Electrochemical reduction of CO_2 (CO_2E) to minimise environmental impact

With a focus on CO_2-eq emissions

Thesis Msc. Sustainable Energy Technology

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Style:	TU Delft Report Style, with modifications by Bing Thio

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Preface

This work presents the outline of my master's thesis project at the University of Technology in Delft. This thesis is the final step in completing my MSc. Sustainable Energy Technology curriculum. However, I could not have conducted the research in this project without the guidance and knowledge from various people. This section aims to acknowledge and thank these people.

First of all, I would like to express my gratitude towards Thijmen Wiltink for his daily supervision. The countless hours spent reviewing and feedback have added significant value to my work. Your persistence regarding the modelling in GAMS has helped me in making the steps I've been able to take. Apart from the hours spent on the content and research of the thesis, we really got along and that is very much appreciated. I wish you all the best in the further progress of your PhD and I am looking forward to the publication of your next and future paper(s).

Second of all I would like to thank Mar Pérez-Fortes for her guidance as supervisor of my thesis project. From the first meeting we had in June 2023, I was hooked on the field of research you are conducting and was sure I'd like to contribute to this. Your knowledge, organisational skills and feedback pushed my thesis to the end product it is now. A big and warm thank you for all your feedback and guidance.

Third of all, I would like to thank Wiebren de Jong as my second supervisor and for participating in my thesis committee. With a clear and fresh perspective, you were able to really broaden the horizon of the research conducted, for which I'm really grateful.

Furthermore I would like to thank Özlem Mahmutoğulları and everybody from the Energy Systems & Services group at the Faculty of Technology, Policy & Management. The group meetings were always interesting and had a sparkling academic debate. It was always interesting to see how all individual research projects connected to the bigger picture and made a coherent and common goal in science. From the Secret Santa Claus lunch to the NWO-NERA symposium in Utrecht, I always felt welcome.

B.L.P. Thio
Delft, June 2024

Summary

Carbon dioxide (CO_2) is a greenhouse gas (GHG) that causes an increase in the surface temperature of our planet. Due to human activities, the concentration of this GHG has increased over the past centuries. To limit the impact of this temperature rise, carbon capture is a high-potential solution. To capture CO_2 from carbon-intensive processes, release into the atmosphere can be prevented. After capture, two different routes are possible: storage or utilisation. The supply chain infrastructure wherein CO_2 is captured and stored is referred to as carbon capture and storage (CCS). The chemical conversion of CO_2 is referred to as carbon capture and utilisation (CCU) since the CO_2 is converted into a valuable feedstock. The electrochemical reduction of CO_2 (CO_2E) is a pathway wherein carbon dioxide is electrochemically reduced in combination with water and electricity into chemical compounds that can act as feedstock for the chemical industry. One of the chemical compounds of interest is synthesis gas (syngas). This gas is a mixture of CO and H_2. Syngas can act as a base component for many different applications. Syngas derivatives can range from methanol to aviation fuels or other hydrocarbons.

CO_2 is the necessary feedstock for the electrochemical production of syngas, it is estimated that the Benelux emits around 18.3 Megatonne of CO_2 from biogenic sources every year [121]. Biogenic CO_2 sources are CO_2 emission streams based on biomass processing. The CO_2 emissions caused by the processing of biomass will even in a circular economy exist based on European legislation. Life Cycle Assessment (LCA) studies focus on quantifying the environmental footprint of products, processes and services. The goal of this thesis is to understand how the conceptual supply chain infrastructure for biogenic CO_2 sources in the Benelux can be configured in the near-term future to minimise the environmental impact. To answer this question the studied supply chain infrastructure of a CO_2E system consists of 4 main components. The carbon is *(i)* captured, *(ii)* transported and at an *(iii)* electrolyser plant converted into syngas, from this plant the product is *(iv)* transported to the syngas demand site which in this case are chemical companies. Each of these components within the supply chain has an environmental footprint. These environmental impacts can come in many forms. This thesis will give a first insight into the environmental impact of the carbon footprint of the CO_2E supply chain infrastructure considered within the Benelux.

To answer this question, a Mixed-Integer Linear Problem (MILP) was formulated in General Algebraic Modelling System (GAMS) to minimise the CO_2-eq footprint of the supply chain which resulted in a minimal objective criterion of 32.92 [kg CO_2-eq per kg syngas]. For this model, a Gate-to-Gate (G2G) system within a CO_2E SC infrastructure was considered assuming direct and indirect CO_2-eq emissions. This optimum is achieved at a 15% market penetration in the syngas demand market. Validated with alternative syngas production routes such as biomass gasification and Steam Methane Reformation (SMR) with CCS this value is relatively high. After obtaining this optimum a sensitivity analysis was conducted, from which it can be concluded that the dominant contributor regarding the environmental impact is the electricity consumption of the electrolyser in the CO_2E SC infrastructure.

Secondly, a cost minimisation was conducted on the exact same G2G system for a CO_2E SC infrastructure, in order to assess the financial feasibility. Based on an additional optimisation problem formulated in GAMS a levelised cost of syngas was found at a minimum value of 0.67 €/kg syngas produced. This minimal value of levelised cost was reached at a market penetration of 8%.

In order to assess and compare these two different objective functions metrics are introduced to compare the CO_2E supply chain configurations. Both models show certain similarities and differences which can be distilled into lessons learned for the Benelux authorities who are responsible for operating the CCU networks.

Keywords: Carbon Capture and Utilisation, Electrochemical reduction of CO_2, Optimisation, Environmental Impact, Cost reduction, Life Cycle Assessment, GAMS, ArcGIS Pro.

Contents

Nomenclature

Abbreviations

Abbreviation	Definition
Benelux	The Union of Belgium, Netherlands and Luxembourg
CAPEX	Capital Expenditures
CBS	Centraal Bureau voor de Statistiek
CCS	Carbon Capture and Storage
CCU	Carbon Capture and Utilisation
CCUS	Carbon Capture Utilisation and Storage
CO_2E	Carbon dioxide electrochemical reduction
DAC	Direct Air Capture
DEA	Diethanolamine
EU	European Union
FT	Fischer-Tropsch
GAMS	General Algebraic Modelling System
GWP	Global Warming Potential
GDX	GAMS Data eXchange
G2G	Gate-to-Gate
HHV	Higher Heating Value
ISO	International Organization for Standardization
IEA	International Energy Association
ISPT	Institute for Sustainable Process Technology
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
f LCOSG	Levelised Cost Of Syngas
LHV	Lower Heating Value
LSM	Lanthanum Strontium Manganite
MEA	Monoethanolamine
MDEA	Methyldiethanolamine
MILP	Mixed-Integer Linear Programming
PPM	Parts Per Million
PSA	Pressure Swing Adsorption
RE	Renewable Energy
REE	Rare Earth Elements
RES	Renewable Energy Source
SC	Supply Chain
SG	Syngas
SMR	Steam Methane Reforming
SOFC	Solid Oxide Fuel Cell
SOE	Solid Oxide Electrolyser
SOEC	Solid Oxide Electrolysis Cell
TRL	Technology Readiness Level
YSZ	Yttria Stabilised Zirconia

Mathematical & Modelling Symbols

Symbol	Definition	Unit
α_i	Efficiency of carbon capture unit within set i	[%]
β_i	Energy consumption factor within set i	[MWh / Mtonne CO_2]
ϕ_i	CO_2 footprint due to construction within set i	[Mtonne CO_2 -eq/ build unit]
GWP$_{H_2}$	Global warming potential of hydrogen	[-]
GWP$_{CO}$	Global warming potential of carbon monoxide	[-]
GWP$_{CO_2}$	Global warming potential of carbon dioxide	[-]
m_i	Mass flow within set i	[Mtonne/yr]
ρ	Density	[kg/m^3]
C	Set of CO_2 sources	-
Cap$_{Tot}$	Capture costs	€
CCI	Individual CO_2 emission locations	-
CIE	Transport of CO_2 from individual CO_2 source to electrolyser	Mtonne CO_2-eq
CIE$_{Tot}$	Total costs generated by the transport of CO_2 from individual CO_2 emission to the electrolyser	€
E	Electrolyser	-
CEH	CO_2 emission locations that can be clustered	-
EH	Exclusive CO_2 Hub	-
EHE	Transport of CO_2 from exclusive hub to electrolyser	Mtonne CO_2-eq
EHE$_{Tot}$	Total costs generated by the transport of CO_2 from exclusive hub to the electrolyser	€
Elyzer$_{Tot}$	Total costs generated by the electrolyser	€
ES$_{Tot}$	Total costs generated by the transport of syngas	€
S	Syngas demand location	-

1 Introduction

This chapter will introduce the field of research for this thesis. The first section will give further background regarding the electrochemical reduction of CO_2 with water into syngas within CCU infrastructures. Section 1.2 will discuss the motivation for a further understanding of this field of research. Section 1.3 will formulate the research question that this thesis will answer. Lastly, section 1.4 will give an outline of this report and therefore the structure of this thesis. It will highlight the different chapters and the content of each chapter.

1.1. Background

In the context of the European Union's (EU) efforts to mitigate carbon dioxide emissions, the Benelux region, with its annual emission of approximately 232 million tonnes, accounts for an 8.3% share of the EU's total CO_2 emissions [21]. Therefore, the Dutch, Belgian and Luxemburg governments are facing the challenge of reducing this emission within the climate goals set in the Paris Agreement. While fossil fuel companies are initially responsible for the CO_2 emissions they produce, large-scale implementation of Carbon Capture Utilization (CCU) networks requires government leadership due to the significant investments and nationwide impact on the chemical industry [29][46]. Therefore, the authorities of these countries can be identified as problem owners regarding the reduction of these GHG emissions and are obliged to look for solutions on how to reduce the footprint of the main contributors. The primary sectors contributing to these emissions include the steel industry, the petrochemical industry, and energy generation. A paradigm shift towards a circular economy suggests the transformation of CO_2, currently regarded as a waste byproduct in these carbon-intensive industries. One possible solution exists through electrochemical reduction processes. This approach not only offers a method to repurpose CO_2 emissions but also aligns with the principles of the circular chemical industry by converting waste streams into resources. Within the scope of this thesis, attention is focused on biogenic sources of CO_2 [90]. The focus on biogenic CO_2 sources stems from their continued presence in a future circular economy. According to EU legislation, these biogenic CO_2 sources will emit carbon in the long term and therefore form a perfect CO_2 supply in future CCU supply chains [52][90]. There is a wide variety of different biogenic CO_2 sources, however for the scope of this thesis there is a distinction and focus on 4 sources. The sources considered are waste incinerators, bioethanol, biomethane, and the pulp and paper industry. The production of ethanol and methane will continue to rely on biomass feedstock. Similarly, within a circular economy, the pulp and paper industry and biogenic waste incineration will persist in generating CO_2 emissions [90][91][109].

Therefore, with an eye on the future perspective and available CO_2 streams that will persist, these distinct 4 biogenic CO_2 sources lend themselves as the perfect feedstock for a CO_2E SC infrastructure.

Now it is concluded that biogenic CO_2 sources can play a role in the circular chemical industry, further processing of this CO_2 is the next step. Based on the type of CO_2 source different capture technologies can be applied to reach the highest efficiency. To fulfil the inevitable shift towards a more circular economy different capture technologies need to be used based on the CO_2 source. Once the CO_2 is captured, it can be transported in the supercritical phase to other locations. The goal of this transport is to centre and gather the CO_2 in one central location where further processing is made possible. One of these potent and promising processing pathways is the electrochemical reduction of CO_2 with water (CO_2E). Many different products can be formed from the electrochemical reduction of CO_2 with water. However, for the scope of this thesis, the focus will be on syngas because it is a chemical building block used today in the chemical industry. Syngas is a mixture of carbon monoxide (CO) and hydrogen (H_2). Syngas is a widely used chemical building block which can act as a feedstock for many derivatives. A schematic overview is given in figure 1.1. As it can be seen in the figure the captured CO_2 can be electrochemically reduced with water into syngas. Syngas can subsequently be processed into derivatives such as methanol, ethanol, hydrogen, and hydrocarbons via Fischer-Tropsch or used for power generation [42]. The big advantage is that syngas can replace fossil fuels as feedstock in these synthesis routes. With the right treatment of the carbon released during further processing of the syngas, the environmental footprint of these chemical processes can be reduced. Therefore, syngas can contribute to the circularity of the chemical industry.

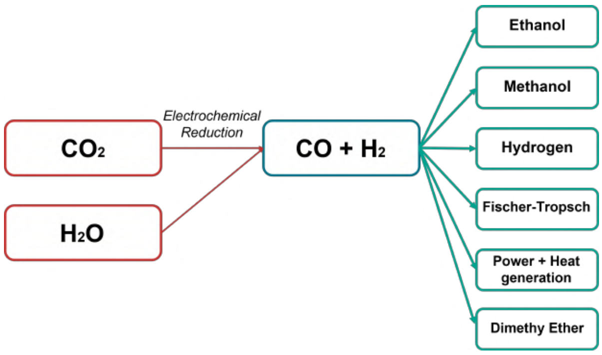


Figure 1.1: A schematic overview of a possible CO_2E to syngas and corresponding derivatives [42]

The last component in a CO_2E SC infrastructure would be the transport of the syngas from the electrolyser location to the syngas demand location. Current syngas demand in the Benelux is dictated by many factors. One of the main drivers of syngas demand is the production of methanol.

A key challenge with CO_2E SC infrastructure is the limited understanding of its environmental impact. It is the goal of the EU to mitigate global temperature rise well below 2 °C due to international agreements such as the Paris Agreement and the European Green Deal [9][20]. Therefore, a clear strategy on how to tackle CO_2 emissions that will exist after 2050 is of inevitable importance. One of the key drivers in these CO_2 reduction strategies is possible CO_2E SC infrastructures. Different policy instruments can be identified to implement CO_2E SC infrastructures, however, it is confirmed that they can have a significant share in reaching reduction targets [105][13].

The chemical industry, research institutes and international organisations (e.g. EU) are stakeholders in a CO_2E SC infrastructure as well. However, due to the limited scope of the chemical industry and the primary focus on the profit of private companies, an incentive from Luxemburg authorities is inevitable. Research institutes are essential for advancing and innovating CCU technologies, however, their capacity is limited in deploying and operating such a CO_2E SC infrastructure. Lastly, international organisations such as the EU can be problem owners and responsible, however, due to the geographical scope Luxemburg's authorities are considered. CCU networks will inevitably ask for a combination of high initial investment costs, long-term strategy and nationwide deployment asking for authority input and responsibility [17][93]. Therefore, the local authorities are responsible operators of the CO_2E SC infrastructures wherein the CO_2 is converted into a valuable feedstock for the chemical industry which can form an economically feasible solution.

However, to make this possible strategy compete with other possible solutions, the environmental impact needs to be clear and show a net benefit when compared to peers. Pros and cons of each solution in environmental impact of the CO_2E SC infrastructure need to be identified to form the lessons learned. A cost-minimised model can be of additional support. Can this CO_2E SC compete with other similar production routes for syngas? What are the possible risks associated with this particular strategy?

This thesis evaluates the environmental impact regarding CO_2-eq emissions of a CO_2E SC infrastructure within the Benelux. An optimisation model will be formulated to minimise the CO_2-eq emissions per functional unit which will be defined as the amount of syngas produced. An optimisation regarding costs will be conducted subsequently. Lastly, additional environmental criteria, such as water consumption and material criticality, will be briefly discussed. All these factors combined will be distilled into the lessons learned for the Benelux authorities. Now that an overall background of the problem and corresponding challenges has been given, the next section will discuss the corresponding motivation.

1.2. Motivation

Different aspects need further research before large-scale implementations of CO_2E SC infrastructures will be used. Some technological advances and/or economic advances have been made in academic research[121][64][85]. Main developments include the field of cost minimisation, efficiency of transport and total CO_2 reduction. These advances can act as a building block for further research. However, only a small number of academic publications are dedicated to the environmental impact of these CO_2E SC infrastructures, something that is the key motivation for the research in this master thesis.

The goal of this master thesis is to evaluate the conceptual CO_2E SC infrastructure based on biogenic sources within the Benelux with a minimal environmental impact. For the scope of this research, the main environmental impact category considered is the CO_2-eq emissions. The lessons learned from the research conducted in this thesis research can support Benelux authorities in pushing emitting industries into a more sustainable and circular configuration. To minimise its CO_2-eq footprint a further understanding is needed which forms the guideline for the research questions answered in this thesis.

1.3. Research Question

This thesis will answer the following research and corresponding subquestions:

What is the optimal CO_2E supply chain infrastructure for biogenic CO_2 sources in the Benelux to minimise the environmental impact?

Subquestions

- Which CO_2-eq footprints contribute the most in a gate-to-gate system within a CO_2E SC infrastructure based on biogenic CO_2 sources?
- How can the minimum environmental impact in a CO_2E supply chain infrastructure be explained and assessed using multiple metrics?
- What are the lessons learned based on the optimum obtained and the metrics used to assess a CO_2E SC infrastructure?

