deficit of €11,343,499 will be incurred. These elevated costs in combination with the high capital expenditures (CAPEX) at €58,095,739 cause for the project to be classed as non-profitable. Digging deeper into what these costs are made up of, it can be seen in Figure 8 that the biggest portion, 73%, of the OPEX are made up of electricity costs. With an electricity cost of €20/kWh in this case and the high amounts of energy needed for the formation of ethylene, this portion will automatically become large. The cost of acquiring CO₂ captured from emissions of other businesses amounts to 8% of the total OPEX of this project.

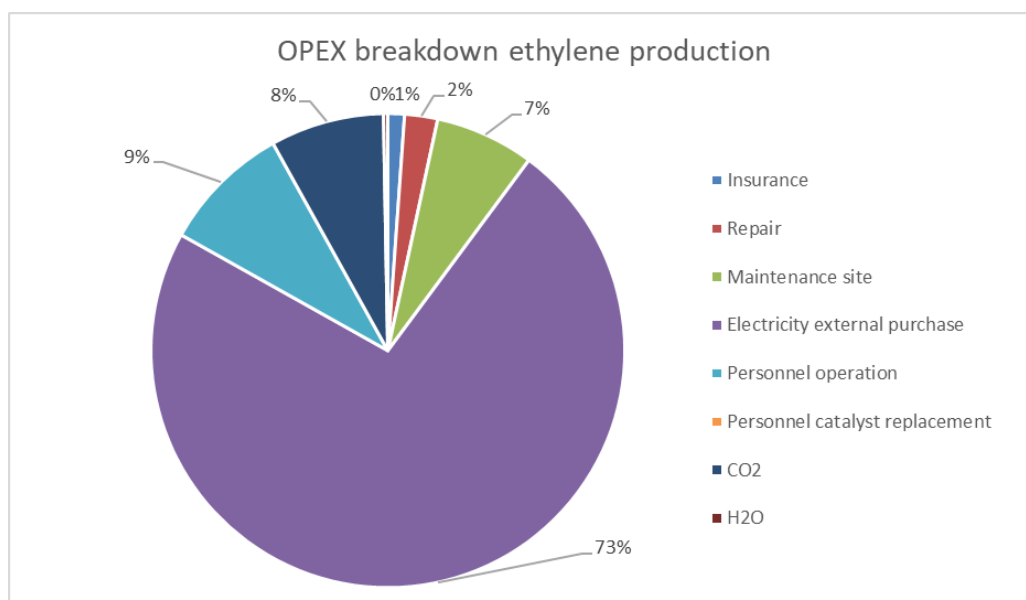


Figure 8: Operational expenditure breakdown base case

When the CAPEX part of the cost analysis is added in order to get the total cost breakdown, it is annualized in order to be able to compare the cost directly to the OPEX. This brings the discounted initial investment to over €16 million. As can be seen in Figure 9, the main costs of this project consist of the investment of the equipment and the electricity costs combined contributing to 39% and 45% of the yearly costs respectively.

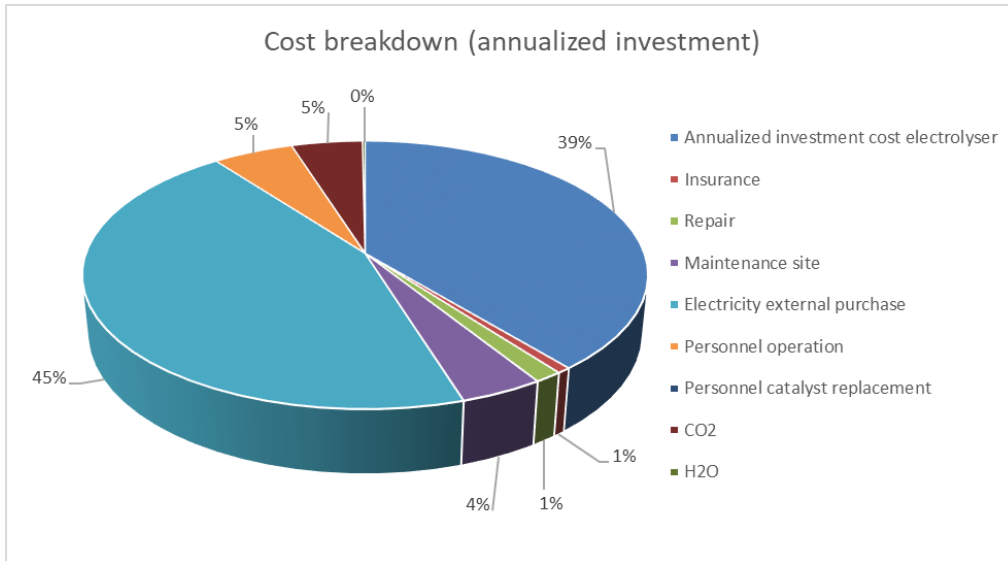


Figure 9: Total yearly cost breakdown

Breaking all these costs down into its CAPEX and OPEX components, provides us with costs per tonne ethylene. At a current market price of ethylene of approximately €1,000 per tonne, this is the total production cost that should be aimed at. However, at a CAPEX per tonne of €490 and OPEX of €2,307 this is still not achieved. Even when applying a price premium of up to 30% to ethylene because of sustainable production, the market value is not achieved (Iles and Martin, 2013). Another detailed view of these cost and revenues broken down is shown in figure 10. There it can be seen that, even when in this case the side products are sold at their respective market values, costs still exceed overall revenues. The benefit of ETS is also marginal and will not contribute enough to turn the production costs into the range that is required. In the section below different suggestions will be made to alter the base case in order to optimize the cost compared to the revenues. Since the NPV is negative and no profit will be made throughout the years, no initial rate of return (IRR) or payback period (PBP) can be reported.

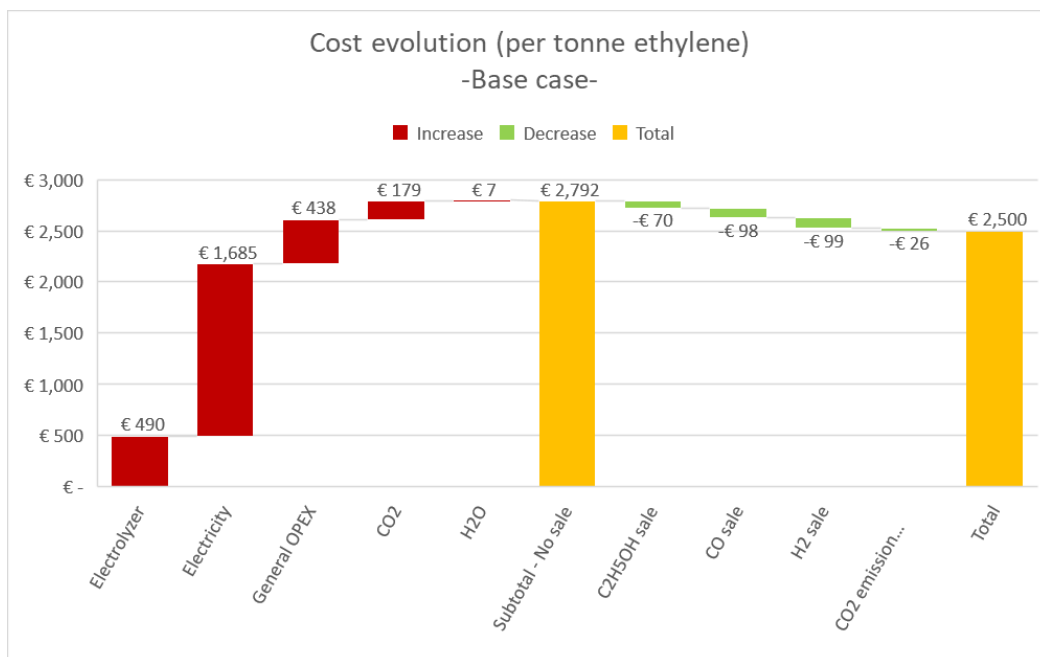


Figure 10: Cost allocation overview

3.1.2 Sensitivity analysis

3.1.2.1 Overall sensitivity

As has been shown above, the base case of producing ethylene electrocatalytically does not seem to be profitable. In 100% of the scenarios, NPV will prove to be negative (figure 11). This assessment has been performed through a Monte Carlo analysis which will also be used to identify the main hotspots on which should be focused when trying to improve the perspectives of the technology. All continuous parameters were varied on a triangular distribution of +/-10%.