Now that the research question and its corresponding subquestions are formulated, a clear goal is set. The next section will describe the structure used in this report to answer the research question.

1.4. Thesis Outline

Firstly, Chapter 2 will identify the knowledge gaps based on the literature review conducted. This chapter will give a current status regarding the advances and innovations of the technologies used for CO_2E SC infrastructures. Subsequently, the trends within the latest publications will be identified and displayed.

Chapter 3 will give an overview of the methodology used to answer the research question. Firstly, this chapter will define different environmental impact indicators and prioritise them. Secondly, a model is proposed in General Algebraic Modelling System (GAMS) to minimise the environmental impact of this indicator. Chapter 4 will elucidate on the methodology used to verify the mathematical model proposed using different scenarios. Chapter 5 will present the results obtained from the mathematical model constructed in the previous chapter. It will assess and evaluate the obtained values and insights regarding the topology of the proposed CO_2E SC infrastructures. Chapter 6 will discuss further insights based on these results. It will identify similarities and differences and based on these aspects form key takeaways. The conclusion that can be drawn from the research conducted is described in Chapter 7. Lastly, chapter 8 will give recommendations for further research. At the back of this thesis report are the appendices wherein the model employed within GAMS 45 Studio is detailed in Appendix A. Appendix B will display the different tables and data used for the research. An overview of the data extracted from SimaPro Multi-user version 9.4.0.2 used to access the Idemat database, is presented in Appendix C.

2
Literature Review

This chapter will dive deeper into the academic research conducted in the field of CCU, CO_2E, supply chain and Life Cycle Assessment studies with corresponding impact categories. Section 2.1 will discuss the knowledge gaps identified. In section 2.2 the current status of carbon capture technology is discussed, which forms the first echelon in the supply chain. Section 2.3 will elaborate on the state-of-the-art application of CO_2E. Section 2.4 will display the supply chain considered for these CCU networks. Section 2.5 details the various CO_2E SC design options for this type of infrastructure. Section 2.6 will discuss the framework used in LCA studies. To conclude, section 2.7 will give an overview of the trends within research and identify the research gaps.

2.1. Knowledge Gaps

The research conducted falls within the scope of the NWO project of the Energy Systems & Service research group within the Faculty of Technology Policy and Management. The goal of this project is to explore the different implementations of CO_2 electrolysis for syngas production. The goal of this project is to explore the various methods of CO_2 electrolysis for syngas production. Within this research, the focus is on application approaches and the tradeoffs associated with them. However, the foundation for adopting a specific approach is based on the knowledge gaps identified in this section.

Firstly the knowledge gaps will be enumerated and subsequently elaborated on with corresponding academic literature. The knowledge gaps identified in this thesis are:

1. **There is a lack of understanding regarding different impact categories in Life Cycle Assessment (LCA) methodology in CCU frameworks [62]:** *As stated by Müller et al. 2020 and Cruz et al. 2021 a range of frameworks and LCA studies have been conducted regarding the environmental impacts of CCU networks, however, scientific gaps have been identified in the transparency, boundary statement and limiting the comparability of LCA studies [22][73]. Additionally, as mentioned by Leonzio et al. 2022 future research in the LCA of CCU networks is a crucial element in their social acceptance and therefore their implementation [81].*
2. **There is a deficiency in measuring the full environmental impact of all relevant processes in CO_2 supply chains for CCU [62][7] [4]:** *As stated by Desport et al. 2022, the conversion of CO_2 into fuels is modelled but still is poorly quantified regarding its environmental impact in the overall decarbonisation of the industry [25]. This is confirmed by the research conducted by Leonzio et al. 2023 wherein it is stated that further research is needed to overcome the limited amount of data regarding the environmental impact of different CCU network components in their corresponding LCA stages [62].*

The two identified knowledge gaps form the validation of the research conducted in this thesis. Different impact categories can be taken into account regarding the environmental impact. This is one of the main drivers since the syngas (SG) produced will have to compete with alternative synthesis routes such as biomass gasification and Steam Methane Reforming (SMR) with CCS and prove to be truly beneficial to these processes regarding its ecological effect. Therefore, a full understanding of the impact categories in LCA methodology within CCU frameworks helps address this scientific knowledge gap. This thesis will address the different impact categories and provide a further understanding of the most urgent one(s).

Once an understanding is constructed, a quantification in measuring this environmental impact in CO_2 supply chains in CCU can benefit in overcoming the limited data. This thesis will provide insights into measuring the impact category or categories. By determining the order of magnitude of these impact categories, a more detailed overview of the different LCA stages will be discussed.

To sum up, it can be concluded that there are two knowledge gaps within academic research regarding the environmental impact of CCU networks. This environmental impact can be assessed using an LCA approach, wherein in this specific use case, priority should be given to the most prominent and urgent impact categories. The most urgent impact categories will subsequently be assessed in order to quantify and measure their environmental footprint in all relevant processes in CO_2 supply chains. To elaborate on this supply chain a chronological literature review will be given of all relevant components segmented into capture, transport and electrolysis.

2.2. Current Status Carbon Capture

Carbon capture and utilisation will inevitably play a major role in the goal of reaching a circular economy within the chemical industry [34][53]. Therefore, carbon capture is the primary component in these supply chains and thus an understanding is crucial. In many chemical processes, CO_2 is a waste stream typically released into the atmosphere with no alternative utilisation. Different technologies in the field of carbon capture exist, each having its unique characteristics regarding efficiency, energy consumption and material use.

The first categorisation in carbon capture and the corresponding technologies is the distinction between the different types of sources. Based on literature, three different sources of CO_2 can be classified, these subsequently are atmospheric, fossil-based and biogenic-based [86][71]. Atmospheric CO_2 emissions occur from natural sources. One can think of these as the decay and decomposition of organic matter. Fossil-based CO_2 emissions originate from the combustion of fossil fuels. Examples are the conversion of natural gas or diesel. The last classification of CO_2 sources are biogenic ones. These CO_2 emissions occur due to the processing of biomass species. Production of ethanol and methane based on biomass input such as corn, sugarcane or sugar beet are examples of biogenic CO_2 sources [69]. Each source of CO_2 has its own corresponding capture technology. Direct Air Capture (DAC) is the technology that captures CO_2 directly from the ambient air [133] [79]. Most of these DAC technologies rely on the fact that CO_2 can be chemically absorbed once the air is sucked into the device in which a solvent is present. However, this technology poses some lack inefficiencies due to low concentrations of CO_2 in ambient air but can be used for the atmospheric CO_2 sources [59][57][119]. Fossil fuel and biogenic CO_2 sources ask for different capture technologies, this is mainly due to the concentration of their CO_2 emission streams. This poses the way for the second categorisation in carbon capture technologies and its current status.

The second categorisation is made on the capture technology which is based on the volume of the emission and the concentration of the CO_2. Fossil fuel and biogenic-based CO_2 sources pose a higher volume and concentration of CO_2. Based on these criteria fossil fuel and biogenic CO_2 sources are in this classification of carbon capture technologies. Different technologies are present in this categorisation. However, these technologies rely on two main distinctions. The CO_2 released can be captured either pre-combustion or post-combustion. Post-combustion capture uses the exhaust gases of combustion processes and uses absorption techniques to capture the carbon in these streams [67][70]. Pre-combustion capture is a different approach. This technique relies on the capture of the syngas produced during the gasification of for example coal or biomass before it is burned. Via this route the net CO_2 emissions can be reduced [48][104]. A technology that cannot be classified as either pre- or post-combustion is oxy-fuel combustion carbon capture. This is a technology that relies on the fact that the combustion of the feedstock is conducted in a pure O_2 environment instead of air. Pure oxygen causes a flue gas stream that is primarily composed of CO_2 and water vapour. The main advantage of this type of combustion is, that it paves the way for more easy CO_2 separation and capture [12][96].

The third categorisation of carbon capture is technology-specific and varies per timing (pre- or post-combustion) or whether it is suitable for oxy-fuel combustion. In this section, an overview will be given of the most prominent and widely used ones. Note needs to be taken into account that other technologies are present. However, according to the literature, the main carbon capture technologies used are:

1. **Amine scrubbing:** This capture technology is mostly used for post-combustion capture. It involves the use of an amine liquid solution to absorb CO_2 from the flue gas streams. The CO_2 rich amine is heated afterwards to release the CO_2 [89][92].
2. **Pressure Swing Adsorption (PSA):** This technology uses the different adsorption characteristics of gases onto solid materials (adsorbents) At high-pressure certain chemicals adsorb which can be later on be released at low pressure. This process is repeated in cycles to separate gases [36][118].
3. **Membrane Separation:** Membrane-based carbon captures uses the fact that certain semi-permeable membranes can be used to selectively separate CO_2 from gas mixtures [11][1]. This separation method makes use of the difference in permeability.
4. **Physical Sorption (Physisorption):** Physisoprtion is a method of capturing carbon dioxide (CO_2) that relies on the physical interaction between CO_2 molecules and the surface of a sorbent material. This technique is distinct from chemical sorption (chemisorption), where chemical bonds are formed between the CO_2 and the sorbent e.g. sorbents are methanol [6] [10].

Now an overview has been given of the different possible capture technologies a link has to be made to the specific biogenic CO_2 sources.

4 different types of biogenic CO_2 will be considered, and their corresponding carbon capture technology based on literature is displayed in table 2.1

Table 2.1: Efficiency of different carbon capture technologies.

Type of Unit	Type of capture technology	Efficiency	Reference
Pulp & Paper	Post-Combustion Amine Scrubbing	80%	(Xiangping Zhang 2014)
Waste Incineration	Post-Combustion Amine Scrubbing	85%	(Xiangping Zhang 2014)
Biomethane	Only compression needed	95%	(Farla 2019)
Bioethanol	Only compression needed	95%	(Farla 2019)

The flue gas streams exiting biomethane and bioethanol biogenic sources are relatively pure [33] [127]. Therefore, it can be assumed that not a capture unit needs to be installed but only a compressor unit. The compressor unit is needed to pressurize the gas and make it ready for transport [130]. However, a further understanding of the exact process of the post-combustion amine scrubber is needed.

A schematic overview of a carbon capture unit based on the technological principle of amine scrubbing can be found in figure 2.1. One can see that CO_2 rich gas (flue gas) enters the absorber on the left side, after which it is brought in contact with a lean amine solution. Different solutions exist but the most used one is Monoethanolamine (MEA), this amine can bind to the CO_2. The specific energy consumption of MEA is around 3.1 GJ/Tonne CO_2, this is relatively low compared to other amine solutions such as diethanolamine (DEA) and methyldiethanolamine (MDEA) [115][2]. This solvent is chosen since it has a lower specific energy input. Via a pump and a heat exchanger the flow of rich amine is brought to the regenerator where the carbon dioxide is separated. The CO_2 is brought to a condenser where the final product of CO_2 is obtained. The amine is brought with a reboiler to its lean state and pumped back into the absorber. The process is not able to work on a 100% efficiency, resulting in a spent solvent stream in the bottom right. In the left top, it can be observed that the exhaust gas exits the system, which is much lower in CO_2 concentration.

A thorough understanding of different carbon capture technologies has been displayed. Furthermore, the corresponding capture technology has been linked to the right biogenic CO_2 source. After capture the CO2 is transported to the electrolyser. The next section will elaborate on the electrochemical reduction of CO_2 (CO_2E) with water into syngas.

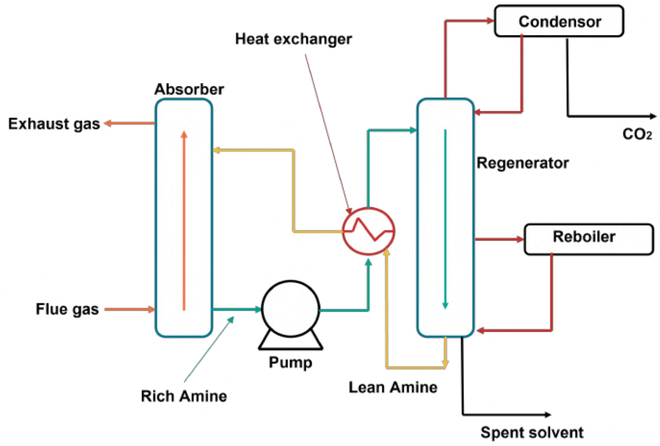


Figure 2.1: A schematic overview of a carbon capture unit

2.3. Current Status CO_2E

The conversion of CO_2 into valuable chemicals and fuels through electrolysis, particularly using solid oxide electrolysers (SOEs), represents a promising future for carbon recycling and synthetic fuel production. The choice for SOEs is because of relatively high efficiencies and reaction rates [8]. In the context of CO_2 electrolysis, solid oxide electrolysers offer an efficient pathway for converting CO_2, often in combination with water (H_2O), into syngas—a mixture of hydrogen (H_2) and carbon monoxide (CO) [76][58]. Efficiency rates differ but according to different sources, a 65% on an industrial scale is doable [102]. Efficiency is here defined as a percentage of the Lower Heating Value (LHV), this means the energy content of the product versus the feed. Syngas is a versatile intermediate that can be further processed into a wide range of chemicals and fuels, including methanol.

Solid oxide electrolysers operate at high temperatures (typically between 700°C and 1000°C), which significantly enhances the kinetics of the CO_2 reduction reaction, leading to higher conversion efficiencies compared to other types of electrolysers, such as polymer electrolyte membrane (PEM) and alkaline electrolysers [99][58]. Chemical reactions taking place in these temperature ranges always pose challenges, however, note needs to be taken that the temperature is constant since dynamic systems are not possible. Problematic challenges can occur in the form of keeping a constant and uniform temperature over the entire electrolyser, therefore, a detailed and sophisticated heat exchanger network is needed. Moreover, the ability of SOEs to co-electrolyse CO_2 and H_2O into syngas offers a flexible adjustment of the H_2/CO ratio in the produced syngas, which is crucial for the downstream synthesis of different chemicals and fuels, including methanol [23][51]. A schematic overview of such an electrolyser can be found in the following figure 2.2.

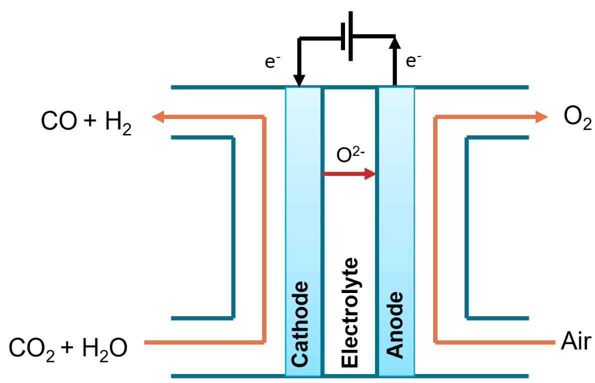


Figure 2.2: A schematic overview of an electrolyser unit

As displayed in the figure, there is an input of air, CO_2 and water. These two separated mass flows come in contact with a cathode and an anode. A current is flowing through these two electrodes via an external power source. The anode electrode is positive during operation. At this electrode, the oxidation reaction occurs. The cathode electrode is negatively charged, at this side of the electrolyser the reduction reaction takes place. During this reaction, it is possible to reduce an oxygen atom from the CO_2 and water. Therefore, the exit stream of the Solid Oxide Electrolysis Cell (SOEC) becomes an enriched oxygen flow. The concentration of oxygen present in the air is therefore greater at the outlet than compared to the inlet air stream. On the opposite side, it can be concluded that CO_2 is chemically reduced into syngas. Syngas can have different molar ratios of their components (CO and H_2) based on the chemical treatment [126].

Recent developments in solid oxide electrolyser technology have been centred around improving durability, lowering the expenses associated with electrode and electrolyte materials, and enhancing the efficiency and scalability of the system. Despite these advancements, challenges such as high operating temperatures leading to material degradation, and the need for further improvements in long-term stability and cost reduction, remain. Research and development efforts continue to address these challenges, to make CO_2 electrolysis via solid oxide electrolysers a commercially viable technology for large-scale deployment [99][16]. SOEC is a rapidly developing technology with significant potential to combat climate change. It allows the sustainable production of chemicals and fuels from CO_2, offering a path towards a cleaner future.

Note needs to be taken into account that no industrial-scale applications of this technology exist. It is expected that the technology readiness level (TRL) of SOECs will reach level 9 in 2030 [68]. A TRL of 9 indicates that the actual system has been proven through successful mission operates and is at the highest level. Currently, the SOEC technology is on TRL 6-7 [68]. Therefore, one of the main assumptions made is that our electrolysers operate at the same configuration as proposed in figure 2.3 [102]. The Institute for Sustainable Process Technology (ISPT) report referenced assumes a SOEC that is ready for large-scale implementation.

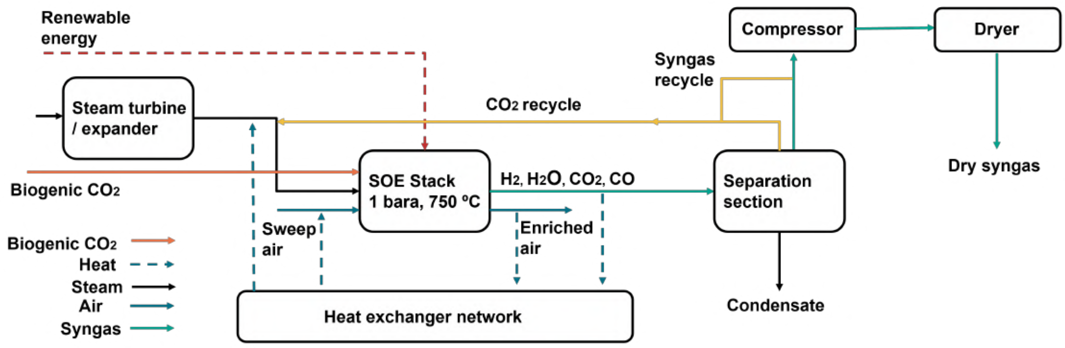


Figure 2.3: Process overview electrolyser [102]

This detailed report was published in 2023 about the industrial application of high-temperature CO_2 electrolysis [102]. The proposed Solid Oxide Electrolyser in this report is a tailor-made configuration use case for the petrochemical company British Petroleum (BP). In this use case, renewable energy is used in combination with steam to produce syngas. This report is one of the first analyses made regarding the industrial-scale application of this technology. As can be seen in figure 2.3 different components are present in the process. Certain components such as a steam turbine, compressor or dryer are common practices within the chemical industry. The main engineering challenge is hidden in the configuration of the pieces of equipment regarding the SOE Stack.

Of which different arrangements can be made regarding the stack. As a baseline, the ISPT report is used, a visual representation can be found in figure 2.4. As can be seen from the figure there is a single cell placed in a horizontal position on top of each other. These repetitional units are placed within these so-called Hot-Box Modules. The CO_2 enters together with the water from the left side of the hotbox. As they continue to the right, there is an exchange of heat with the surroundings due to reaction and current flow. Therefore, it is important to control the exact temperature along the pathway. The temperature affects the energy consumption and the conversion rate of the reaction. To keep maximum control, a heat exchanger is applied to each side. The conversion of CO_2 into syngas happens at high temperatures. According to the ISPT report, these can range from 700 to 800 °C. Subsequently, it is an energy-intensive process to commence the reaction. Once the electrolyser is in operation, a new equilibrium will hold wherein the electrolyser will settle in a thermo-neutral voltage. This means that no additional heat is needed. Additionally, the phase transition of water into the vapour phase consumes as well a lot of energy. The significant latent heat of vaporization associated with water in the combustion products lowers the measured Lower Heating Value (LHV)

A detailed overview of all components considered within the process can be found in Appendix B.

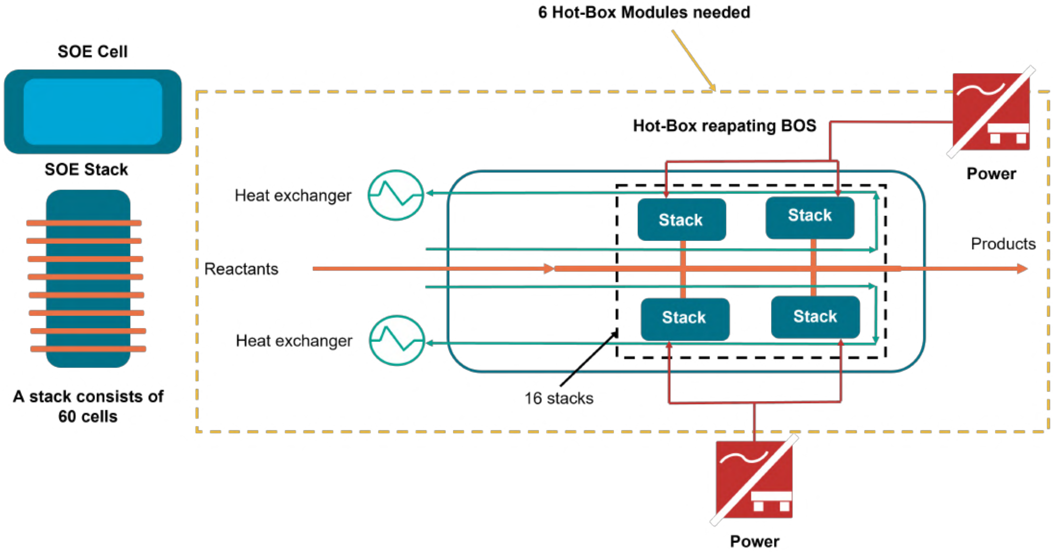


Figure 2.4: Repetitional unit within the SOEC [102]

This section has elaborated on the technology of electrochemical reduction of CO_2 with water to form syngas. This chemical conversion is conducted in a SOEC. The ISPT report forms a baseline for the industrial-scale implementation of such a plant. The next section will elaborate on the supply chain to link the capture of CO_2 and the conversion of CO_2 into syngas.

2.4. Supply Chain

This section will give a further understanding of the supply chain needed to make supply meet demand in a circular CO_2 economy. As stated earlier, biogenic CO_2 sources are allowed under EU policy to emit CO_2 by 2050. Section 2.2 discussed the possibility to capture this CO_2 and Section 2.3 discussed the possibility to electrochemically reduce this CO_2 into syngas. CO_2 transport will be necessary between capture sites, electrolysers, and syngas demand locations, resulting in a supply chain. This forms the supply chain that has to be studied within this CO_2E SC infrastructure. Different configurations of this CO_2E SC infrastructure can be operated concerning different tradeoffs. The supply chain consists of the following components as displayed in figure 2.5. In this figure 2.5 the blue blocks represent the capture, transport or conversion of CO_2. Whereas the orange blocks represent the production or transport of syngas.

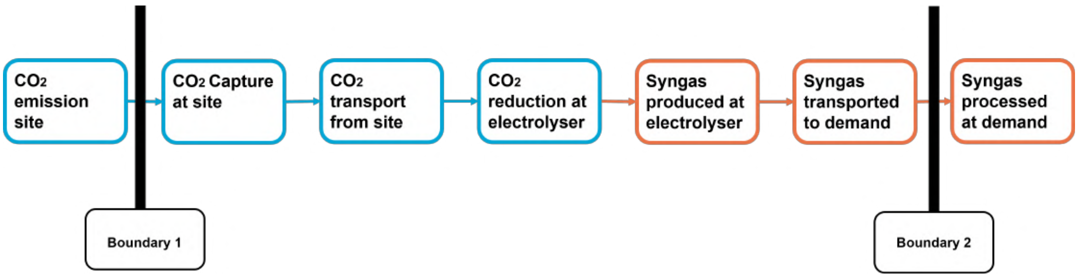


Figure 2.5: Schematic overview of the supply chain considered with corresponding system boundaries

After capture the CO_2 has to be transported to the electrolyser. Different ways of transportation can be used but the most preferred way of transport is via pipelines wherein CO_2 is in the supercritical state.

The main advantage of transporting CO_2 in the supercritical state is that it shows a higher density and lower viscosity which makes it more energy efficient during transport [131][98]. Once the CO_2 has been converted at the electrolyser, the product (syngas) has to be transported to the demand locations. It is important to notice that these are the set boundaries considered in this supply chain as displayed in figure 2.5. For the infrastructure of this supply chain, different components are needed. These can come in the form of capture and electrolyser units, but the amount of pipeline built as well. This supply chain covers the entire supply (CO_2 from biogenic sources) to the demand (syngas demand by the chemical industry). The construction and design of such a SC however poses challenges. Orders of magnitude of supply, demand and the distance between these nodes pose certain tradeoffs between the infrastructure. The next section will elaborate on this SC infrastructure design.

2.5. CO_2E SC Infrastructure design

This section will elaborate on the tradeoffs that come into play for different CO_2E SC infrastructure configurations. Major developments have been made mostly focussing on the supply chain organisation of these CO_2E SC infrastructures. Most of these academic publications analyse these complex structures with decision-making models where the optimal planning and application of these infrastructures are made. Most of these studies rely on the fact that CO_2 sources are present and these so-called ”sinks”, which represent storage sites. Note needs to be taken into account that this is only for the situation regarding Carbon Capture and Storage (CCS). Empty salt cavities or empty gas fields are examples of sinks in these models [101][103]. In certain studies, utilisation sites are used as intermediate nodes in these structures to convert the captured CO_2 into a new usable feedstock [38][66].

These problems are often described in a programming model and approached with the linearization of certain variables. Different models are proposed depending on the specific use case. An optimisation model regarding the infrastructure of SC for CO_2E mostly consists of several components that act as variables. Often modelled are capture, utilisation, storage and transport units, wherein the model can decide whether or not to utilise them. By turning the knobs of these variables and staying within the constraints a feasible solution might be found that satisfies the goal. The goal for CO_2E SC infrastructure design can vary depending on the scope of the project. Often chosen objective functions that are taken into consideration when designing infrastructure for CCU networks are cost minimisation or maximisation of CO_2 reduction [123] [124]. Multi-objective function optimisation is possible as well since this can provide a valuable tradeoff between the two of these single objectives. Multi-objective modelling involves creating models that can evaluate and optimise multiple objectives, often conflicting, simultaneously. This type of modelling is used when decision-makers need to consider several criteria that are important for the success of a project or solution. Multi-objective SC design for CCU networks makes the modelling complex and can even push for machine learning solutions [125]. An optimisation goal that has been lacking within academic literature though is the environmental impact of these possible CCU networks [63][25].

2.6. Life Cycle Assessment

A Life Cycle Assessment (LCA) is the systematic and analytical procedure to extensively quantify and interpret a product, process or service’s environmental consequences. This covers every phase, starting from the extraction of raw materials (the cradle) and continuing through material processing, manufacturing, distribution, usage, upkeep, and disposal or recycling (to the grave). Assessing the environmental costs connected to particular products or processes and identifying areas for environmental improvement are the main objectives of life cycle assessment or LCA [107] [40] [54].

The International Organisation for Standardization (ISO) has standardized the LCA approach in the ISO 14040 and 14044 series. These standards offer a structure and instruction for carrying out LCA, guaranteeing the evaluations’ uniformity, openness, and comparability. The three primary stages of the LCA process are displayed in figure 2.6.

The framework displayed in figure 2.6 can be explained as follows.

1. **Goal and Scope Definition:** This is the first and foundational stage of LCA where the purpose of the assessment is clearly stated. The scope includes defining the system boundaries, which outline the parts of the product’s lifecycle that will be included in the assessment. It also determines the level of detail, assumptions, and limitations of the LCA. The objective criterion, which

is a quantified description of the service that the system provides, is established here, allowing for a consistent basis of comparison. In this section, the functional unit is defined as well, which is a quantified description of the function or service that the product system delivers.

2. **Inventory Analysis (Life Cycle Inventory, LCI):** During this stage, data is collected and calculations are performed to quantify relevant inputs and outputs of the system. Inputs may include raw materials, energy, water, and other resources. Outputs can include emissions to air, water, and soil, as well as co-products and waste. The inventory analysis involves compiling and quantifying inputs and outputs for the product system throughout its life cycle. During the LCI section of the LCA, all impact categories are defined and weighed. After selected they can be analysed either midpoint or endpoint. Midpoint analysis assesses environmental impacts at an intermediate stage (e.g., the amount of greenhouse gas emissions), while endpoint analysis evaluates the final consequences of these impacts on areas of protection such as human health.
3. **Impact Assessment (Life Cycle Impact Assessment, LCIA):** This phase involves evaluating the significance of potential environmental impacts based on the LCI flow results. It translates emissions and resource extractions into a limited number of environmental impact scores by using predefined models. These models consider the contribution of each input or output to a range of impact categories such as global warming, ozone depletion, eutrophication, acidification, and resource depletion. Which specific impact categories are taken into account depends on the LCIA method chosen. Therefore, it is important to clearly state the goal and scope definition of the LCA before this step. An overview of all impact categories is stated in table B.11 which can be found in Appendix B. This table displays an overview of the different impact categories their description and the unit used to quantify these impact categories.

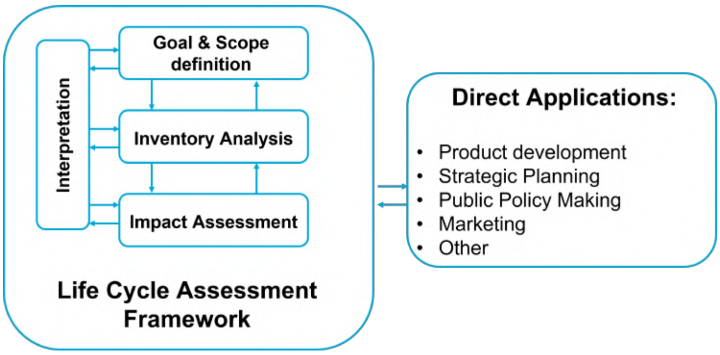


Figure 2.6: The LCA framework applied in this research [94] [30]

2.7. Trends in academic literature

This section will discuss the trends identified in the literature and the shortcomings of the corresponding literature. The trends in literature can give an insight into the direction in which the field of research is headed and as well support shortcomings such as the knowledge gaps proposed earlier.

2.7.1. Trends in Literature

The main trend that can be identified in the academic literature considered within this research is that there is a definite increase in the popularity of CCU networks, but little is known about the environmental impact of these networks nor what chemical product is the most favourable. Little research has been conducted in the field of a full LCA for these networks, however, more and more publications are being released regarding their implementations and cost-benefit analyses [64] [65] [63]. This trend in academic literature is confirmed by various sources but as well based on the interview with Grazia Leonzio. Leonzio is a research associate of Imperial College London and specialised in the modelling of CCU networks and their environmental impact.

The following main shortcomings identified during the interview with Grazia are defined as follows:

- There is insufficient research regarding the environmental impact of CCU infrastructures forming a public acceptance barrier [41].

- LCA can give a first insight into this environmental impact but it is unknown what impact category should be the main focus [81] [62].

This is in line with industry behaviour since most of these projects are in collaboration with private companies motivated by profit. The amount of publications for the following grouped keywords shows a major increase over the past years in academic research. Group 1 for the keywords: LCA, CCU and Modelling has tripled over the past 5 years. The amount of publications for the keywords: CO_2, Electrochemical reduction and Syngas has doubled over the past 5 years.

The amount of publications per group as a function of time has been displayed in figure 2.7.

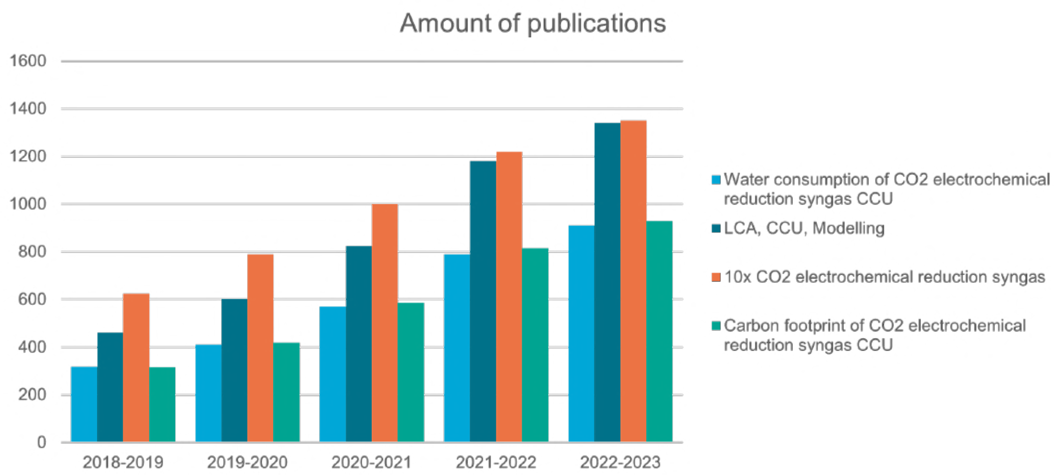


Figure 2.7: Amount of publications per year on different keywords

However, due to the governmental funding and general goal to cut CO_2 emissions a further understanding is needed within the environmental impact of this energy transition solution. Based on the chart displayed in figure 2.7 one can see that there are in the year 2022-2023 almost 10 times more publications on Google Scholar regarding CO_2, Electrochemical Reduction and Syngas as combined keywords. Now one can see that the light blue bars and dark green bars increase as well but not at the same rate as the previously mentioned keyword groups. This shows that there is research conducted regarding the environmental impact of these CCU networks but that it is limited compared to the general research of these CCU networks. Therefore, a trend can be identified in academic publications wherein there is an unparalleled rate between different keywords. This supports the trends found in academic literature and the information obtained from the interview with Grazia.

3
Method

This chapter will elaborate on the methodology applied for the research conducted in this thesis. Section 3.1 will give an overview of the environmental impact assessment and the corresponding environmental impact indicators. Section 3.2 will clarify the modelling conducted in GAMS in order to minimise the CO_2-eq footprint. Section 3.3 will elaborate on thisthe mathematical formulation in GAMS. Subsequently, section 3.4 will elaborate on the evaluation of these proposed optimisation models. Lastly, section 3.5 will discuss additional environmental criteria such as water consumption and criticality of materials.