First, all possible varying parameters were included to later on start excluding the most significant ones in order to get a clearer view of the underlying variables. An extremely high influence of a specific parameter might dominate other important parameters which would be skipped if this method were not applied. By including all possible scenarios and assumptions to run through each other and taking 1,000 samples, a wide array of possible outcomes was found. The NPV for this project will be between approximately -316.8 million euros and -91.3 million euros. This is a wide range of values with even the most optimistic one resulting in a negative NPV.

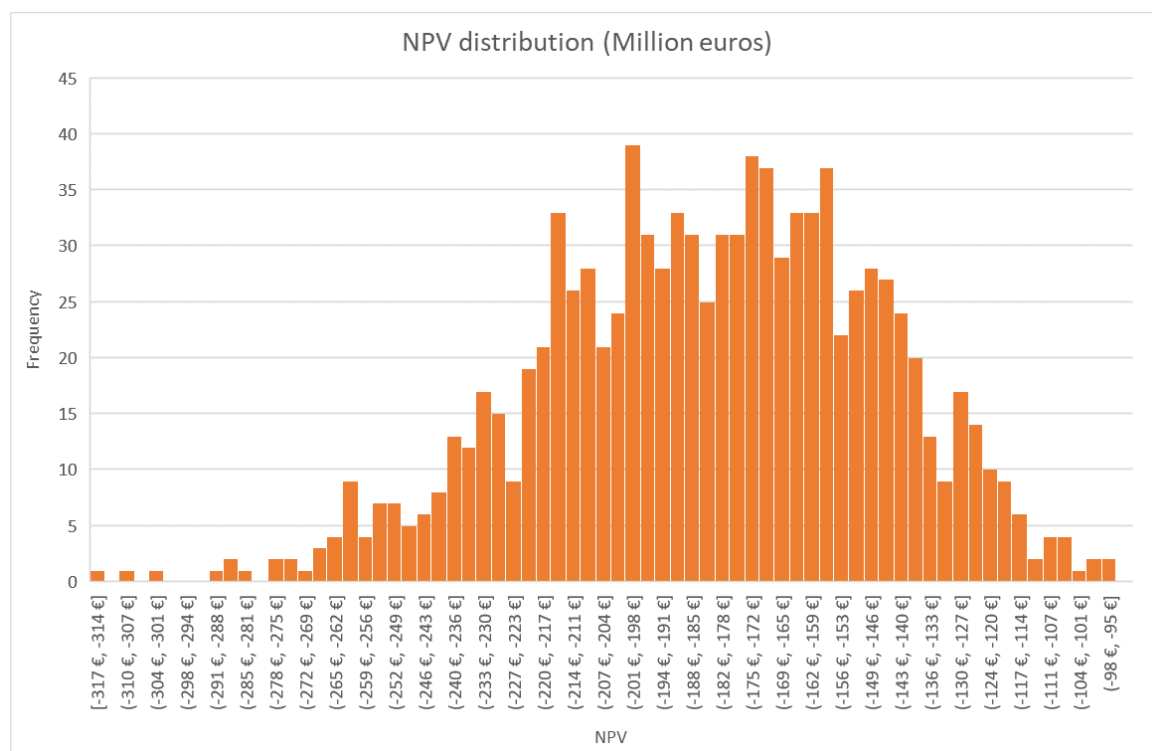


Figure 11: NPV probability distribution

When the variables with the highest influence on this variance are analyzed, it is mainly the electricity price which has a large negative influence of -32.6%. In second place the selectivity proves to be one of the most important factors, contributing to the variance for 32.1%. Of course also the amount of CO₂ used will have an impact. In this case, as costs exceed revenues, it will be a negative relationship between the amount of CO₂ used and the NPV of -12.8%. With almost equal contribution to variance, the applied potential will also have a negative impact as a lower value would approach the theoretical value more. Therefore a negative contribution to variance of -12.6%

can be noticed for the applied potential. 2.6% if variance is explained by the market value of ethylene. A higher value will automatically yield higher revenues and thus a higher NPV. Finally, the initial investment cost of the installation seems to have an inferior role contributing to the variance of NPV. That is mainly because the cost of the investment will be discounted over its lifetime. Only -2.3% of variability in NPV will be explained by the investment cost (figure 12).

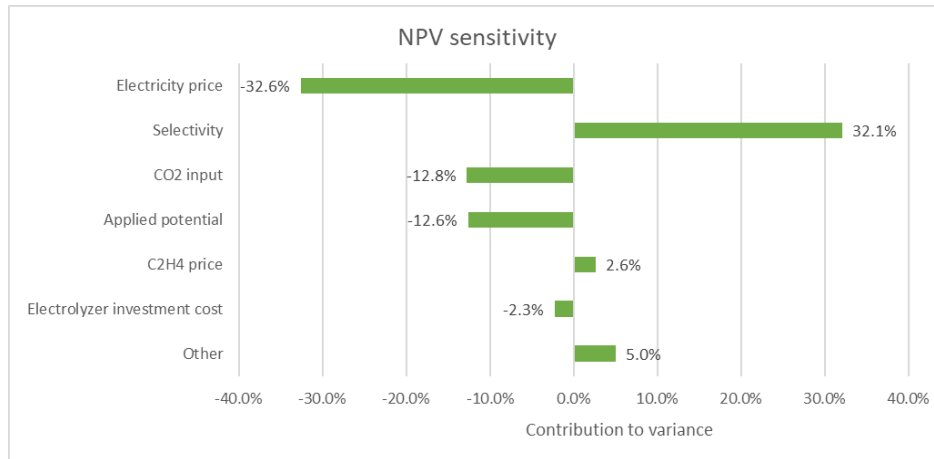


Figure 12: Most important variance contribution parameters

Finally, sensitivity based solely on financial parameters, the top contributor will naturally again be the electricity price, having a negative influence on NPV variance of -82.7% (figure 13). As other parameters' significance is suppressed by this large influence of the electricity price, a sensitivity chart has been created omitting the electricity price.

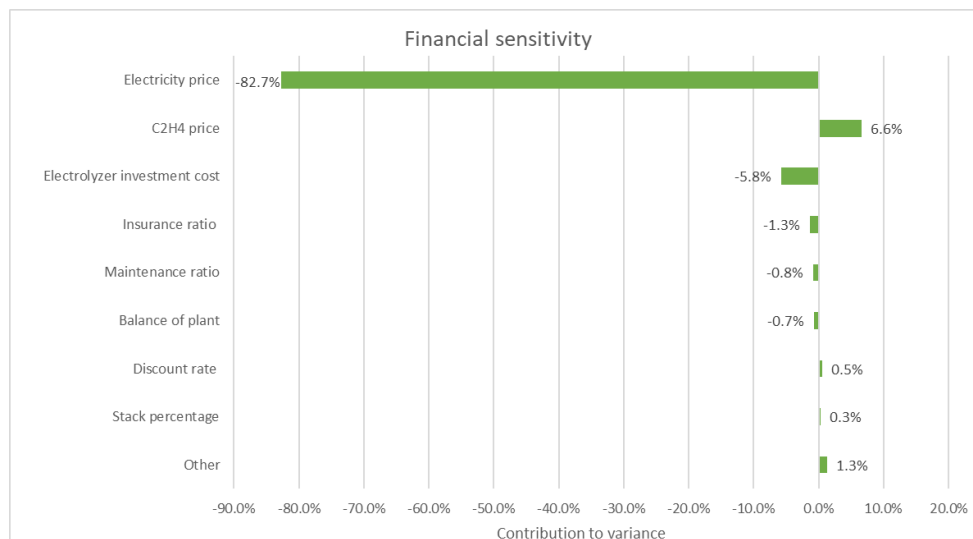


Figure 13: Financial sensitivity: contribution to NPV variance

Now it shows more clearly the influence of underlying parameters. The price of ethylene stands at the top with 38.3% influence on NPV variance, while the elektrolyzer investment cost is not far behind, with an influence of -33.3%. Ratios of the initial investment such as the insurance, maintenance and balance of plant to significantly influence NPV as well, amounting to a contribution to variance of NPV of -7.5%, -4.4% and -3.9% respectively (figure 14).