3.1. A framework for environmental impact assessment

A Life Cycle Assessment (LCA) acts as a framework to give insight regarding the environmental impact of a product or service. For the research conducted in this master thesis, SimaPro 9.4.0.2 Classroom Multi-user is used to access various databases that contain the environmental footprint of different components in the CO_2E SC. Section 3.1.1 will elaborate on the goal and scope set for the G2G CO_2E SC infrastructure. Section 3.1.2. will discuss the Life Cycle Inventory Assessment for a G2G CO_2E SC infrastructure. The LCA framework proposed is the first step in the methodology applied in this research in order to answer the research question.

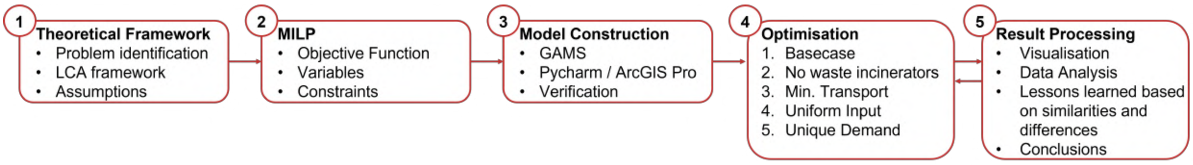


Figure 3.1: The methodology applied to structure the research in this thesis.

As described in the previous chapters this thesis will analyse the environmental impact of a CO_2E SC infrastructure. Therefore, the LCA framework for this methodology is defined as follows.

1. **Goal and Scope Definition:** This LCA aims to assess the total environmental impact of CO_2E SC, wherein the ecological footprint is minimised. Different impact categories can be taken into account based on the table B.11. Based on the impact categories: Global Warming Potential, Stratospheric Ozone Depletion, Ionizing Radiation, Ozone Formation (Human Health), Fine Particulate Matter Formation, Ozone Formation (Terrestrial Ecosystems), Terrestrial Ecotoxicity, Freshwater Ecotoxicity, Marine Ecotoxicity, Human Carcinogenic Toxicity, Human Non-Carcinogenic Toxicity, Land Use, Mineral Resource Scarcity, Fossil Resource Scarcity and Water Consumption a priority needs to be made due limited time for this thesis. Based on the knowledge gap proposed in Chapter 2 and on the academic literature read, a preference is given to the impact category of Global Warming Potential followed by Water Consumption. As proposed by academic literature, additional research is needed to see the true added value of CCU infrastructures in the carbon cycle, thus validating the main priority of GWP [65][62][63]. Therefore, the main goal of the LCA in this thesis is to assess the GWP of the CO_2E SC infrastructure. As secondary goals, the water

consumption is assessed since the literature states that scarcity in freshwater consumption could possibly be a bottleneck in the upscaling of CO_2E [106][61][117].

2. **Inventory Analysis (Life Cycle Inventory, LCI):** Data is collected from the Idemat 2022 and 2023 databases which are accessed via a SimaPro multi-user account at the university. Assumptions made for the different components in this analysis are stated in the corresponding section. If not found in the Idemat 2022 and 2023 database, academic literature was used to estimate the values used in the LCI. For a more detailed examination of the gate-to-gate system as delineated in section 3.1.2, a thorough elaboration on the specific inputs and outputs is warranted. As stated goal and scope definition, the focus is on the impact categories of CO_2-eq emissions.
3. **Impact Assessment (Life Cycle Impact Assessment, LCIA):** The assessment of the obtained results from the model will first be evaluated in GAMS. The results will be visualised in ArcGIS Pro via PyCharm. The CO_2E SC infrastructure proposed will be visualised for different market penetration values. This market penetration analysis is conducted to see for which optimum the CO_2E SC can deliver the functional unit to the demand positions. Subsequently, the model will be verified by varying input and observing its behaviour. Lastly, it will be validated using a comparison to alternative syngas production routes.

The next sections will elaborate on each specific part of the framework individually.

3.1.1. Goal and Scope within a G2G CO_2E SC Infrastructure

The scope of the system proposed is a gate-to-gate (G2G) system within the supply chain of biogenic CO_2 sources wherein, all captured CO_2 will be as efficiently as possible converted into syngas. Within this system there are different footprints taken into account, these can be categorized as direct or indirect CO_2-eq emissions. However, before an elaboration on these different types of emissions can be given, a total overview of the supply chain is needed. Figure 3.2 gives an overview of all different components and the different aspects of the CO_2E SC infrastructure that have an environmental impact. The cradle in the supply chain is defined as the excavation and processing of raw materials. In this part of the process, one can think of metals, sand or Rare Earth Elements (REEs) used for the electrodes of the electrolyser.

After processing and construction of each CO_2E SC infrastructure echelon, there is still additional environmental impact. During Operation and Maintenance (O&M) extra materials are used. During the demolition and construction of CO_2E SC infrastructure components, an additional environmental impact is caused. An example of environmental impacts can be in the form of heat and/or electricity used for the O&M or demolition phase. The demolition phase is reached for a component when it is at the end of its lifetime.

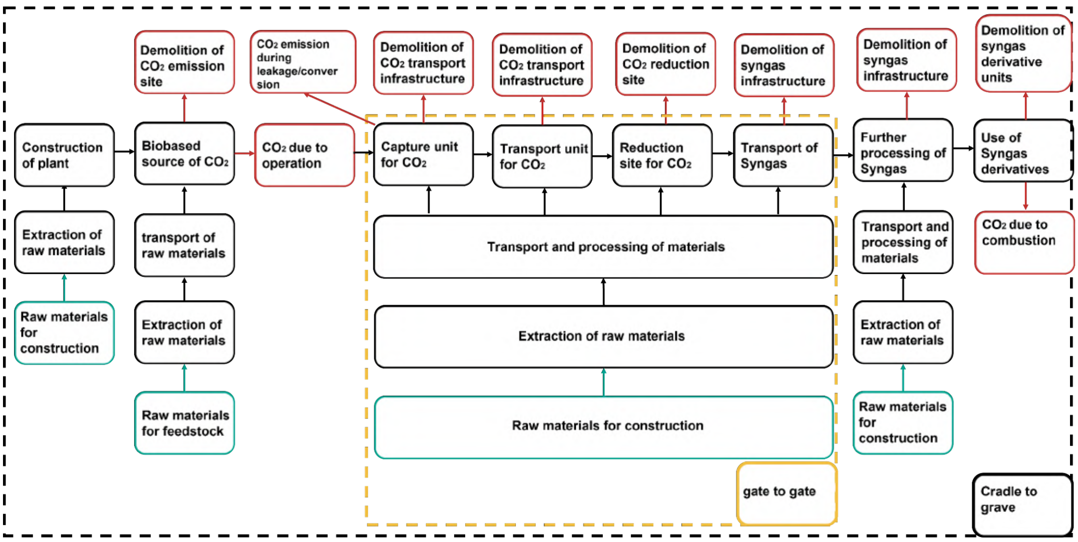


Figure 3.2: The SC system considered in this research

Within this system, a subsystem is defined as the G2G system indicated by the yellow dashed part displayed in figure 3.2. This research does not consider the CO_2-equivalent footprint resulting from demolition or waste production associated with various echelons in the CO_2E SC infrastructure and its corresponding units. The boundaries set by the system are indicated in the yellow dashed area, with a focus to minimise the CO_2-eq footprint per functional unit. Additional scenarios were considered wherein constructional, O&M and other footprints are neglected. For the G2G system defined it can be concluded that only short-cycle CO_2-eq emissions are considered (emissions occur over a relatively short period of time). Since the demolition and decomposition are not considered, the long-cycle CO_2-eq emissions are neglected.

Possible footprints at the biogenic source are not taken into account, nor are the further processing footprints of the syngas once delivered at the demand site. Subsequently, the demolition and corresponding footprints within the CO_2E SC infrastructure are left out of scope as well. The choice for this G2G subsystem within the system is for the scope of the research conducted in this thesis. After syngas production, the additional conversion steps used in the chemical industry are roughly the same, since they all rely on the formation of hydrocarbons. Therefore, it is validated to put the gate of the system at the delivery of syngas at the demand location. The biogenic CO_2 sources vary in size, type of machinery and energy consumption resulting in a wide range of environmental footprint per location that is complex to calculate. This results in the validation to take this part of the SC out of scope for the research conducted in this thesis. The demolition of our G2G is left out of scope since little is known about the demolition of especially the electrolyser units. Therefore, it is validated to leave out the environmental impact of the demolition phase. Now that strict boundaries have been defined within the scope of this research, it is time to identify the different environmental footprints within each echelon of the CO_2E SC infrastructure.

Direct CO_2-eq emissions

During the operation of the supply chain, direct CO_2-equivalent emissions arise from inefficiencies in capture, leakages during transportation, and inefficiency due to not full conversion during electrochemical reduction. Another component taken into account as direct emissions is the electricity consumption and the corresponding carbon footprint of this electricity. Note needs to be taken into account that for the research conducted in this thesis, it is assumed that the electricity consumed is generated by renewable energy sources and will always be available. Still, this electricity has a certain footprint due to construction and modifications of the materials. For sense of scale, the carbon footprint of the current Dutch Electricity mix is on average 373.21 [g CO_2/kWh] [78] whereas it is estimated that the carbon footprint of e.g. PV Solar electricity in The Netherlands in 2013 on average was 26.38 [g CO_2/kWh] [120]. It's crucial to bear in mind these orders of magnitude during the Life Cycle Impact Assessment (LCIA) phase of the LCA.

Figure 3.3 gives a schematic overview of all the different direct CO_2-eq emissions. From the figure, it can be concluded that there are 8 different types of emissions. The direct emissions indicated in red on top of the CO_2E SC echelons are emissions due to the fact of inefficiency during capture, leakage during transport and inefficiency of the electrolyser.

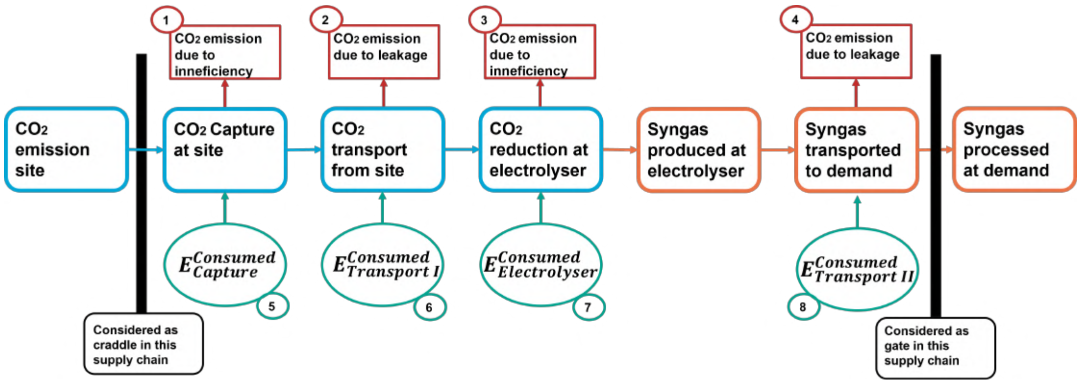


Figure 3.3: Schematic overview of the direct CO_2-eq emissions

Additionally, each component in the supply chain consumes electricity resulting in 4 additional direct CO_2-eq emissions displayed at the bottom of the CO_2E SC echelons. Electricity is for example consumed during transport, heat during electrolysis or during compression at the capture location.

Indirect CO_2-eq emissions

Apart from direct CO_2-eq emissions, there are 8 indirect CO_2-eq emission streams identified within G2G subsystem of the CO_2E supply chain. A schematic overview of these streams, depicted in figure 3.4, illustrates each different component of the supply chain. Each of these components has its constructional footprint due to the use of materials. During the operation and maintenance of these components certain parts might need replacement and therefore this will have an additional CO_2-eq footprint. It is assumed for simplicity that the CO_2-eq footprint due to O&M equals 4% of the constructional footprint.

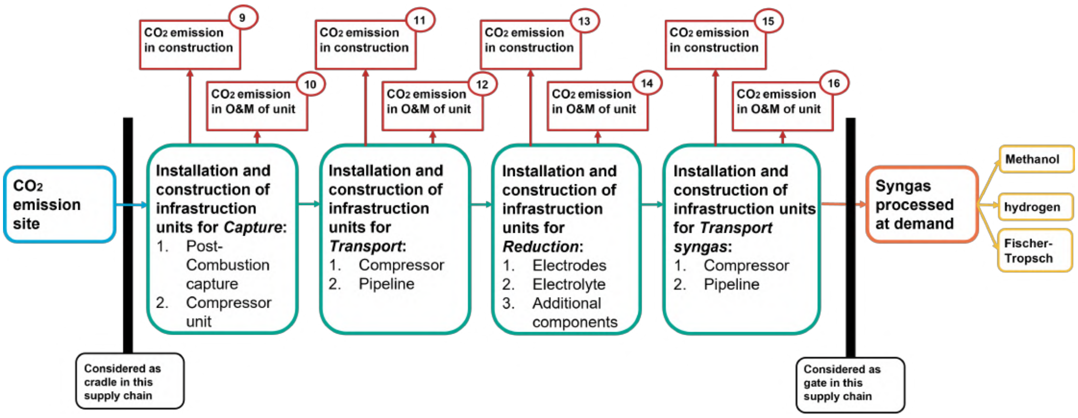


Figure 3.4: Schematic overview of the Indirect CO_2-eq emissions

For the scope of this thesis, other direct or indirect CO_2-eq emissions are not considered. Any additional indirect emissions, such as those related to transportation, distribution, or disposal of materials for O&M, are intentionally excluded from consideration.

Different analyses can be used in order to define the goal of the LCA for this CO_2E SC infrastructure. The two main methods are midpoint analysis and endpoint analysis [45]. Midpoint analysis puts the focus on intermediate environmental indicators, such as greenhouse gas emissions, water consumption, or acidification potential. Endpoint analysis on the contrary puts the focus on more comprehensive environmental impacts, often expressed in terms of human health and ecosystem quality.

The method chosen was the ReCiPe2016 midpoint. The choice for midpoint is validated since it enables a specific assessment of the GWP and is relatively less complex to interpret compared to an endpoint analysis [24][14]. The comprehensive and up-to-date data of the Idemat databases make it a good candidate for the environmental assessment of a CO_2E SC infrastructure. The ReCiPe2016 midpoint method is renowned for its comprehensive environmental impact categories, enabling precise identification of key impact areas. This feature is crucial for developing focused strategies to minimise environmental impacts effectively.

The combination of the defined scope and set goal forms the first step of the LCA conducted in this thesis, however, the next steps are needed in order to quantify the different environmental impact factors.

3.1.2. Life Cycle Inventory Assessment for a G2G CO_2E SC Infrastructure

For the Life Cycle Inventory Assessment, each individual echelon within the CO_2E SC Infrastructure will be discussed and visualised in bar plots using the Idemat databases, validating the main focus on global warming potential. If not applicable in the database, academic literature will be used in order to estimate the impact category.

Life Cycle Inventory Assessment of a Capture unit

For the scope of this thesis, the LCI data for a carbon capture unit based on an amine solution is used and applied to all biogenic sources just as described by Koorneef et al. 2008 [55]. In this paper, thorough research has been conducted on a post-combustion capture unit used for a power plant.

It is within the research of Koorneef et al. 2008, assumed that for the construction of a carbon capture unit, 235 tonnes of steel for the absorber and stripper is used. 82 additional tonne for piping and smaller equipment. Lastly, it is assumed that there is 1 cubic meter of concrete used, and together with the transportation footprint, the assumed lifetime of the capture unit is 30 years. See figure C.3 in Appendix C for a more detailed overview.

Based on the data obtained from the Idemat database, it is calculated that the constructional footprint regarding CO_2-eq footprints is 0.28 Mtonne CO_2-eq per build capture unit. For the scope of this thesis, it is estimated that the CO_2-eq footprint for O&M is 4% of this value for constructional footprint. Thus, it is assumed that the annual O&M CO_2-eq footprint of a capture unit corresponds to 0.01 Mtonne.