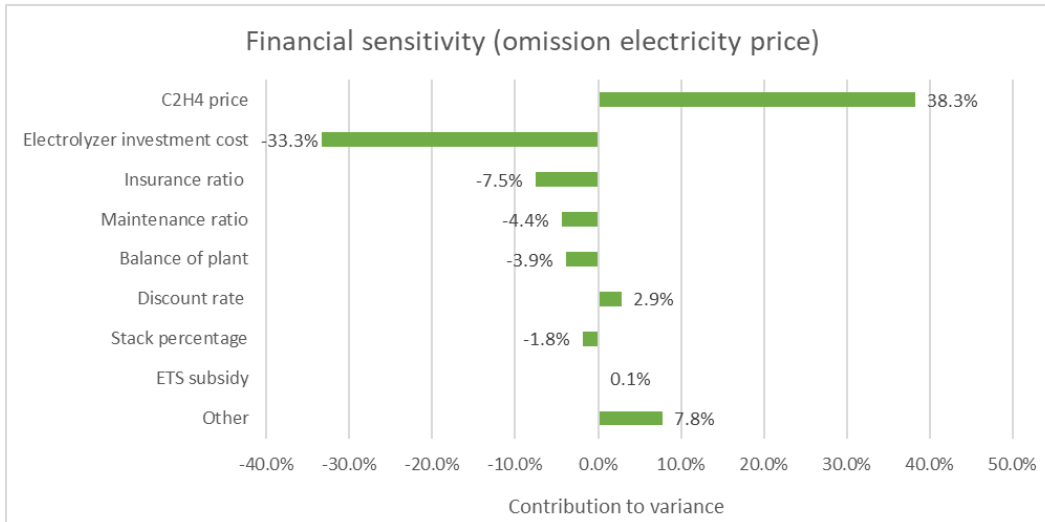


Figure 14: Financial sensitivity: contribution to NPV variance (electricity price omitted)

Discount rate does not seem to have the most significant effect, however this effect is positive because of the negative overall NPV estimation. Another surprising parameter that is of low influence, is the subsidy. Based on the saved amount of carbon dioxide equivalent emissions, the ETS subsidy-like benefit was calculated. It however seems from these analyses that those financial aids do not hold enough weight in order to be significant towards the NPV (figure 11).

Taking the analysis above into account and considering the range of possible NPV's, it can already be concluded that a positive NPV can only be achieved when other factors are taken into account. In the uncertainty scenario analysis, different assumptions will vary uncertain parameters to simulate certain possible NPV's.

3.1.2.2 Local sensitivity

In order to quantify the effects of the most important parameters, a local sensitivity analysis will shed more light on the most significant once that have been identified above. To be more specific, mainly the electricity price, selectivity and potential will be varied.

The most obvious and self-explanatory variable to change throughout the process, is the selectivity towards the target product ethylene. Increasing the FE towards 100% will increase the NPV towards the positive range (Figure 15). It will be however impossible to reach that full selectivity, a more realistic aim would be around 80% (Sapountzi et al., 2017). These higher selectivity levels might prove to be achievable in the future, depending on further technological developments. This also means however that if no other parameter is changed, the cost per tonne will remain higher than the current market value at any level of selectivity (Figure 16).

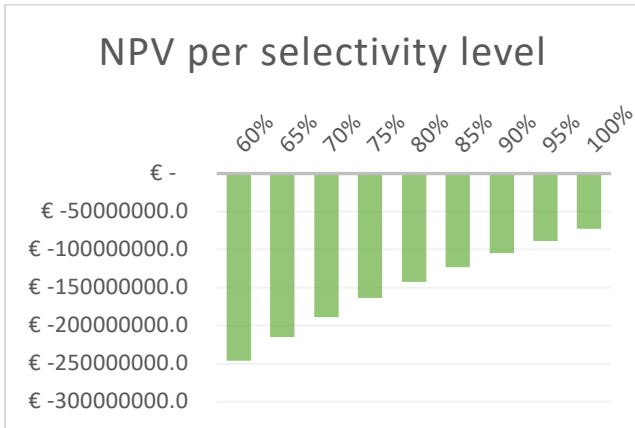


Figure 15: Local sensitivity: effect of selectivity variation on NPV

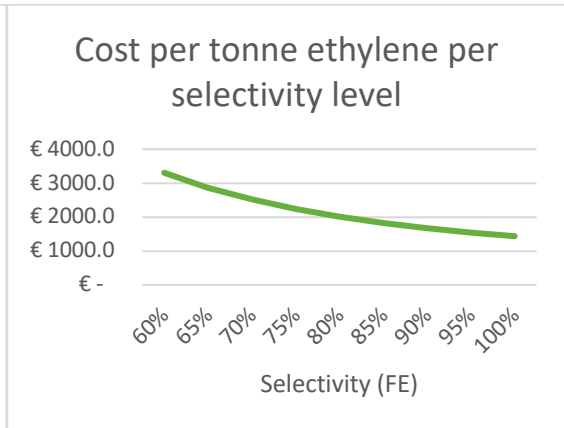


Figure 16: Local sensitivity Effect of selectivity variation on production cost per tonne

If another parameter with high influence is changed next to the selectivity level, more positive ranges can be attained. The two parameters which will be altered next, are the electricity price and applied potential. As was shown before, the electricity price will have high influence on the overall NPV of the project. Taking a look at the evolution of NPV over possible prices, it can be noticed that at a low enough electricity bid and high enough selectivity level, OPEX per tonne will be lower than the market price of ethylene, albeit only marginally (figure 17 and 18). The lowest currently reported energy bid for photovoltaic electricity supply can be found in Saudi Arabia and lies at €10/MWh (Bellini E., 2021). Take with that the annualized investment costs of the electrolyzer and there is almost no point where production costs are lower than the market value. If only the OPEX is aimed towards market value of ethylene, the electricity price should be kept below €20/MWh with selectivity at least 85% in order to break even (figure 17). Taking into account the annualized investment as well, it can be seen that only selectivity of 95% or above combined with an electricity price of €10/MWh or below will yield a break even production of ethylene (figure 18). However, as mentioned earlier, these values will not be realistic to achieve.

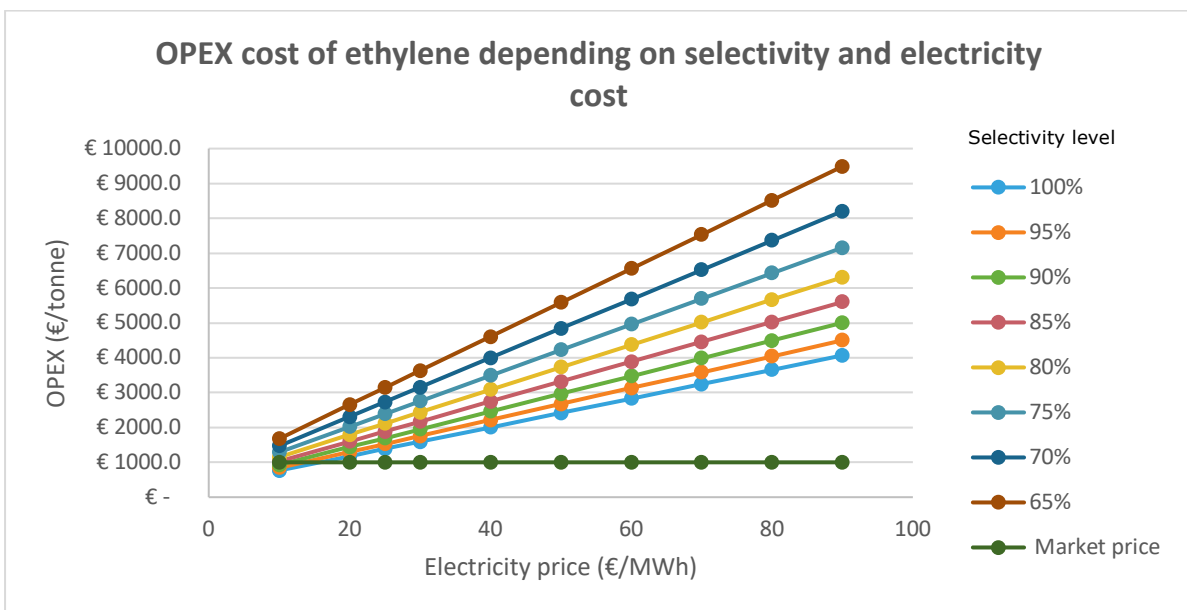


Figure 17: OPEX cost of ethylene per selectivity level to market value of ethylene

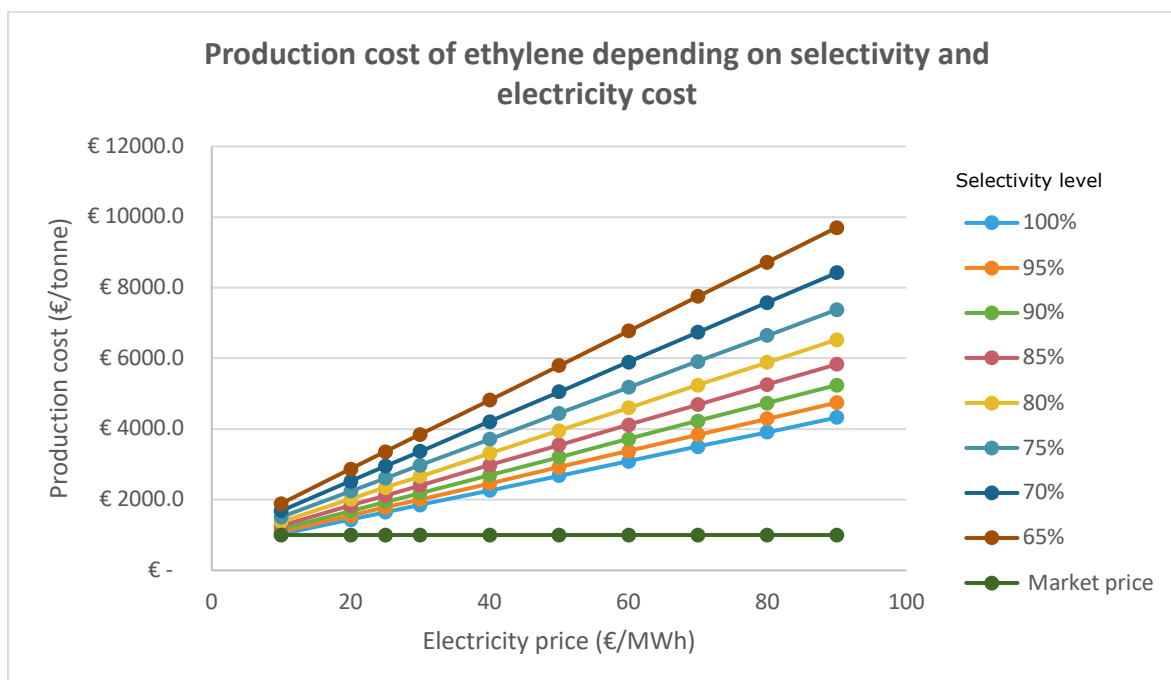


Figure 18: Total production cost of ethylene per selectivity level to market value of ethylene

This implies that either another technical parameter like the applied potential needs to improve or another element needs to be altered in order for the project to become more profitable. First delving deeper in the possibility to improve on the applied potential. With a current overpotential of 0.65V, there is still some room for improvement even though there will always be losses throughout the process, making a perfect theoretic potential of 1.15V not realistic. However, just like with the electricity price variation, a production cost below market value seems to be unachievable and profits are not within reach without other variables changing (table 7). Another possibility is to ask a price premium of up to 30% like described in Iles and Martin (2013). This would increase the production cost margin and make more realistic ranges possible. It would however still mean selectivity needs to increase to almost its maximum attainable value while keeping the electricity price low.

Table 7: Cross sensitivity: impact of selectivity level and potential to cost/tonne of ethylene

		SELECTIVITY LEVEL							
Cost/tonne (€)		100%	95%	90%	85%	80%	75%	70%	65%
POTENTIAL (V)	1.15	1,028	1,097	1,178	1,274	1,390	1,530	1,711	1,926
	1.25	1,092	1,167	1,256	1,362	1,488	1,641	1,838	2,073
	1.5	1,249	1,341	1,450	1,578	1,731	1,916	2,153	2,436
	1.75	1,406	1,514	1,641	1,791	1,971	2,189	2,464	2,795
	2	1,560	1,684	1,830	2,003	2,209	2,459	2,773	3,151

3.1.3 Uncertainty scenario analysis

The above-mentioned assumptions each have an influence on the NPV of the project, contributing to its variance. Figure 19 clearly shows that the possibility of avoiding unnecessary import costs plays an important part in improving the NPV with a contribution to NPV variance of 91.7%. As stated earlier, this would only apply for those companies that already import ethylene or would have to consider importing ethylene. The possible sale of side products will also be a significant factor to consider, meaning the purity of all end products is something to strive for. Learning effects on the other hand will not contribute a significant amount to the NPV variance, with only 0.2% of all the variance declared by uncertainty assumptions stemming from this parameter (figure 19).

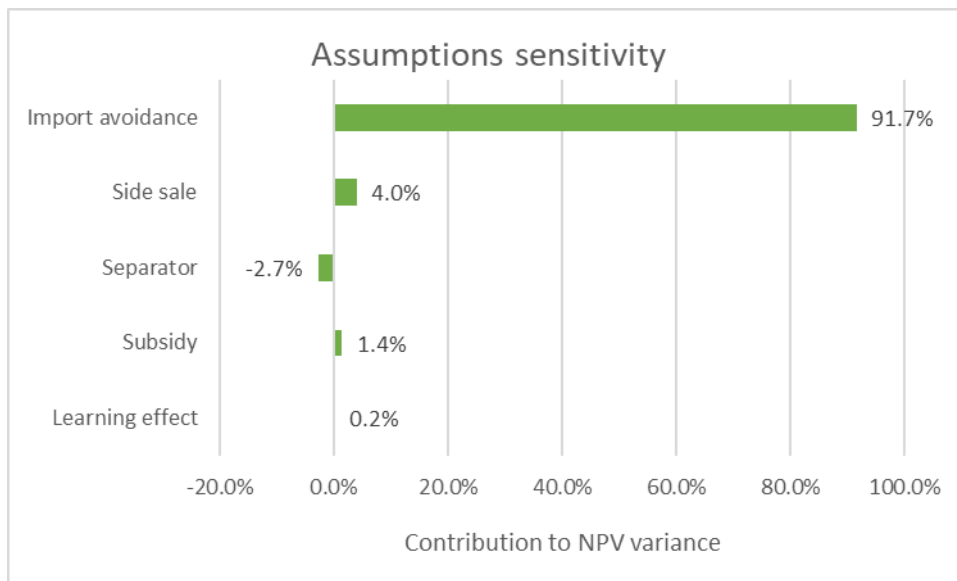


Figure 19: Contribution to variance of uncertainty assumptions

Table 8 gives an overview on different possible scenarios benchmarked to the base case which has been treated before. The first two scenarios prove to be profitable. This requires however for the electricity cost to go as low as €10/MWh and selectivity to reach 85% with the required overpotential limited to only 0.35V. As it stands these values are not achievable, but it is promising to know that with technological improvements, the case might become more feasible.

As mentioned earlier, the import benefit is only applicable to specific situations, which is why it is only included in one scenario. The difference between the two positive cases is significant however, solely due to this import benefit being included in the first scenario, proving the findings from the sensitivity analysis in figure 19.

As also has been shown before, the electricity price plays an important role. If the current market price of the Belgian electricity mix is used like in scenario 4, the NPV greatly decreases (table 8). Indicating that this factor should be a top priority to get into lower ranges in order to make green electricity accessible and cases like this one more viable.