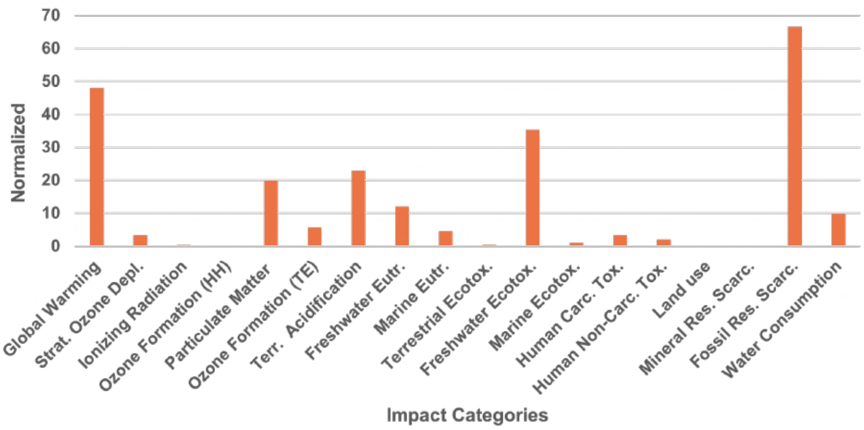


Figure 3.5: The normalized bar chart of the inventory analysis for a carbon capture unit

Figure 3.6 displays the normalized inventory analysis for a carbon capture unit and the characterization of the inventory analysis. Normalization in LCA studies involves comparing the obtained results to a reference value, such as the average environmental impact caused by an individual over a specific timeframe, to contextualize and assess the relative significance of the environmental impacts identified [110]. These reference values are used to make the data dimensionless and more easy therefore to interpret. This reference situation could be one person´s resource use and emissions released in the world during one year. Normalization therefore converts complicated units into fractions of this average person´s score per impact category. For the normalization factors used, the ReCiPe 2016 scores by the RIVM are used [88]. This is in line with the methodology proposed by Simapro.

From the normalized inventory displayed in figure 3.5 one can see that the Fossil Resource Scarcity, Global Warming Potential and Terrestrial Acidification are the most prominent impact categories. This observation validates the main focus on Global Warming Potential.

Life Cycle Inventory Assessment of a Transport unit

Due to limited data on the transport of syngas, it is assumed that all transport for the LCIA of this thesis is the same as for a transport pipeline of natural gas. Several studies model CO_2 transport via pipelines just the same way as natural gas transport [72]. However, little is known regarding the transport of syngas via pipelines. The main reason for this is that it is mostly used as an intermediate on-site and therefore transportation is minimal. The lack of academic literature regarding syngas transport via pipelines validated that it is assumed that syngas can be transported similarly to natural gas. For the LCIA of these onshore pipelines different studies have been used to calculate their footprints [55] [27].

It is assumed that there is a 2% leakage during the transport of CO_2 or syngas due to handling, compressing and permeation through cracks and imperfections of the transport pipeline [112]. Additionally, it is assumed that syngas and CO_2 will have the same degree of leakage during transport. However, for the leakage of syngas, a correction factor is applied in order to convert the mass amount of syngas leaked for its Global Warming Potential into CO_2-eq. The molar ratio of CO:H_2 in syngas is assumed to be 1:2 just as proposed by the ISPT report [102]. For this part of the CO_2-eq emissions, it is assumed that the GWP of syngas can be estimated as the average of the molar ratio of the binary mixture of syngas with respect to their individual global warming potentials. It is in this assumption important to note that it is assumed that hydrogen and carbon monoxide leak and permeate in the same order of magnitude. However, due to the size of the hydrogen, it is much more likely that it will leak and permeate at a higher rate than carbon monoxide [83][84]. Based on the assumptions mentioned and the GWP values provided for hydrogen and carbon monoxide, it is estimated that the GWP of syngas is 4.5 as 20 years of carbon dioxide [116][87].

The transport of CO_2 is in the supercritical state and of syngas in the gas phase. Based on the literature found, it is assumed that a transport unit has a heavy 914mm wall piping, with a corresponding thickness of 20 mm [27] [47]. As a base case for this research, the Prince Rupert 2 pipeline project in Canada is taken as an example. The factor for the carbon footprint has been scaled down to the capacity of the maximum transport of mass in this specific use case. Based on the literature found and its corresponding scaling it is estimated that there is a 0.03 [Mtonne CO_2-eq per Mtonne transported per km]. This factor includes all possible CO_2-eq emissions (constructional, O&M and energy consumption). The values regarding footprints for the construction footprint of Di Lullo et al 2020. are compared to the LCI data proposed by other studies and are in the same order of magnitude [55].

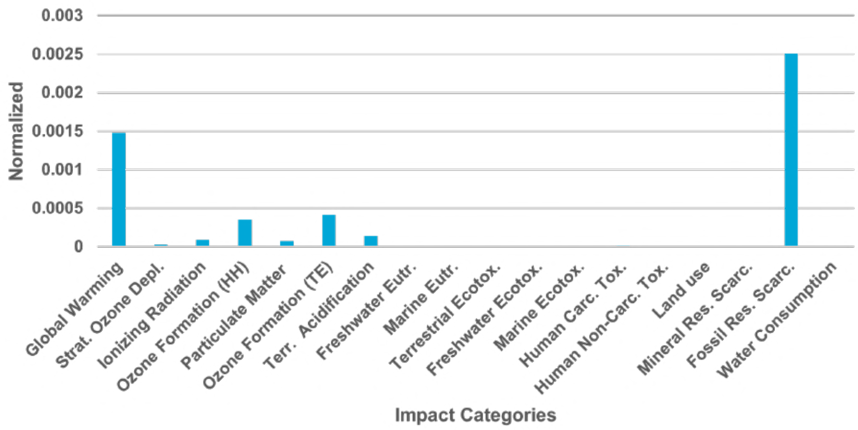


Figure 3.6: The normalized bar chart of the inventory analysis for a Transport unit

However, to validate the constructional footprint of a natural gas pipeline transport unit a normalized inventory was used from the Idemat database. From the normalized inventory displayed in figure 3.6 one can see that the Fossil Resource Scarcity, Global Warming Potential and Ozone Formation (Terrestrial Ecosystems) are the most prominent impact categories. This observation validates the main focus on Global Warming potential. For the modelling, the Prince Rupert 2 use case is used as an Inventory Assessment due to its distance dependence and more accurate assessment compared to the Idemat database.

Life Cycle Inventory Assessment of an Electrolyser unit

The electrolyser constitutes a sophisticated and multifaceted facility, yet industrial-scale deployments remain unavailable. Consequently, a combination of a chlor-alkali plant alongside a custom-engineered Solid Oxide Electrolyser Cell (SOEC) to a CO_2electrolysis plant application for BP is used to approximate the CO_2-equivalent footprint of such an electrolyser.

As mentioned in the previous chapter a configurational hot-box module is assumed as in the ISPT report wherein a module has a capacity of 9MW. This is referred to as the standardized capacity of one single module. These modules are assumed to be scaleable linearly to gigawatt scale These stacks can be scaled up to a maximum capacity of 900MW [102].

Different materials can be taken into account for the construction of an electrolyser plant. A Solid Oxide Fuel Cell (SOFC) is an electrochemical device that converts chemical energy directly into electricity by oxidizing a fuel, typically hydrogen or hydrocarbons, at high or low temperatures using a solid oxide electrolyte [113]. Various literature sources have been utilized to explore the use of construction materials like steel, concrete, and iron in Solid Oxide Fuel Cell (SOFC) applications [50] [80] [50]. These materials are considered ancillary materials. An overview of these materials is displayed in table

B.7. An additional focus regarding materials is put on the modules wherein the choice of REEs for the electrode plays a vital role.

Different types of materials can be used as electrodes in the SOEC. Most of the materials used that can form a bottleneck are Rare Earth Elements (REEs). This is a group of 17 chemical elements that are unique regarding their properties and therefore their high-tech applications. For the REEs considered academic literature will be used in order to find the optimal configuration of these REEs. Further analysis of the REEs used for the electrodes and their abundance, distribution, CO_2-eq and cost footprint is in section 6.3.2.

Stijn Yska addressed the potential of alternative configurations for CO_2ER supply chains in his master thesis conducted at the Delft University of Technology for the MSc. Complex Systems Engineering [128]. The field of research conducted in this research has a lot of common ground with the research conducted in this thesis. In an interview with Stijn, he pointed out that a nickel-YSZ cathode and LSM-ScSZ are preferred. In this notation, LSM is an abbreviation for Lanthanum Strontium and Manganite and YSZ is an abbreviation for Yttria Stabilised Zirconia. The choice was based on their abundance and relatively low carbon footprint. A further elaboration of this choice is made in section 6.3.2.

The combination of ancillary materials and the choice of REEs for the module displayed in tables B.7 and B.1 gives rise to the normalized bar chart for the inventory analysis in figure 3.7 of an electrolyser unit.

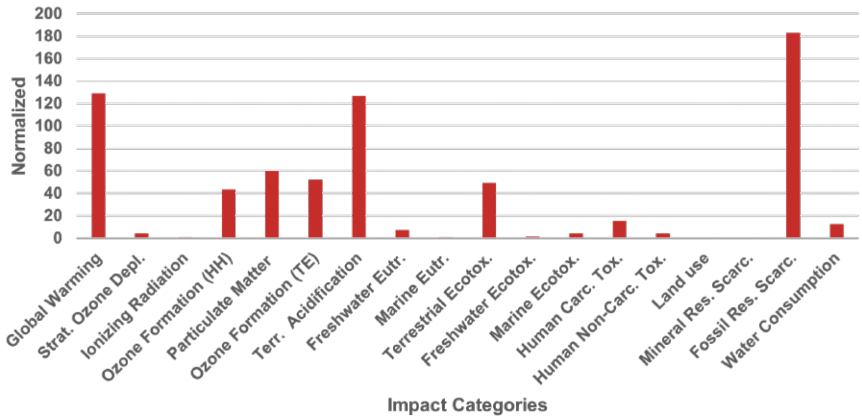


Figure 3.7: The normalized bar chart of the inventory analysis for an Electrolyser unit

Based on this figure it can be concluded that again fossil resource scarcity, global warming potential and Terrestrial Acidification are the most prominent and urgent impact categories for the electrolyser. It can be concluded based on the order of magnitude of the y-axis scale in figure 3.7 in comparison to figures 3.6 and 3.5 the electrolyser has a higher normalized environmental impact compared to the capture and transport unit.

Now that insight has been given regarding the LCI for a G2G CO_2E SC infrastructure, a mathematical model will be discussed in order to reach the final step of the LCA, the LCIA.

3.2. A carbon minimisation model in GAMS

GAMS is a modelling system for mathematical programming problems which has a main focus on optimisation problems and therefore lends itself as a perfect candidate regarding the minimisation of the environmental impact of a CO_2E SC infrastructure. Different models and structures can be used to address such a SC, based on the criteria and objective. For the scope of this master thesis, it was chosen to use a Mixed-Integer Programming (MILP) approach to formulate the problem and use the CPLEX and GUROBI solver. These two solvers are selected due to their efficiency and robustness [56]. A fundamental understanding of the core concept of system optimisation is inevitable in order to formulate a MILP in GAMS. All optimisation problems consist of variables, the objective function and the corresponding constraints. The three main components for formulating such an optimisation problem are:

1. **Variables:** Set of variables that reflect the degrees of freedom or decisions within the problem. There are different types of variables with each having its own form. Example variables come in the form of free, binary, or integer variables. There are two sub-classifications made for the variables used in the MILP proposed.
   (a) Decision Variables: Are linked to a certain decision and the corresponding choice of the model. These variables are binary and can therefore only take the value of 0 or 1. An example decision is, for example, the choice to construct an electrolyser at a specific location or not.
   (b) Regular Variables: Are linked to non-decisive parameters. If capturing from a specific emission location, there is flexibility in determining the quantity of CO_2 to be captured, thereby categorizing it as a regular variable.
2. **Objective Function:** In this specific context, the objective function embodies the overarching objective of the problem, which is to minimize the total environmental impact given the set of variables. The objective function is defined as the minimal amount of CO_2-eq needed to fulfil all syngas demand.
3. **Constraints:** Constraints resemble the boundaries that need to be satisfied within the problem. Constraints can be either linear or non-linear and come from the problem statement. An example in this use case could be the need to always fulfil a certain fraction of syngas demand within the market.

A simplified overview of an optimisation model can be seen in fig 3.8.

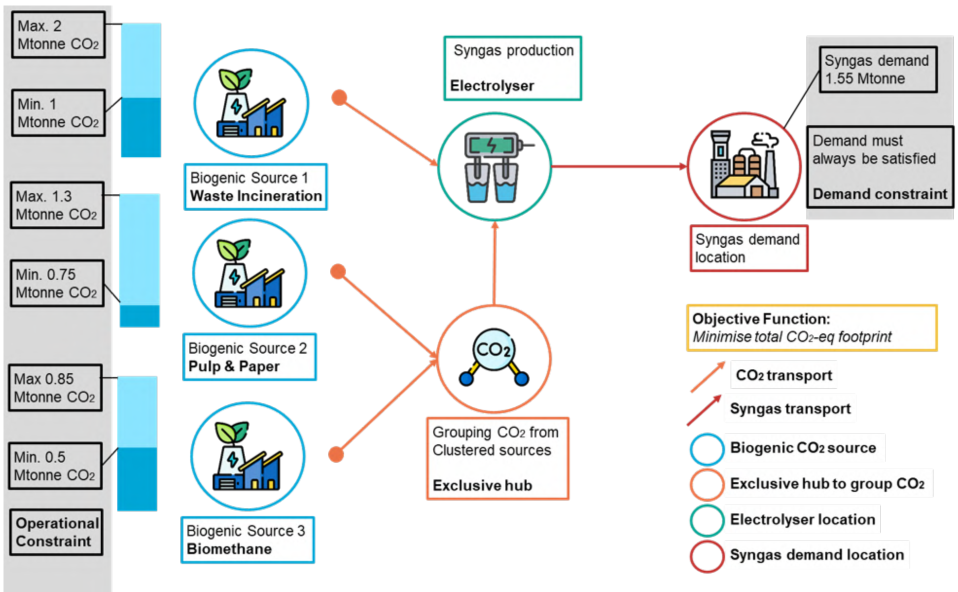


Figure 3.8: A visual representation of variables, constraints and objective function

In this example, three different biogenic CO_2 sources are given which represent the possible supply of CO_2 to the SC. Each of these sources has a specific minimum and maximum amount of CO_2 that can be captured, these resemble the operational constraints. Within these constraints, the model is free to choose and therefore this is a parameter, which can take different values. CO_2 can be captured, transported and converted at an electrolyser. If it is favourable to either construct a capture, transport or electrolyser is denoted by a decision variable. If the decision variable takes the value 1 it chooses to construct that specific unit. If it takes the value 0 it decides to not construct that specific unit. The syngas produced will be transported to the demand location. The demand location has a certain degree of demand that always has to be met, this forms the demand constraint in the supply chain. Lastly, the box in yellow represents the objective function. This minimisation aims to choose the variables in such a configuration that all constraints are satisfied but the total CO_2-eq footprint is minimised.

Note needs to be taken into account that there are two different routes of the CO_2 to be transported to the electrolyser location. As can be seen in the configuration, there is an exclusive hub where the

CO_2 of two separate biogenic CO_2 is collected before it is transported to the electrolyser. This way of transport is possible if the biogenic sources are within a 25 km radius of each other and it is beneficial to capture CO_2 from both sources. The exclusive hub saves transport pipelines and therefore the path length. If it is more efficient to capture from only one single biogenic CO_2 source, or there are no other biogenic sources within the 25 km radius, there is direct transport of CO_2 to the electrolyser.

The point of CO_2 collection is referred to as the exclusive hub. These are located as the point of center between the used biogenic CO_2 sources.

An overview of this mathematically proposed topology can be seen in figure 3.9. In this topology, the different sets can be seen and how they can be divided into subsets. For example, Set C contains all possible biogenic CO_2 sources. From this set, two subsets can be defined. Subset CI represents all individual CO_2 sources from which (if beneficial) CO_2 will be transported directly to the electrolyser. Subset CEH represents all CO_2 that can be used in an exclusive hub. Additionally are sets EH, E and S. Set EH represents all exclusive hub locations in the model. These are dedicated to the point of centre of the corresponding biogenic CO_2 sources in set CEH. Set E represents all possible locations to construct an electrolyser. Electrolyser locations are pre-defined at all CO_2 sources, syngas demand positions and uniformly over the geographical scope of the Benelux. Set S represents the syngas demand positions. These are fixed by their amount of demand and location. For lower market penetration, there are no constraints on where to decrease the amount of syngas demand to be satisfied, neither at which specific location. Therefore, different demand configurations can be beneficial for different CO_2E SC infrastructures.

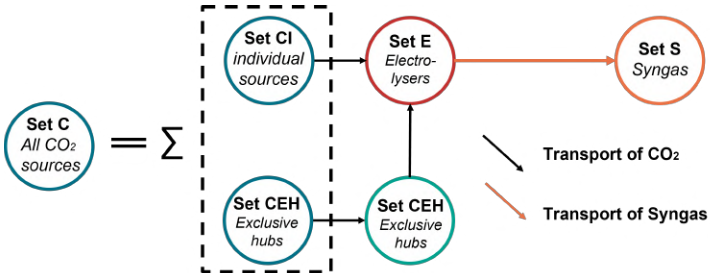


Figure 3.9: The topology of the CO_2E SC for the Benelux usecase

From this schematic overview, it can be concluded that there are multiple possible routes for the CO_2 to be transported from the source to the electrolyser. There are 4 distinct transport routes that can be identified in this topology.