Table 8: Uncertainty scenario results

<i>Variable</i>	<i>Base case</i>	<i>Scenario 1</i>	<i>Scenario 2</i>	<i>Scenario 3</i>	<i>Scenario 4</i>
<i>Import benefit</i>	0	1	0	0	0
<i>Price premium</i>	0%	20%	20%	15%	0%
<i>Side product sale</i>	1	1	1	1	0
<i>Separator unit</i>	0	1	1	1	0
<i>ETS subsidy</i> (€/tonne CO ₂)	25	50	50	25	25
<i>Learning effect</i>	0	20%	20%	10%	0
<i>Electricity price</i> (€/MWh)	20	10	10	25	50
<i>Selectivity</i>	70%	85%	85%	75%	70%
<i>Potential</i>	1.8	1.5	1.5	1.8	2
<i>CAPEX per tonne (€)</i>	490	341	341	548	530
<i>OPEX per tonne (€)</i>	2,309	930	930	2,076	5,323
<i>Total cost/tonne</i> <i>C₂H₄ (€)</i>	2,799	1,271	1,271	2,623	5,853
<i>NPV (€)</i>	-188,517,782	167,125,201	4,196,317	-184,768,853	-584,422,714

3.2 Environmental

3.2.1 Base case

3.2.1.1 Midpoint categories

The technical framework with the mass and energy balance has already been linked to the economic parameters in the TEA part, but now it will get linked to the environmental impacts. The base case which has been described above will be compared to the traditional ethylene production method (i.e. cracking of naphtha). Values for the traditional production were taken from the EcoInvent database in SimaPro as the market relevant ethylene produced from naphtha, which considered the entire production process. As can be seen in table 9, there are certain midpoint categories where the new electrolysis technology is superior, but there are also some where this is not the case. In terms of global warming potential (GWP), it seems to be confirmed that producing ethylene through electrolysis emits less carbon dioxide, at least when using green electricity like in the considered base case. The value of 472kg CO₂ per tonne is in range of the expected values as provided by Khoo et al (2020). In that case however, it was not specified green energy would be used, which could explain the better value in this study. This GWP difference between electrocatalysis and the cracking of naphtha means that the ETS can be used as a benefit in a similar way as a subsidy (Ellerman et al., 2010). With current ETS valuation at approximately €25/tonne, this would make for approximately a one on one ratio compared to the ethylene production, with 1,040kg of CO₂ equivalents saved per tonne ethylene compared to the traditional technology (Business insider, 2021). This would elevate the subsidy to €289,602 per year.

As expected, the fossil fuel potential (FFP) will yield a value in favor of the electrolysis, as no fossil fuels are being used during the process. It is remarkable that both the marine ecotoxicity potential (METP) and freshwater ecotoxicity potential (FETP) are positive in the direction of electrolysis, while the terrestrial ecotoxicity potential (TETP) is the most negatively reported value across all the impact categories. This can be attributed to the use of a photovoltaic installation (Milousi et al., 2019). Finally, the water consumption potential (WCP) value is also noticeably higher with the electrolysis case compared to the traditional cracking process. This can be attributed to the fact that water will be used as one of the main input streams in the electrolyzer.

Table 9: Environmental impact of electrocatalytic vs cracking production of ethylene

Parameter ¹	Unit	Base electrolysis	Traditional cracking	Delta
GWP	kg CO ₂ eq	4.72E+02	1.51E+03	-1.04E+03
ODP	kg CFC11 eq	2.43E-04	2.58E-06	2.40E-04
IRP	kBq Co-60 eq	-3.50E+02	1.29E-01	-3.50E+02
HOFPP	kg NO _x eq	3.94E+00	2.67E+00	1.27E+00
PMFP	kg PM2.5 eq	3.30E+00	1.01E+00	2.29E+00
EOFP	kg NO _x eq	4.35E+00	2.91E+00	1.44E+00
TAP	kg SO ₂ eq	3.82E+00	3.07E+00	7.50E-01
FEP	kg P eq	-1.19E+00	1.07E-02	-1.20E+00
MEP	kg N eq	-1.82E-01	1.65E-03	-1.84E-01
TETP	kg 1,4-DCB	8.76E+04	1.01E+01	8.76E+04
FETP	kg 1,4-DCB	-2.57E+02	2.76E+00	-2.60E+02
METP	kg 1,4-DCB	-2.91E+02	3.74E+00	-2.95E+02
HTPC	kg 1,4-DCB	-1.07E+02	1.64E+01	-1.23E+02
HTPnc	kg 1,4-DCB	-2.42E+03	5.89E+01	-2.48E+03
LOP	m ² a crop eq	-3.14E+02	7.14E-01	-3.15E+02
SOP	kg Cu eq	7.64E+01	9.20E-02	7.63E+01
FFP	kg oil eq	4.03E+02	1.43E+03	-1.03E+03
WCP	m ³	2.48E+04	1.16E+01	2.48E+04

¹GWP=Global warming potential; ODP=Ozone depletion potential; IRP=Ionizing radiation potential; HOFPP=Photochemical oxidant formation potential for humans; PMFP=Particulate matter formation potential; EOFP=Photochemical oxidant formation potential for ecosystems; TAP=Terrestrial acidification potential; FEP=Freshwater eutrophication potential; MEP=Marine eutrophication potential; TETP=Terrestrial ecotoxicity potential; FETP=Freshwater ecotoxicity potential; METP=Marine ecotoxicity potential; HTPC=Human toxicity potential cancer; HTPnc =Human toxicity potential non-cancer; LOP=Agricultural land occupation potential; SOP=Surplus ore potential; FFP=Fossil fuel potential; WCP=Water consumption potential.

If hotspots of environmental impact want to be identified, it is necessary to normalize these values so they can be compared directly as per normalization factors (Sala et al., 2017). Figure 20 represents all 18 midpoint categories, but with all the values normalized so they can be compared without worrying about the different units. In this image, once again, the TETP, FETP, METP and WCP values jump out above the others, making it impossible to draw conclusions about the other categories. When these outliers are omitted and the normalized naphtha cracking case is included as well, we can conclude that GWP does not contribute the most to the environmental impact in the case of electrolysis. Also, due to using emitted CO₂ (captured either via DAC or point source), both the ionizing radiation potential (IRP) and freshwater eutrophication potential (FEP) contributions will be negative, indicating an optimistic environmental effect for both these cases. Like mentioned above, the fossil fuel potential of the naphtha cracking process will be the main contributor to the environmental impact in that scenario (figure 21).

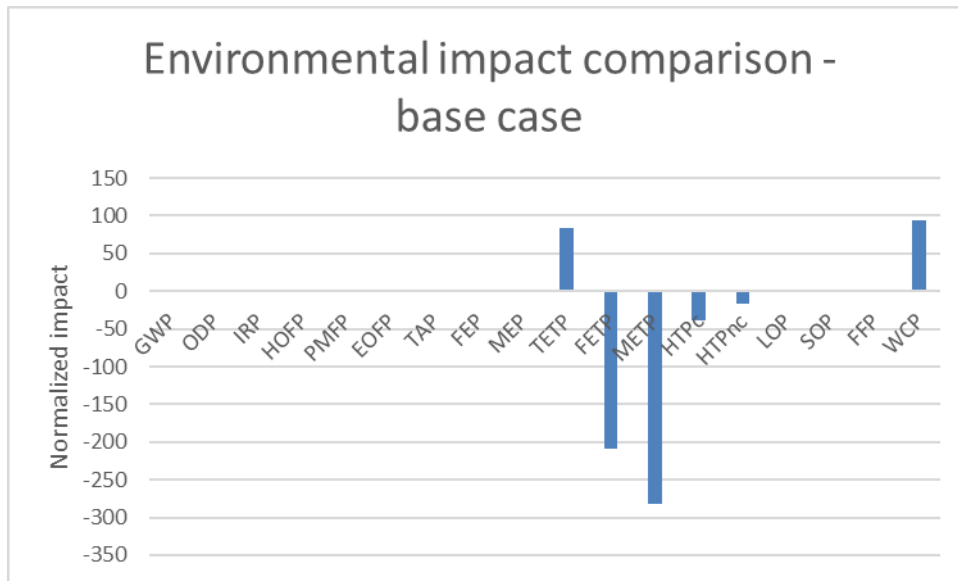


Figure 20: Normalized environmental impacts per midpoint category

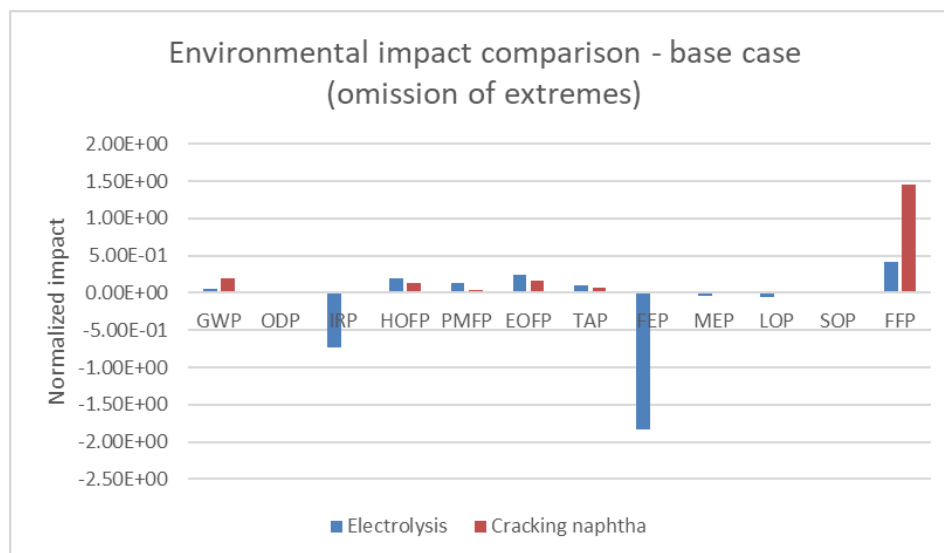


Figure 21: Comparison most significant midpoint categories: electrolysis vs cracking

3.2.1.2 Endpoint categories

After analyzing those midpoint categories, damage pathways can be investigated per impact category in order to aggregate these 18 values to 3 more general values. In figure 1 earlier, it could be seen how every midpoint category contributes to the specific endpoint category. The first endpoint category, damage to human health, is described in terms of DALY (disability-adjusted life years). The damage to ecosystems category will be described by the species loss per year and the final category, damage to resource availability, will be expressed by the resource availability (RA) (Huijbregts et al., 2016).

The aggregation of all these midpoints into their respective damage provides us with an overview, allowing for hotspot identification and comparison to the traditional production method. First, assessing the endpoint category "Damage to human health", it can be concluded that depending on the damage pathway, different technologies will come out on top (figure 22 and 23). Because of the

large water consumption in the electrolysis installation, the distribution is skewed, therefore, in order to make a better estimation, it has been left out for figure 23. A positive environmental effect (negative value) can be noticed on both human health toxicity levels. On the other hand, particulate matter formation will be a big contributor to the human health category. The main contributor to this high value is the extremely high energy demand as mentioned earlier. The global warming potential effect on human health is noticeably lower for the electrolysis case (figure 23).

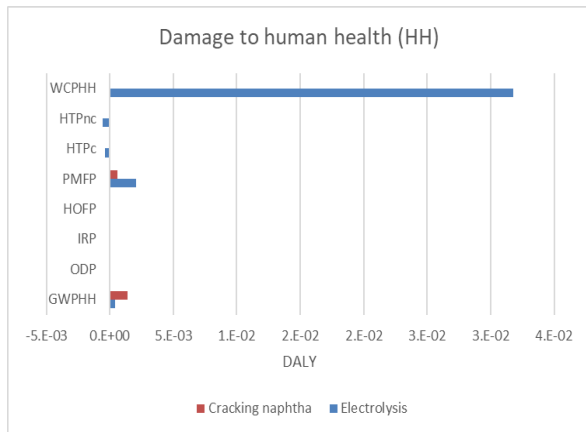


Figure 22: Ethylene production: Human Health

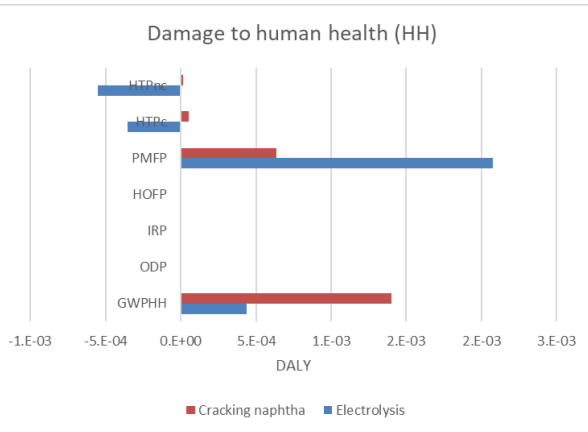


Figure 23: Ethylene production, omission WCP Human Health

The second endpoint category to consider, is "Damage to ecosystems". Here the water consumption of the electrolysis installation will play an important role as well, leading to high assumed damage to the ecosystem (Figure 24). Based on figure 25, it can be distinguished that the land occupation potential will be much better in the electrolysis case because of the use of captured CO₂. Terrestrial ecotoxicity on the other hand proves to be more damaging opposed to the traditional cracking of naphtha. Finally, the global warming potential will also be lower compared to cracking of naphtha in this endpoint category, just like in the human health category (figure 25).

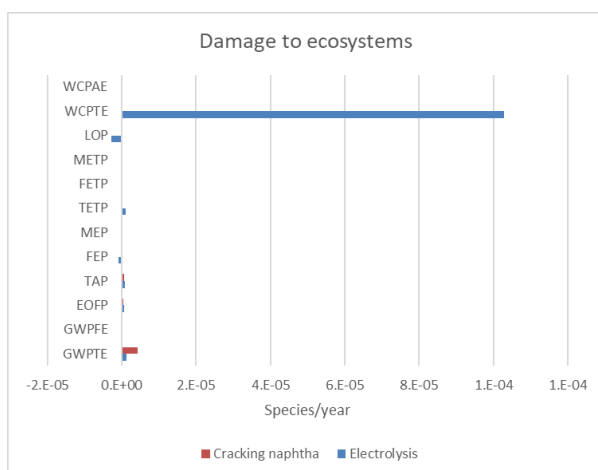


Figure 24: Ethylene production: Ecosystem damage

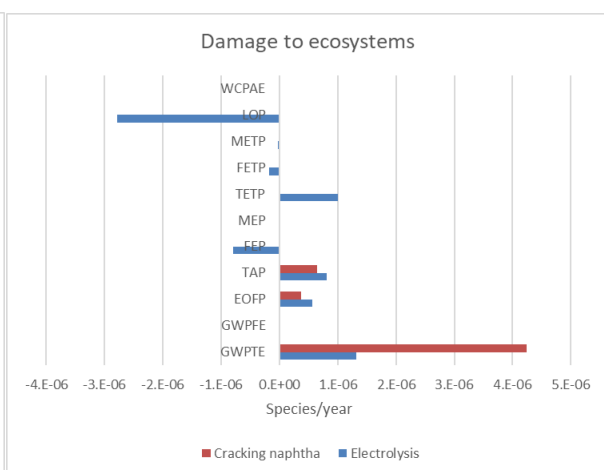


Figure 25: Ethylene production, omission WCP Ecosystem damage

Finally, the third endpoint category, which only consists of two damage pathways, focuses on the fossil resources. This means that, as little to no fossil resources are needed, the electrolysis case will prove to score better (figure 26). In both cases though, it will be the fossil fuel potential (FFP) outscoring the surplus ore potential (SOP) (figure 27).

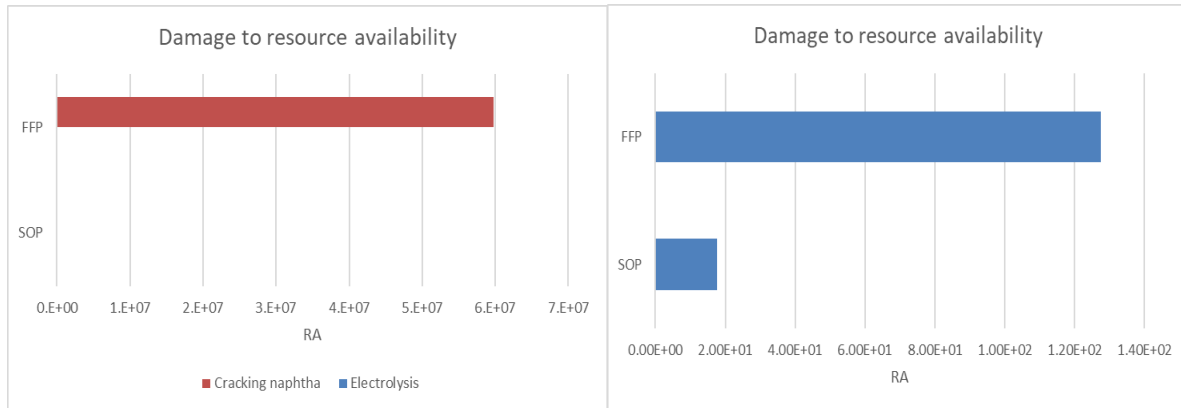


Figure 26: Ethylene production: Resource availability electrolysis vs cracking

Figure 27: Ethylene production: Resource availability

Combining all damage pathways into their respective endpoint category, these different categories can be compared to each other (figure 28). Here it can be seen that only in the resource availability department, electrolysis will score better. It should however be mentioned that the main contributors to this unexpected relationship is due to the large amount of electricity needed and the H₂O that is used as an input stream, making for a lot of water to be used across the process.