These routes are defined as the following:

1. CI - E: The CO_2-eq footprint due to CO_2 transport from individual CO_2 source to the electrolyser.
2. CEH-EH: The CO_2-eq footprint due to CO_2 transport from CO_2 source to the exclusive hub.
3. E-S: The CO_2-eq footprint due to SG transport from electrolyser to the syngas demand position
4. EH-E: The CO_2-eq footprint due to CO_2 transport from the exclusive hub to the electrolyser position.

If it is beneficial to choose a certain connection and construct a specific electrolyser a binary variable is connected to this decision. The existence of this decision is connected to an indicator constraint. Since this variable can only have integer variables, the problem becomes a MILP where some values are continuous, integer or binary. an overview of these variables is displayed in table 3.1.

Variable	Type	Description	Number of Variables
x(CCI,E)	Free	Amount of CO_2 from individual source to electrolyser	469
x(CEH,EH)	Free	Amount of CO_2 from individual source to exclusive hub	469
x(EH,E)	Free	Amount of CO_2 from exclusive hub to electrolyser	469
y(E,S)	Free	Amount of SG from electrolyser to syngas demand	470

Table 3.1: Overview of All Variables Used

The problem is formulated in GAMS. The output was collected in a GAMS Data Exchange file (.gdx). This .gdx file is reformatted using pycharm Edu.2022.2.2. The executed file from this script is finally visualised using ArcGIS Pro. A schematic overview of this process is displayed in figure 3.10

Figure 3.10: Schematic overview of the software used in the LCIA

Figure 3.11 shows a base scenario within the Benelux. In this scenario, all locations of sources, electrolysers and syngas demand have been displayed. From the map it can be seen that there are sources and syngas demand locations mainly in the western part of the Benelux.

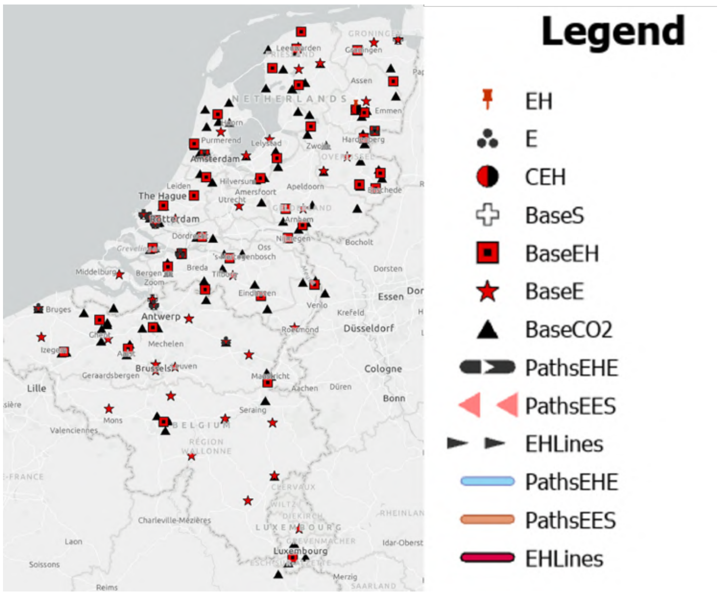


Figure 3.11: All supply and demand locations displayed in the Benelux

Each position has its tradeoffs regarding the variables in the minimisation problem. Examples can be the size and type of biogenic CO_2 source, distance to syngas demand and the size of syngas demand. Table 3.2 displays all syngas demand locations based on the order of magnitude. The values displayed are based on the work of Wiltink et al. 2023 [121]. In this publication, the syngas demand was estimated based on the current syngas use or methanol output of that specific plant. From this table, it can be concluded that the majority of the syngas demand is located in the port of Rotterdam (Botlek), followed by the Moerdijk and the port of Antwerp area. The last syngas demand position is in the north of The Netherlands located in Delfzijl.

GAMS will consider all possible tradeoffs in this configuration wherein syngas demand is always satisfied. On the contrary, the CO_2-eq emission locations might not be close or in the corresponding size near the syngas demand locations. Table 3.3 gives for example an overview of the 5 largest CO_2 emission locations based on biogenic sources within the Benelux. One can immediately conclude that all of these are waste incineration plants that are located in the Netherlands.

To sum up, most of the demand and supply of the Benelux is located in the western part of the Benelux with a major share of supply by waste incinerators. Different topologies are possible where for higher market penetrations transport via exclusive hubs possibly is beneficial to minimise the environmental impact.

CompanyName	Country	Mtonne	S
Shell Nederland Chemie BV (Moerdijk)	NL	2.49	s31
BP Rotterdam Refinery	NL	2.03	s35
EVONIK ANTWERPEN	BE	0.48	s30
Lyondell Chemie Nederland Bv	NL	0.274	s15
Huntsman Holland BV	NL	0.2039	s20
Dynea (Delfzijl)	NL	0.9915	s38
Hexion	NL	0.5524	s41
Caldic Chemie	NL	0.3045	s46
BASF ANTWERPEN	BE	0.12	s19

Table 3.2: Syngas demand data for Chemical Companies [121]

FeatureName	CO_2Source	Mtonnes
AVR NV (Rijnmond)	Waste Incineration	1.73
Afval Energie Bedrijf (Amsterdam)	Waste Incineration	1.31
HVC (Alkmaar)	Waste Incineration	0.981
Attero BV (Moerdijk)	Waste Incineration	0.942
Twence BV Boeldershoek	Waste Incineration	0.897

Table 3.3: 5 Biggest CO_2 Emission Locations concerning waste incinerators [121]

3.3. The Mathematical Formulation

This section will dive deeper into the mathematical formulation of the optimisation model proposed in GAMS based on the variables, constraints and objective function. It will summarize the key takeaways of each component and the reasoning behind the code.

To model the CO_2E SC infrastructure proposed, a fixed-charge facility location problem (FLP) is proposed in GAMS, within this problem there is a finite number of suppliers, plant locations and demand points [60]. The distinctive distances between source, plant and end-use are pre-defined. The electrolyser has a maximum capacity of 100 stacks, therefore the model is referred to as a capacitated multiple allocation problem. To make sure that the logistic transport works, mass balance constraints are present to set an equilibrium between the amount of CO_2 entering the SC versus the amount of SG arriving at the demand positions.

Table B.15 in Appendix B displays an overview of all sets used, table B.16 displays the variables used and figure 3.12 gives a simplified overview of the objective function defined in GAMS. However, the terms applied in the objective function can be classified into 4 different categories.

$$Objective\ Funtion = min\{ \left(\sum m_1 (1-\alpha_{1.j})\right) + \left(\sum m_2(1-\alpha_2)\right) + \left(\sum m_3(1-\alpha_3)\right) + \left(\sum m_4(1-\alpha_4)GWP_{syngas}\right) + \left(\sum E_4\ \beta_4\ m_1\ \alpha_{1.j}\right) + \left(\sum E_5\ \beta_5\ m_2\ \alpha_2\right)$$

$$+ \left(\sum E_6\ \beta_6\ m_3\ \alpha_3\right) + \left(\sum E_7\ \beta_7\ m_4 GWP_{syngas}\right) + \left(\sum \varphi_8 + m_9\varphi_9\right) + \left(\sum \varphi_{12} + m_{13}\varphi_{13}\right) + \left(\sum \delta_{Transport} * m_i\right)\}$$

Inefficiencies in CO_2E SC infrastructure footprint

Energy consumption footprint

Constructional and O&M footprint

Transport footprint

Figure 3.12: Simplified overview of objective function regarding direct and indirect CO_2-eq emissions

As displayed in figure 3.12, the objective function mainly is a function of inefficiencies in the CO_2 SC (Not full capture, leakages, not a full conversion at the electrolyser), the energy consumption of each echelon, constructional and O&M footprints and a transport footprint to include pathlength and mass flow dependencies.

The electrolysis plant can be situated in one of three locations: *(i)* at the source of the feedstock, *(ii)* at a designated intermediate point between the feedstock source and the end-use site, or *(iii)* at the end-use site. Figure 3.13 displays these 5 different supply chain stages, wherein an electrolyser (e_n) can be constructed at stages 1, 3 and 5.

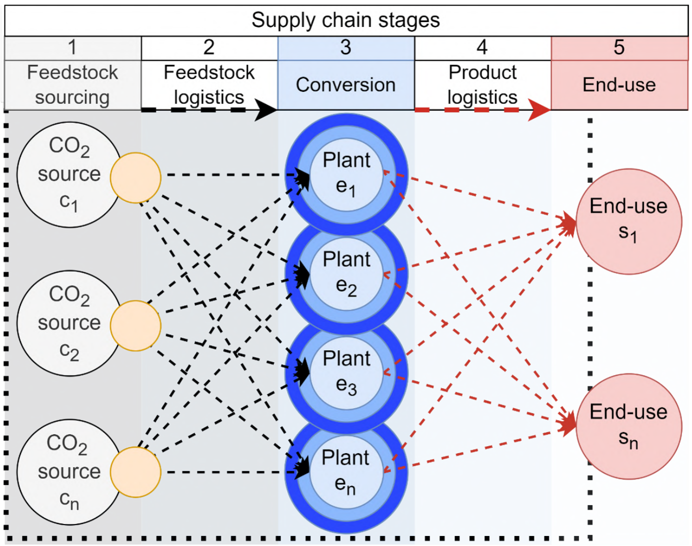


Figure 3.13: The fixed charge facility location problem wherein an optimal SC configuration is the objective function [121]

Additionally, location constraints are established in the mathematical formulation to specify the exact location of electrolysers. The formulation in GAMS is for a Mixed-Integer Linear Problem wherein a linear sum of all direct and indirect CO_2-eq emissions is taken.

In mathematical formulations, several constraints can be identified, but the most prominent and important ones are the following. The demand constraint ensures that all syngas demand must be satisfied to achieve a certain market penetration. The mass balance constraints maintain that mass cannot be created or lost, ensuring the conservation of mass throughout the system. The operational constraints stipulate that at each stage of the supply chain, a certain fixed inefficiency occurs, impacting overall performance.

The objective function is defined as the sum of all direct and indirect CO_2-eq emissions per stage of the SC. A general overview of the objective function applied is given in the following figure 3.12.

3.3.1. A cost minimisation model in GAMS

Apart from the environmental impact assessment, a levelised cost of syngas minimisation problem formulated by Thijmen Wiltink was conducted in order to gain further insights into the economic feasibility of this CO_2E within the Benelux. This specific optimisation aims to see similarities and differences compared to the environmental optimisation model. This is why this specific model was applied to the use case proposed. Similar input, problem formulation and output formatting were used to analyse similarities and differences between the two different optimisations. This optimisation problem is used as well to gain insights regarding the water consumption of CO_2E. However, additional metrics are needed in order to compare and assess the CO_2E SC infrastructures proposed by both models.

3.4. Evaluating optimisation models

In order to evaluate the optimisation models proposed there will be a focus on objective criteria and corresponding market penetration, topology analysis and transporting preference. Additional metrics can be identified to compare and assess CO_2E SC infrastructure configurations, however, these 4 are chosen due to their robustness and effectiveness.

3.4.1. Objective criteria and corresponding market penetration

For each optimisation problem, an individual type of objective criterion can be defined to evaluate for which market penetration the functional unit is delivered at a minimal environmental impact and costs to the demand positions.
The goal of this objective criterion metric is to measure the total environmental impact of the supply chain by calculating the CO_2-eq emissions per kilogram of syngas produced. It provides a direct measure of the efficiency and sustainability of the supply chain in terms of greenhouse gas emissions.
The objective criterion for the CO_2-eq minimisation problem is defined as the total CO_2-eq footprint emitted due to either direct or indirect emissions, divided over the total amount of syngas delivered, see equation 3.1

$$\text{objective criterion carbon minimisation} = \frac{m_{\text{CO}_2\text{ emitted}}}{m_{\text{syngas produced}}} \tag{3.1}$$

The unit of the objective criterion for the CO_2-eq minimisation is in kg CO_2-eq per kg syngas.

The objective criterion for the cost minimisation problem is defined as the total cost of the CO_2E SC infrastructure divided by the total amount of syngas delivered, see equation 3.2.

$$\text{objective criterion cost minimisation} = \frac{\text{CIE}_{\text{Tot}} + \text{EHE}_{\text{Tot}} + \text{ES}_{\text{Tot}} + \text{Cap}_{\text{Tot}} + \text{Elyzer}_{\text{Tot}}}{\text{m}_{\text{syngas produced}}} \tag{3.2}$$

The unit of the objective criterion for the cost minimisation is in € per tonne of syngas, representing the levelised cost of syngas delivered. The levelised cost of syngas (LCOSG) accounts for the total costs over the lifetime of the syngas production facility, including capital, operating, maintenance, discounted to present value and averaged over the total syngas produced. In other words, it provides a measure or indicator of the cost-effectiveness of syngas production. An additional unit used for both objective criteria is to express the environmental footprint and/or costs per unit of energy of syngas. For this conversion, a fixed value will be used based on either the Lower Heating Value (LHV) or the Higher Heating Value (HHV).

Apart from the objective criteria defined, based on the product delivered at the end of the supply chain, additional metrics can be used in order to assess the configurational design of the CO_2E SC infrastructure. The objective criterion will be assessed as a function of market penetration. Market penetration is defined as the percentage of syngas demand that is met. The chosen methodology allows the model to freely determine which demand to satisfy, at which location, and to what extent. Thus, this is referred to as market penetration. The correlation between the objective criterion and the market penetration can be of added value to the Benelux authorities since it will provide them insights into whether full market penetration is needed. This can be of interest since these CO_2E SC infrastructures can due to their size have a big impact on the Benelux. Additionally, other metrics will be introduced in the next subsections.

3.4.2. Topology Analysis

Based on the work of Wiltink et al. 2023, a framework based on co-location, decentralization and centralization can be used in order to classify different CO_2E SC infrastructures [121]. These three classifications have their own further classifications as specified in figure 3.14.
The aim of this metric is to examine the spatial arrangement of the supply chain components, particularly focusing on the proximity of CO_2 sources and syngas demand points to the electrolysers. It also assesses the connectivity of the electrolysers to multiple sources and demand points.

What is important to notice, is that the radius around the electrolyser is set at a value of 10 kilometres. This is a methodological choice and can be varied. However, this specific value was chosen due to the isolated local areas of Botlek and Moerdijk. The purpose of this exact radius is to allow a classification of different topologies. Based on these topologies an examination and comparison of different CO_2E SC infrastructures can be made.

The framework presented in this topology analysis is a first insight into the configuration of a CO_2E SC infrastructure but additional assessment can be conducted in order to analyse the exact transport impact or source mix.

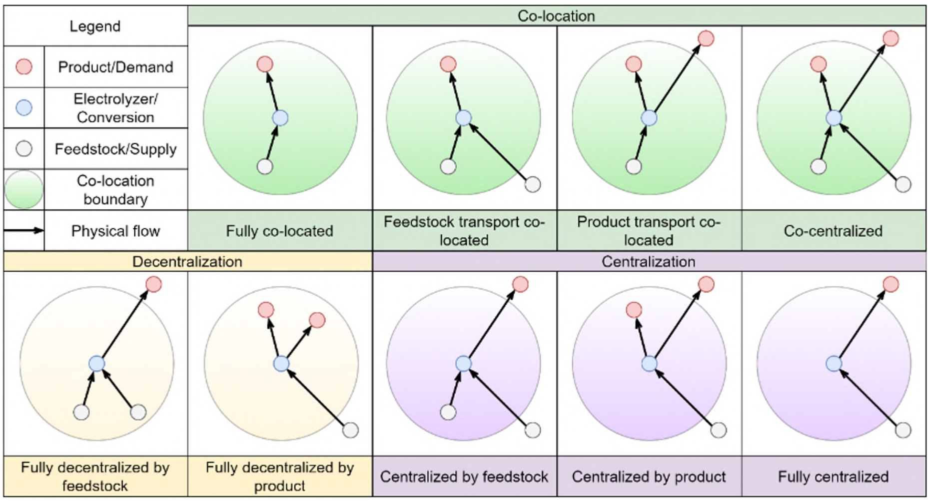


Figure 3.14: Characterization of different supply chain configuration [121]

3.4.3. Other metrics

Additionally to the topology analysis, a quantitative analysis can be conducted based on the exact transport footprint per possible route and the variety of sources chosen. Each of these metrics provides further insights into an understanding of the CO_2E SC infrastructure and enables comparison of specific configurations and identify similarities or differences.

The transport footprint metric

Apart from the topology analysis, the transport footprint per route can give a further understanding of lessons learned from the optimisation model provided. As stated earlier in section 3.2, four different routes are possible each with its footprint depending on the distance covered in kilometres and the amount of mass transported through it. An analysis in the transport footprint of each different route as a function of market penetration can give insights regarding the tradeoff between the size and distance of certain routes in the model.
This metric examines the preferences and efficiencies in transporting CO_2 versus syngas within the supply chain. This process considers three factors: travel distances, transportation emissions, and whether the CO_2 is brought together at central locations before being delivered to the electrolysers.