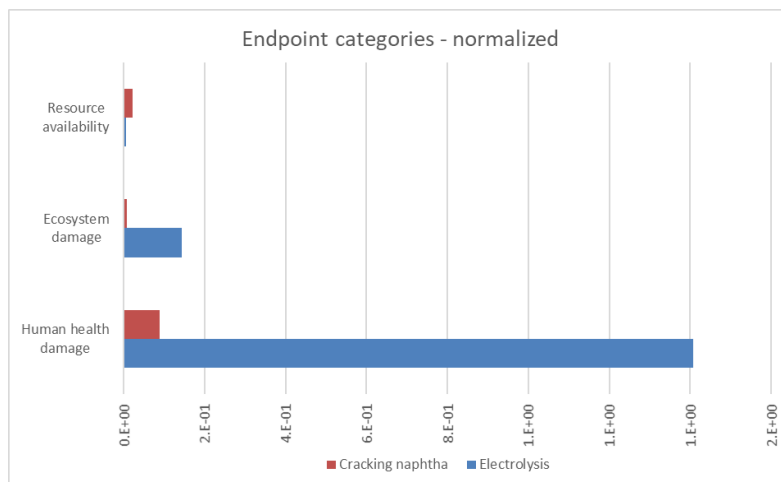


Figure 28: Environmental impact ethylene: endpoints

3.2.1.3 Single score

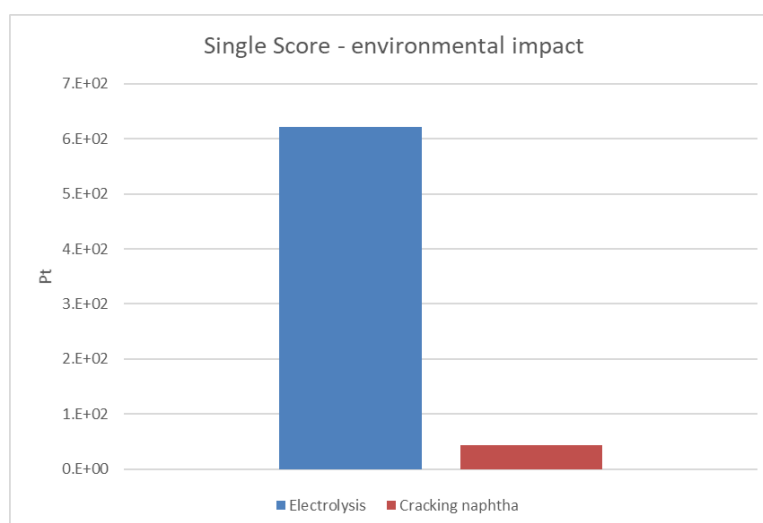


Figure 29: Environmental impact electrolysis vs cracking: single score

Performing another aggregation step, the trends which started becoming clear in the earlier sections, electrolysis gets a higher final score and is therefore seen as performing environmentally less optimal compared to the traditional cracking of naphtha (figure 29). It should however be noted that in this base case, tap water was used as an input stream and that the single score representation does not provide the full scope of both processes.

3.2.2 Scenario analysis

Four different scenarios have been identified for the electrocatalytic production of ethylene which can be put against the traditional production method by cracking naphtha (table 10). The first scenario is the case where a photovoltaic source of electricity is used throughout the process and where the side products that get formed will not be sold afterwards. In this case those side products will be looked at as waste and allocated based on mass (Zimmerman et al., 2018). The second scenario will change from solar energy to the traditional electricity mix in Belgium, keeping side product management the same as scenario 1. In the other two scenarios, the side product management will change toward not seeing them as a waste stream and thus not taking them into account when calculating the environmental impact of these scenarios. The electricity source of scenarios 3 and 4 will remain the same as in scenario 1 and 2 respectively.

Table 10: Environmental impact: Midpoint parameters per scenario versus traditional cracking case

Parameter	Unit	Scenario 1	Scenario 2	Scenario 3 =base case	Scenario 4	Traditional
GWP	kg CO ₂ eq	9.82E+02	2.47E+04	4.72E+02	2.42E+04	1.51E+03
ODP	kg CFC11 eq	2.65E-03	9.39E-03	2.43E-04	6.98E-03	2.58E-06
IRP	kBq Co-60 eq	-2.56E+02	5.22E+04	-3.50E+02	5.21E+04	1.29E-01
HOFP	kg NO _x eq	5.55E+00	4.62E+01	3.94E+00	4.46E+01	2.67E+00
PMFP	kg PM2.5 eq	4.52E+00	2.47E+01	3.30E+00	2.35E+01	1.01E+00
EOFP	kg NO _x eq	6.02E+00	4.69E+01	4.35E+00	4.52E+01	2.91E+00
TAP	kg SO ₂ eq	7.35E+00	6.84E+01	3.82E+00	6.49E+01	3.07E+00
FEP	kg P eq	-9.40E-01	7.93E+00	-1.19E+00	7.67E+00	1.07E-02

<i>MEP</i>	kg N eq	2.22E-01	8.50E-01	-1.82E-01	4.46E-01	1.65E-03
<i>TETP</i>	kg 1,4-DCB	9.00E+04	-6.20E+03	8.76E+04	-8.69E+03	1.01E+01
<i>FETP</i>	kg 1,4-DCB	-2.33E+02	6.70E+01	-2.57E+02	4.35E+01	2.76E+00
<i>METP</i>	kg 1,4-DCB	-2.51E+02	1.69E+02	-2.91E+02	1.29E+02	3.74E+00
<i>HTPc</i>	kg 1,4-DCB	-8.69E+01	5.89E+02	-1.07E+02	5.69E+02	1.64E+01
<i>HTPnc</i>	kg 1,4-DCB	-1.60E+03	1.32E+04	-2.42E+03	1.24E+04	5.89E+01
<i>LOP</i>	m2a crop eq	1.10E+04	1.10E+04	-3.14E+02	-3.15E+02	7.14E-01
<i>SOP</i>	kg Cu eq	7.89E+01	3.21E+01	7.64E+01	2.95E+01	9.20E-02
<i>FFP</i>	kg oil eq	1.44E+03	8.15E+03	4.03E+02	7.11E+03	1.43E+03
<i>WCP</i>	m ³	2.49E+04	3.18E+04	2.48E+04	3.18E+04	1.16E+01

¹GWP=Global warming potential; ODP=Ozone depletion potential; IRP=Ionizing radiation potential; HOPF=Photochemical oxidant formation potential for humans; PMFP=Particulate matter formation potential; EOPF=Photochemical oxidant formation potential for ecosystems; TAP=Terrestrial acidification potential; FEP=Freshwater eutrophication potential; MEP=Marine eutrophication potential; TETP=Terrestrial ecotoxicity potential; FETP=Freshwater ecotoxicity potential; METP=Marine ecotoxicity potential; HTPC=Human toxicity potential cancer; HTPnc =Human toxicity potential non-cancer; LOP=Agricultural land occupation potential; SOP=Surplus ore potential; FFP=Fossil fuel potential; WCP=Water consumption potential.

Main key findings from these scenarios are that only when a renewable energy source such as solar energy is used a lower global warming potential will be achieved. Something that should be noted as well, is that by using the traditional electricity mix, even higher water consumption is found, making the process environmentally less interesting, as the water consumption in the base case (scenario 3) was already significantly elevated compared to the cracking of naphtha. The benefits acquired in the human health toxicity potential aspects by using a photovoltaic energy supply system will get lost when electricity is acquired from the known Belgian grid (table 10). Terrestrial ecotoxicity potential (TETP) is one of the only dimensions where the use of the traditional electricity mix seems significantly more optimal compared to photovoltaics. A possible reason for this difference lies with the use of specific materials in photovoltaic cells (crystalline) as well as the energy required for the cells to be produced as well.

The viewpoint shift of taking the side products as a waste stream is less optimal in every scenario, but will remain better in the global warming category compared to the cracking of naphtha. To conclude, even if no sale of the side products is possible, the CO₂ emissions will still remain lower. This means however that the potential benefits from ETS will be lower. This in combination with missed revenues by not selling the side products, the NPV will be noticeably lower as well.

4. Discussion

Since it seems like the NPV will be almost impossible to become positive considering the current assumptions and technological status, other possible approaches can be looked at. Results in both the economic and environmental dimension are in line with previous studies which reported a total production cost per tonne of about €3,000 and CO₂ emissions of around 600kg to 3 tonnes CO_{2e} per tonne ethylene (Savaete T., 2016; Khoo et al., 2020). The study of Khoo et al (2020) did include a the environmental impact of capturing CO₂, which explains the slightly higher value.

Of course the investment costs will drop as research will be continued and learning effects will be playing a key role in future installations (Mayyas et al., 2019; Schoots et al., 2008). The amount of electricity that is needed can however not be altered as it is dependent on the Gibbs free energy of a specific element. Therefore, further developments in green electricity and more specifically photovoltaics will allow for this case to become more viable. Belgium is not the ideal region for PV electricity production because of the limited peak sunlight hours. A more realistic region for producing large quantities of PV would be around the equator, in regions such as Spain or the Middle east (Bellini E., 2021; HotSpotEnergy, 2011).

Results from this study are in line with each other for the large part. With a negative NPV and overall no better environmental impact compared to the traditional process when looking at the single score indicator, one would expect the idea to be scrapped immediately. However, when breaking down the environmental impact, it is found that the electrocatalysis indeed emits less carbon dioxide compared to the traditional cracking of naphtha when green electricity (PV) is used to power the process. This means that it is not CCU that should be looked at critically, because it causes a net benefit in CO₂ emissions. The main step to look at, is the electrocatalysis itself and how that can be improved, both on the economic level as well as the environmental level.

Another aspect that can be questioned, is the application and goal of this installation. With electrolysis equipment for conversion towards H₂ already further in development and H₂ holding a higher value compared to ethylene. It might be profitable to shift the focus of production to either H₂ or another product with lower energy requirements and tailor the catalysts in order to still get ethylene as a side product (Alper and Orhan, 2017). The quantities of ethylene produced will be lower, but if smaller players can be found that need the product, it might be more profitable than focusing on the big markets. This is a temporary solution until technological progress enables larger scale ethylene production through electrocatalysis. Possible smaller players that might need ethylene are fruit and vegetable farmers who can use ethylene in small quantities to enhance the ripening of their products (Vanoirbeek L., 2015; Proefstation voor groententeelt, 2017). This approach implies that side products will be of high enough quality to be sold and that the separator installation will inevitably be needed.

The capture of CO₂ was not included, a follow up study could integrate the different possibilities of capturing the carbon dioxide in order for it to be used as input for industrial processes like the one discussed in this study. Main points of interest from that additional research will be the cost of collecting CO₂ and the environmental impact of doing so. The source of energy that is being used and the quantities required would also need to be taken into account and added to the already large quantities for the electrolysis. It should however also be investigated whether these necessary quantities of sustainable energy can be provided. It is essential for a sufficient grid to be developed to sustain the large energy demands of this process with green energy (Bogdanov et al., 2021). In the results above however, the total environmental impact of PV energy provision has been included. However, if only the PV use were considered, only 10% of the total value would have to be considered, proving PV is clearly the more sustainable option and the source to aim for instead of the traditional electricity mix (Reich et al, 2007).

Also not taken into account are the other side products that will get formed. Since no sufficient data was found on what these products were, the total environmental impact might differ slightly. An actual in depth experiment will make it possible to specify these products further and report more detailed numbers for both the economic and environmental dimensions.

The assumptions that have been made, such as the price premium need to be checked through a market research in order to determine the actual willingness to pay (WTP) over market value for these more sustainable products. Learning effects have currently been solely based on literature, but could be analyzed specifically for electrocatalysis for future research. The practical application of the ETS benefit is something that can be investigated in more detail as well, since the current assumption only takes into account the current ETS trading value.

In order to achieve a full 'Techno Sustainability Assessment' (TSA), the social dimension will have to be added as well. It would be a nice additional research to utilize the framework proposed by Rafiaani et al (2019) in order to incorporate that social dimension into the assessment of CCU based technologies such as electrocatalysis.

5. Conclusion

It has been proven that at the current state of technology, the electrocatalysis of CO₂ towards C₂H₄ is not yet viable. The economic dimension reports a negative NPV for every realistic scenario in which selectivity, applied potential and electricity price are the main contributors to the variance. A base case of -188 million euros was found with a selectivity towards ethylene of 70%, 0.65V overpotential and an electricity price of € 20/MWh. The most significant OPEX is the electricity cost, as 84 MWh is needed per tonne of ethylene. Depending on the assumptions chosen in uncertain scenarios, more positive values could be found however. It was proven that the most benefit for this technology can be found for businesses that currently have to import ethylene as they could save on those import costs, causing the NPV to increase into positive values up to 167 million euros.

The environmental dimension proves difficult to make a unanimous statement. CO₂ emissions are down by just over 1 tonne of CO_{2e} per tonne of ethylene when green electricity is used. Due to the large quantity of electricity needed however, the current Belgian electricity mix would cause even more CO_{2e} to be emitted compared to the traditional process of cracking naphtha. Considering the single score environmental impact, the electrocatalytic process seems to perform worse than the traditional process. This can be mainly attributed to the large quantities of water needed in the process, causing the WCP value to be 24,800m³ higher compared to cracking naphtha. Depending on the focus of the environmental impact of both processes, it can be stated that electrocatalytic conversion is definitely more sustainable when it comes to CO₂ emissions when sustainable sources of energy are used. As no toxic substances are emitted like in the case of cracking naphtha, human toxicity, both cancerous and non-cancerous, in the electrocatalytic conversion case has a more sustainable score by 123 and 2480 kg 1,4-DCB respectively. Resource availability also seems to be more problematic in the case of cracking naphtha, as natural gas is used in that case. Combining the economic and environmental aspects, an ETS benefit can be acquired when lower carbon emissions are achieved. These are valued at approximately €25 per tonne CO₂.

Future developments on both the technological dimension of the elektrolyzer as well as the capture of CO₂ as well as on sustainable energy will enable this case to become more relevant and profitable. It is however not clear when these levels will be achieved, this will depend on learning effects specific for those technologies. Starting production in companies currently importing ethylene or solely producing ethylene as a side product in order to develop the technology further in the meantime seem like the most realistic approaches.

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Appendix 1: Mass and energy formulas

Table A1: General formulas mass and energy balance

PARAMETER	FORMULA
Current (A)	$(\text{CO}_2 \text{ input (mol/sec)} * \# \text{ Electrons} * \text{Faraday constant (C/mol)}) / \text{Selectivity ratio}$
Theoretical potential (V)	$\text{Gibbs free energy (J)} / (\text{Faraday constant (C/mol)} * \# \text{ electrons})$
Electrode area (m ²)	$\text{Current (A)} / \text{Current density (A/m}^2\text{)}$
Minimum power (W)	$\text{Current (A)} * \text{Theoretical potential (V)}$
Actual power (W)	$\text{Current (A)} * \text{Applied potential (V)}$
Electricity (MWh/y)	$\text{Actual power (MW)} * \text{Operating hours (h/y)}$
Number of cells (#)	$\text{Electrode area (m}^2\text{)} / \text{Cell area (m}^2\text{)}$
Catalyst loading (kg)	$\text{Electrode area (m}^2\text{)} * \text{Catalyst use (kg/m}^2\text{)}$
Land use (ha)	$\text{Number of cells (\#)} * \text{cell land use (m}^2\text{)}$