Source mix

The size, location and source characteristics can be of interest for the optimum CO_2E SC infrastructure since these can play a vital role in the CO_2-eq and cost minimisation.

As mentioned in section 3.2, the majority of biogenic CO_2 available in the Benelux is from waste incinerators. Their size and location might make them an ideal candidate for capture of CO_2. However, limitations are there in the purity of the outlet CO_2 stream of different sources. For the CO_2-eq minimisation, there is no differentiation between different CO_2 sources. But for the cost minimisation function, a differentiation was made based on the purity of the flue gas exiting the biogenic CO_2 source. It is assumed that the outlet stream of biomethane and bioethanol plants is pure enough that only compression is needed prior to transport, resulting in lower costs [32].

This metric evaluates the diversity and types of CO_2 sources used in the supply chain. It categorizes the sources (e.g., waste incinerators, pulp & paper factories, bioethanol plants, and biomethane plants) and analyses their proportions.

3.5. Additional environmental insights

This section will discuss additional environmental insights regarding the CO_2E SC infrastructure considered, including water consumption and the use of critical materials by the electrolyser, apart from

CO_2-eq emissions. Water consumption by the electrolyser will be considered an additional environmental criterion, as it is estimated to have a significant impact. The water consumption is calculated as a function of the amount of syngas produced and is therefore a linear function of the constraints set for the model. However, this function can still provide valuable insights into the water consumption of the CO_2E SC infrastructure and be put into perspective of the overall water consumption. The water consumption by the electrolyser is estimated as proposed in the work by Detz et al. 2023 in which it is proposed that the [Mtonne SG/yr]/[Mtonne water/yr] can be estimated with the factor 0.86 [26]. Therefore, this constant will be applied.

Subsequently, for the use of SOECs a wide variety of materials are used of which some can have a significant environmental footprint.

First of all, a wide range of metals can be used for the electrode configuration. Based on academic literature the following notation is used to indicate the materials used in a SOEC: *Cathode*|*Electrolyte*|*Anode*, consequently the same notation will be used in this report. Figure B.1 displayed in Appendix B is a first overview of all different possible configurations for the electrode, anode and electrolyte. This table is based on the MSc. thesis work of Stijn Yska conducted in 2022. It is important to note that additional materials are used. Examples are the materials used for the interconnects between the cells, cell sealant and the housing of the stack [97]. For the scope, the focus will be put on the single-cell composition. Based on the conclusion drawn from the research of Yska's thesis, the most common configuration of SOECs for co-electrolysis is Ni-YSZ|YSZ|YSZ-LSM. The specific configuration chosen is validated by academic work [132] [49][39][75]. Based on this specific configuration the following materials are considered for this research: Nickel, Yttrium, Zirconium, Lanthanum, Gadolinium, Cerium, Strontium and Manganese. These materials will be of pivotal function for HT-SOECs in co-electrolysis mode. A schematic overview of such a configuration is depicted in figure 3.15

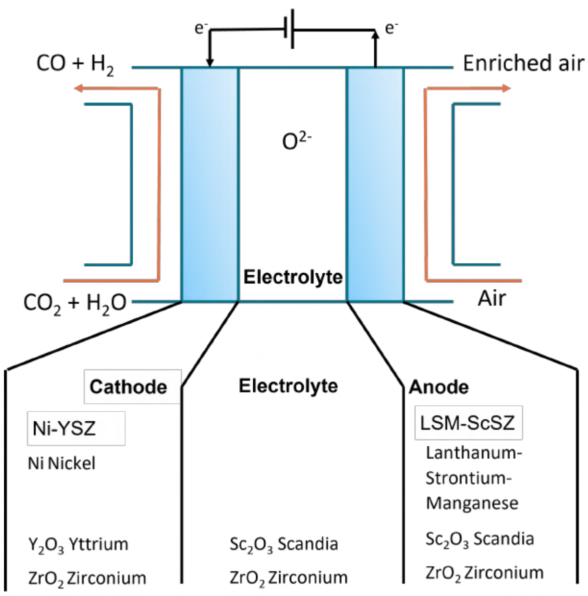


Figure 3.15: A schematic overview of the SOEC and the configurations of materials used

The rest of this thesis will evaluate these materials based on the following criteria:

1. **Abundance:** *Availability and prevalence in nature*
2. **Geographical distribution:** *Distribution worldwide*
3. **CO_2-eq footprint:** *Emissions due to extraction and processing*
4. **Costs:** *Expenses due to extraction and processing*

These 4 criteria are chosen since they can form the main barriers to the implementation of these SOECs and therefore of a potential CO_2E SC infrastructure as well. Chapter 6 will elaborate on these criteria defined, but first, a verification of the mathematical model will be given.

3.6. Verification of model

Next, a framework for environmental impact assessment will be presented, followed by the development of a carbon minimization model in GAMS and its mathematical formulation. Subsequently, the evaluation of this model will lead to the proposal of a strategy to verify its findings. This part of the research is of crucial importance to confirm whether the model corresponds as expected and can compute the initial set goal. While this aspect belongs to the overall methodology, its significance warrants a dedicated chapter for in-depth exploration. The following chapter will elucidate on different scenarios imposed on the model.

4
Verification of the mathematical model

This chapter will focus on the verification of the model optimising for the CO_2-eq emissions. First of all, section 4.1 will display the implementation strategy used to verify the model proposed in the previous chapter. Second of all, section 4.2 will give an overview of the base scenario which will be used as a reference for the rest of this chapter. Third of all, Section 4.3 will give an overview of the different scenarios and parameters used to verify the model.

4.1. Implementation strategy for verification

Figure 4.1 shows a visual representation of the methodology applied in order to verify the CO_2-eq minimisation model wherein a focus is put on the different scenarios and their results in comparison to the base scenario.

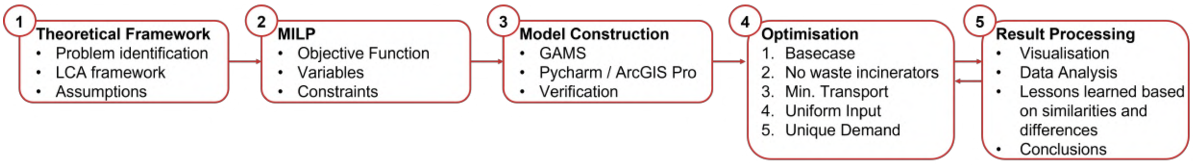


Figure 4.1: Chapter 4 will focus on the 4th step of the methodology strategy proposed.

From this diagram, it can be concluded that after the theoretical framework, MILP and model construction the fourth step is to optimise the model and verify its findings which in this case is conducted via four different scenarios. These scenarios are executed with respect to the base scenario but a solemn variable or constraint is changed. The obtained data is visualised in ArcGIS Pro and the results are compared to the base scenario. The goal of this verification process is to confirm whether the model has been implemented correctly according to its specifications as intended to be. Therefore, a base case simulation is needed as a benchmark.

4.2. A base scenario

In this section, a verification of the base scenario is proposed to minimise the environmental impact of a CO_2E SC infrastructure optimisation model. The base scenario serves as the reference point where all parameters and constraints are set to their initial values. This verification ensures that the model functions correctly under the initial conditions and provides a foundation for comparing various alternative scenarios described later in this chapter.

4.2.1. Default input parameters

The default input parameters for the base scenario are derived from the research conducted by Wiltink et al. 2023. This research prioritises using real-time CO_2 emission data from biogenic sources. In this research it is estimated that the demand for syngas is parallel to current methanol production levels [121]. Additionally, in this study, the distances between potential nodes in the network are quantified in kilometres but are adjusted using a terrain factor. This adjustment accounts for various complexities such as steepness, mountainous terrain, and water bodies. Consequently, constructing a specific SC infrastructure in a densely populated area would be less advantageous compared to the same infrastructure in a less densely populated area due to these terrain factors. The base for this quantification of terrain lies in the work by van den Broek et al. 2013 [108]. The raster proposed has a 325x325 meter resolution for the Benelux scope. With the use of this raster, a basis is constructed for ArcGIS Pro to accumulate the CO_2-eq footprint of distances. ArcGIS Pro uses this output in combination with the final positions to find the optimal path between two different locations in the CO_2E SC infrastructure. This averaging can pose unusual routes for relatively smaller distances.

4.2.2. Model Setup for the Base Scenario

The optimisation model proposed in GAMS (45) is a MILP that focuses on minimising the objective criterion regarding the environmental impact using a CPLEX 22.1.0.0 MILP and GUROBI solver. The system ran with an AMD Ryzen 5 5625U with Radeon Graphics 2.3GHz processor and 8 GB RAM. The problem comprised binary, integer and free variables. The model was solved for a resource limit option of 29000, which constrains GAMS to use only 29000 kilobytes. The convergence criterion is set to 0.0001, resulting in a maximum optimality gap of 0.0001%. The set boundaries resulted in a solve time of 4 minute and 47 seconds.

The output is saved in a Gams Data eXchange (.gdx) file, which is converted using a PyCharm (Edu 2022.2.2, Python 3.9) script proposed by Wiltink et al. 2023 to visualise the obtained configuration in ArcGIS Pro [121].

Lastly, the validation of the base scenario involves several key steps. A comparison is made to alternative syngas production routes to assess and nuance the results obtained from the base scenario. Different syngas transport routes are identified, and for the scope of this thesis research, validation is made by comparing the base scenario to biomass gasification and SMR with CCS. Chapter 5 will further elucidate this validation process and provide a broader perspective regarding the results obtained from the base scenario.

4.3. Different scenarios and parameters

To assess the behaviour of the optimisation problem formulated, visualisations in ArcGIS Pro for different market penetrations are necessary to verify and understand the outcome of the metrics. Therefore, four different scenarios are identified and applied to the model to force unusual configurations, resulting in further verification of the optimisation model proposed.

4.3.1. No waste incinerators Scenario

The exclusion of waste incinerators from the CO_2 input options is validated by the presence of impurities in their flue gas streams, rendering them less favourable as biogenic CO_2 sources compared to other alternatives. This decision is supported by the fact that waste incinerators account for a significant portion, approximately 77%, of all available biogenic CO_2 in the Benelux region, which can push the model towards more unusual configurations. From these new CO_2E SC infrastructure configurations valuable lessons can be learned since not full market penetration will be possible. Therefore, this scenario represents a realistic and practical approach to modelling the CO_2E supply chain infrastructure.

With a back-on-the-envelope calculation, it can be estimated that due to the fact that only 23% of the biogenic CO_2 is available, resulting in less than 28% of the syngas market can be satisfied. A quick overview of the share of each type of biogenic CO2 source can be seen in Figure 4.2, from which the data is based on the work of Wiltink et al. [121].

4.3.2. Minimal Transport Footprint Scenario

The CO_2E SC infrastructure's significant influence on land use in densely populated regions of the Benelux can be the potential bottleneck regarding societal acceptance. This validates the assumption that additional, and hence longer, pipeline transport routes may be necessary to mitigate the impact on densely inhabited areas. Therefore, it is validated to constrain the model to a certain minimal threshold of transport footprint in order to mitigate these additional pipelines. For this scenario, a minimal transport

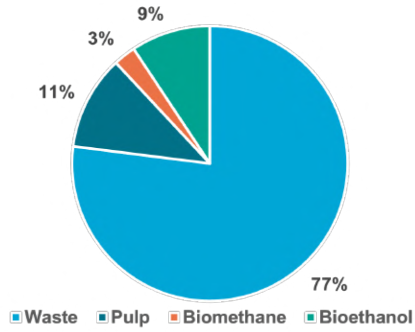


Figure 4.2: Share of every type of biogenic CO_2 source in the Benelux

footprint for the CI-E, CEH-EH and EH-E is set for a minimum of 10 Mtonne CO_2-eq. This means that no matter what the configuration in GAMS is, the system will always build its pipeline structure in such a way or transport enough mass, that the combined CO_2-eq footprint of that specific route in total equals 10 Mtonne of CO_2-eq.

4.3.3. Uniform CO_2 input Scenario

To equalize the preference for sources based on their size, a uniform CO_2 input is validated in order to let a beneficial environmental impact only focus on location and therefore the topology of the source concerning the demand.

For this scenario, all biogenic CO_2 sources available in the input are set to a value of 0.1 Mtonne CO_2 per year. This corresponds to roughly 12.3 Mtonne of CO_2 available in the system.

If waste incinerators are no longer the biggest available sources in the system, equal chances are created based on the size of the biogenic CO_2 sources. For minimising the environmental impact of the CO_2E SC infrastructure the main focus regarding capture is now purely on location, therefore, the topology mix for local sources is of most interest in this configuration. Although this scenario may seem unrealistic due to the improbable uniform distribution of CO_2, it nonetheless offers valuable insights into the advantageous topologies concerning environmental impact, thus providing valuable insights for optimising the transport routes and electrolyser locations in the CO_2E SC infrastructure.

4.3.4. A single demand location in Delfzijl

To comprehensively evaluate potential demand locations not proximate to large sources, this scenario will put focus only on syngas demand from the Delfzijl location. In this scenario, all other demand points, including Botlek, Moerdijk, and Antwerp, are set to zero. Consequently, the only demand originates from the Dynea plant in Groningen, with an annual demand of 0.99 Mtonne of SG.

The selection of Delfzijl as the sole demand location stems from its unique and isolated geographical position. Situated in the Dutch provinces of Groningen, Friesland, and Drenthe a limited amount of small biogenic CO_2 sources, primarily biomethane plants are available. The limited options of large CO_2 sources will push the model towards new configurations from which valuable lessons can be learned based on the similarities and differences compared to the other scenarios.

This chapter verifies the base scenario and outlines four distinct scenarios for the implementation strategy. This forms the last step of the methodology proposed, before moving towards the results.

5
Results

This chapter will elaborate on the final step of the implementation strategy proposed. Firstly, section 5.1 will give the validation of comparable syngas production routes regarding their GWP. Secondly, section 5.2 will give an overview of the results obtained for the base scenario. Thirdly, section 5.3 will give an overview of the results obtained for the four different scenarios. Lastly, Section 5.4 will give an overview of the results obtained from the cost minimisation.

5.1. Validation of model outcome

Based on the academic literature found, it can be concluded that an average objective criterion of 3.47 kg CO_2-eq per kg syngas and 10.2 kg CO_2-eq per kg syngas for SMR with CCS and biomass gasification are obtained. This analysis is displayed in tables 5.1 and 5.2. Note needs to be taken into account that the comparative analysis conducted in this section is based on academic literature wherein a CO_2-eq footprint per mass unit syngas is stated. From these publications it is not always clear the boundaries set for that specific research, therefore, it is recommended that further research is conducted. A more detailed approach can give additional valuable insights regarding the validation of the model proposed.

Deviations in the tables provided are due to the fact that each publication has its own assumptions and system boundaries set. This heavily affects the CO_2-eq footprints found. For biomass gasification, the type of biomass used has a significant effect on the objective criterion. The moisture content, treatment of the feed and handling along the gasification process are some of the factors that come into play.

Reference	Value	Unit
Hospital-Benito 2023 [44]	6	[kg CO_2-eq per kg SG]
Zang 2024 [129]	3.43	[kg CO_2-eq per kg SG]
Afzal 2018 [3]	0.96	[kg CO_2-eq per kg SG]
Salkuyeh 2018 [95]	3.5	[kg CO_2-eq per kg SG]
Average	3.47	[kg CO_2-eq per kg SG]

Table 5.1: Objective Criterion of SMR with CCS

Reference	Value	Unit	Comment
Salkuyeh 2018 [95]	24.5	[kg CO_2-eq per kg SG]	Candian pinewood gasification
Azadi 2015 [5]	2.45	[kg CO_2-eq per kg SG]	Algae gasification
Cho 2023 [18]	3.61	[kg CO_2-eq per kg SG]	-
Average	10.2	[kg CO_2-eq per kg SG]	-

Table 5.2: Objective Criterion of various biomass gasification Processes

Although the definition and gates considered for the systems are different or not always stated clearly, the values provided can give an insight regarding an order of magnitude of the CO_2-eq footprint of these synthesis routes. Based on these 8 papers and the results discussed later in this chapter, it can be concluded that:

1. SMR with CCS produces syngas for the lowest CO_2-eq footprint per mass unit of syngas followed by biomass gasification and CO_2E SC infrastructure (3.47, 10.2, 32.92 kg CO_2-eq/kg SG respectively).
2. A correction should be made for the lifetime of a CO_2E SC infrastructure and the solemn focus on the electrolyser.

This section elucidated the validation of the results obtained from academic literature, however, to compare to these numbers the results of the base scenario are needed.

5.2. Results of the base scenario

The base scenario is the run conducted on all initial inputs and will act as a baseline for all other scenarios. In this scenario, all original input, variables and constraints are formulated and minimised for an environmental impact regarding GWP. According to this scenario, the following values are obtained as displayed in table 5.3.

Metric	Value	Unit
Objective Criterion	32.92	[kg CO_2-eq/kg SG]
Market Fraction	15	[%]
Main Driver in Footprint	Electricity Consumption Electrolyser	-
Topology	1) Fully Co-Located, 2) Fully Decentralized by Product	-
Main Driver transport	E-S, 56	[%]
Source mix	Waste Incinerators, 88	[%]

Table 5.3: Metrics of base scenario

Based on these metrics, the objective criterion is reached at 15% market penetration for a value of 32.9 kg CO_2-eq per kg SG delivered, which will be elaborated on further with the corresponding visualisation in ArcGIS Pro.

The topology of choice is fully co-located and for market penetrations higher than 6% fully decentralized by product is also observed. Lastly, the source mix mostly relied on waste incinerators and the transport of syngas from the electrolyser to the demand location was the main contributor to the transport footprint.

Now an overview has been given of the four metrics defined to assess this CO_2E SC infrastructure, a visual representation is needed to understand why these values and characteristics occur in this scenario.

5.2.1. Visualising the base case scenario

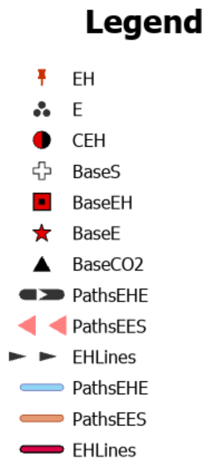


Figure 5.1: Legend to interpret ArcGIS Pro

Figure 5.2 displays visualisations of the base case scenario for the market fractions 25%, 50%, 75% and 100% respectively. In the left top corner is the 25% market fraction penetration, the top right corner displays the 50% market penetration, the bottom left 75% and lastly the bottom right is the 100% market fraction satisfied configuration. It is important to take into account the following legend when observing and analysing the visualisation in ArcGIS Pro (see figure 5.2). For the 25% market penetration in the top left, it can be concluded that there is a co-located topology present for the Botlek area and the Moerdijk area (blue dashed area top corner). This Moerdijk configuration is part of the total configuration found at a 25% market penetration. These CO_2E SC infrastructure configurations are within the 10-kilometre radius. For an increased market penetration it can be observed that there is a connection between the Moerdijk and Botlek area. In this figure in the top right corner (for 50% market penetration), it can be concluded that CO_2 transport is preferred for this distance. From the top right configuration, there are mostly fully co-located and fully decentralized by product topologies present. It can be observed that there is almost no transport of syngas since all syngas are produced directly at the demand position itself. In the bottom left corner (75% market penetration) it can be observed that there is demand in the Antwerp and Delfzijl area. Additionally, it can be concluded that for an increased market penetration syngas transport is preferred for the Delfzijl demand over CO_2 transport. This is an interesting observation since the transport of syngas poses a more environmental impact than the transport of CO_2. Furthermore, it can be concluded that for this market penetration interconnectedness between Botlek, Moerdijk and Antwerp is beneficial in order to minimise the environmental impact. For the 100% market penetration, all demand areas are interconnected and a diverse mix of CO_2E SC infrastructure topologies is observed. The topologies observed are Fully Co-Located and Fully Decentralized by Product (both account for 33.3%), Feedstock Transport Co-Located, Centralized and Product Transport Co-Located (each for 11.1%).

Now the objective criterion, market fraction, main drivers of footprint and the topology of the CO_2E have been discussed, and an elaboration regarding the transport footprint and source mix are the next metrics to discuss.

Figure 5.3 displays the transport footprint of each possible route from which it can be concluded that E-S is the main contributor of the transport footprint regarding CO_2-eq emissions.

The increased and dominant share of the transport footprint by E-S and EH-E transport is in line with the topologies observed. Note needs to be taken into account that the CO_2-eq footprint of the E-S is not scaled for the same linear factor as for the CO_2 transport routes. Since E-S routing has a correction factor that is used for the GWP of syngas during leakage these plots cannot be observed as linear to the total distance of each distinct routing.

Figure 5.4 displays the source mix for the base case scenario for different market penetrations from which it can be concluded that waste incinerators are favoured. For market fractions higher than 55% some large bioethanol plants and/or pulp & paper locations are used. Waste incinerators are preferred due to their size and location. This strong preference and input into the model is the motivation to test its behaviour in new situations wherein this is alternated. Additionally, the flue gas exiting the waste incinerators contains impurities which can pose challenges for the conversion at the electrolyser.

Before proceeding to outline the different scenarios defined in Chapter 4, it is essential to gain a deeper understanding of the optimal outcomes achieved when reaching a 15% market penetration.

5.2.2. Optimum at 15% market penetration

The optimum at the 15% market penetration is obtained due to a perfect tradeoff between a minimal amount of units needed for capture and electrolysis versus a transport footprint. This particular configuration is noteworthy due to the balance between minimizing the number of units required for capture and electrolysis while simultaneously reducing the transport footprint. With this balance, the 15% market penetration scenario maximises the efficiency of the supply chain system. Figure 5.5 displays the CO_2E SC infrastructure visualised in ArcGIS Pro for the 15% market penetration wherein table 5.4 gives an overview of the variables compared to other market penetrations. Based on the figure given

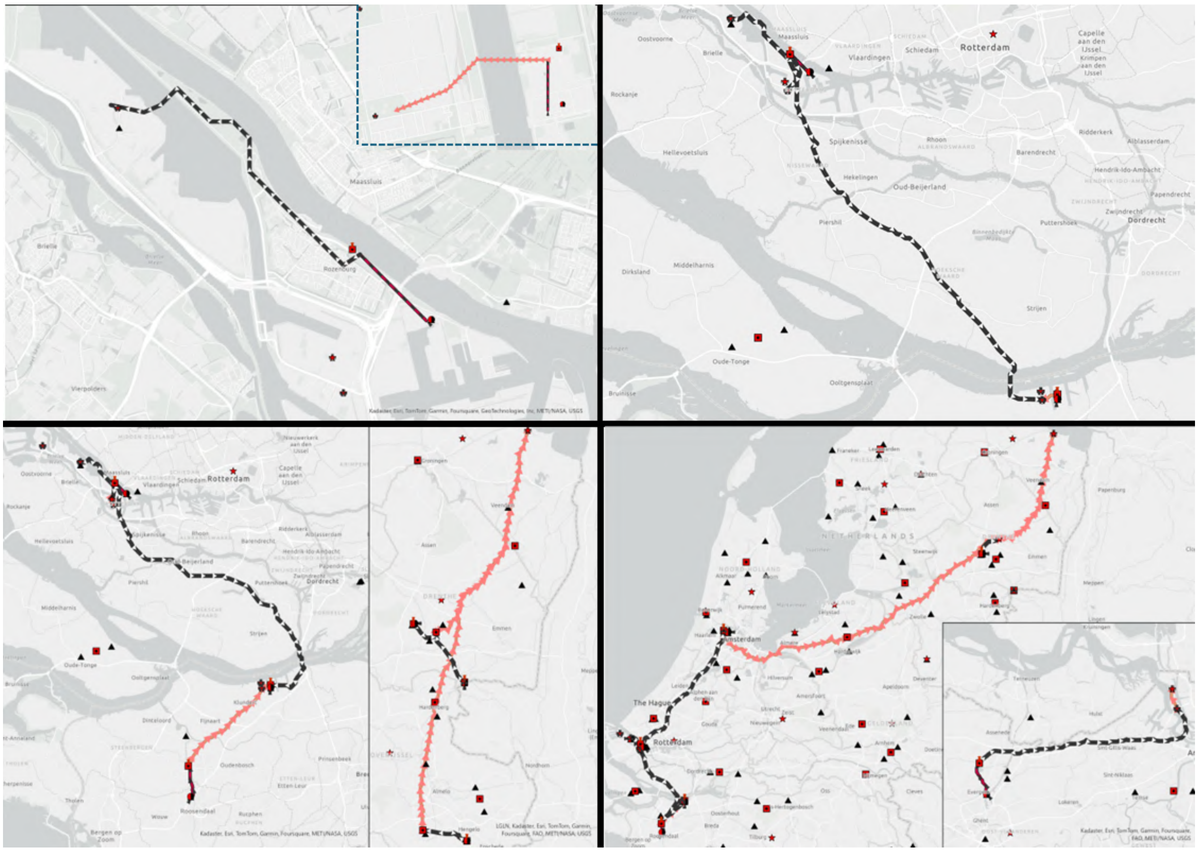


Figure 5.2: Visualisation of base scenario in ArcGIS Pro for 25%, 50%, 75% and 100% market penetration.

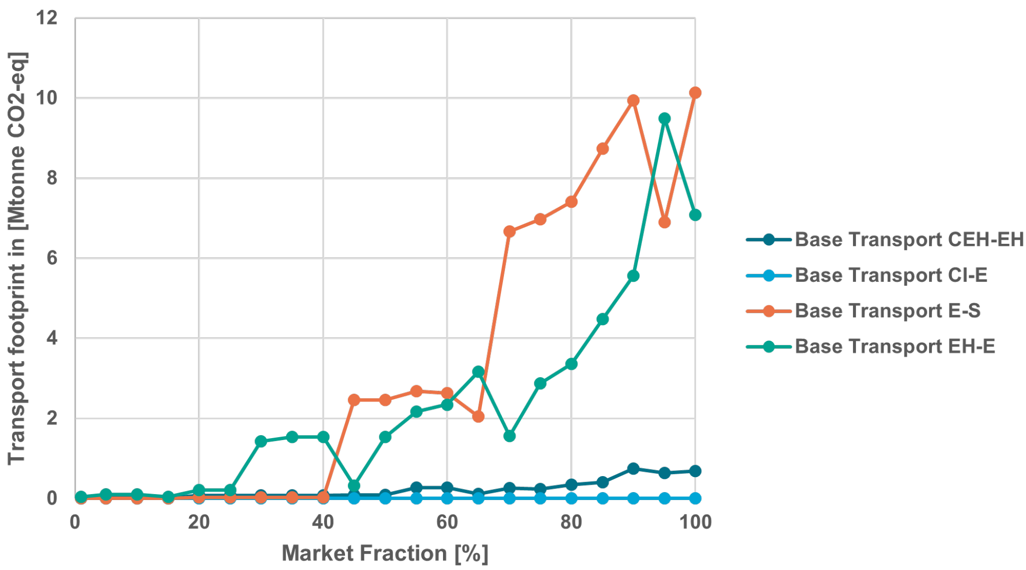


Figure 5.3: CO_2-eq footprint of different transport routes for the base case

and the table displayed it can be concluded that the minimum for the 15% market penetration occurs because there is a perfect balance for only one capture and electrolyser unit for its maximum value of SG produced. Furthermore, it can be concluded that there is a minimum total transport footprint for this particular footprint because this is the last CO_2E SC infrastructure configuration wherein the Moerdijk area is able to configure in a fully co-located topology. For an increase in demand, an additional

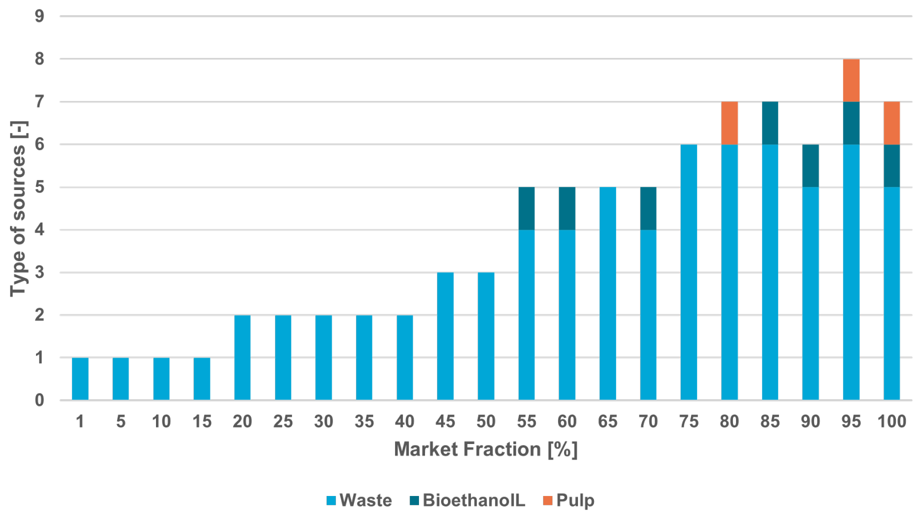


Figure 5.4: Type of biogenic CO_2 sources as a function of market penetration

demand position is needed which in this situation is favourable in the Botlek area which results in an extra capture and electrolyser unit.

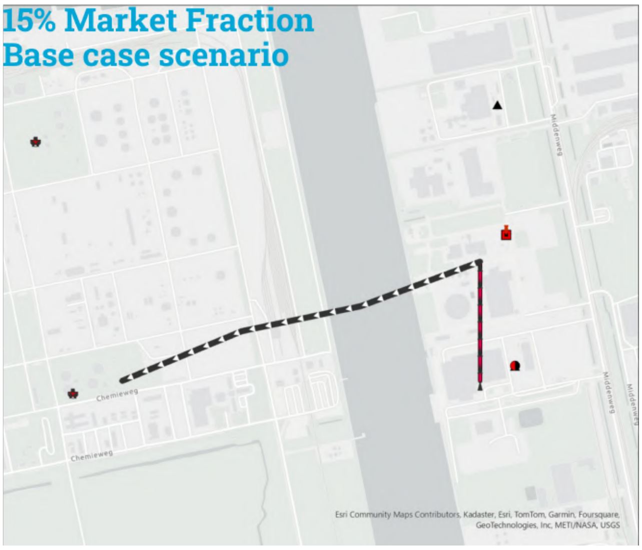


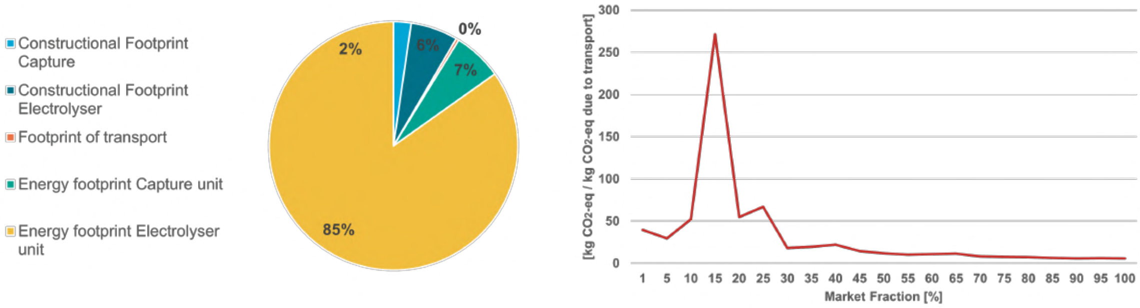
Figure 5.5: Visualisation of the CO_2E SC Infrastructure for 15% market fraction

Therefore, it can be observed that for the 20% market penetration versus the 15% market penetration, the additional production of SG does not trade off versus the constructional footprint of the additional capture and electrolyser unit. With a back-of-the-envelope calculation, this can be validated since the additional capture and electrolyser unit account for roughly 1.03 Mtonne CO_2-eq in total regarding their constructional footprint. In addition to that it would produce around 1.39 Mtonne CO_2-eq via energy consumption. This would make a total of 2.42 Mtonne CO_2-eq. However, an additional amount of 0.05 Mtonne syngas from 0.15 Mtonne of SG at 15% penetration to 0.20 Mtonne of SG at 20% penetration is needed. This results in a footprint of 48 kg CO_2-eq per kg SG, if taking into additional factors along the SC, it can be argued that the objective criterion at 20% is higher compared to the 15% market penetration. As a result, the objective criterion is increasing and the optimum observed at 15% market penetration is validated. Based on table 5.4, an even further increase in market penetration leads to a significant increase in transport footprint and objective criterion. This is because demand positions can no longer just be satisfied with only the fully co-located topology CO_2E SC infrastructure topologies.

Fraction [%]	Capture units	Electrolyser units	Total Transport [Mtonne CO_2-eq]	objective criterion [kg CO_2-eq/kg SG]
1	1	1	0.05	71.91
5	1	1	0.17	39.46
10	1	1	0.17	34.78
15	1	1	0.05	32.92
20	2	2	0.33	34.77
25	2	2	0.33	33.84
30	2	3	1.54	35.77

Table 5.4: Objective criterion for Fraction, Capture Units, and Electrolyser Units

A full overview of table 5.4 for all market penetration can be found in the appendix (see table B.12) Based on the results obtained for the base scenario it can be concluded that the main driver of the environmental impact of a CO_2E SC infrastructure is the electrolyser and its electricity consumption resulting in an objective criterion of 32.9 kg CO_2-eq per kg syngas delivered for a market penetration of 15%. The CO_2E SC infrastructure topology that is most beneficial regarding environmental impact is either fully co-located or fully decentralized by product with a focus on waste incinerators. A contribution of each echelon within the CO_2E SC infrastructure to the objective criterion for the base case scenario at a 15% market penetration can be seen in figure 5.6a.



(a) Share of every echelon to the objective criterion at 15% market fraction in the base scenario

(b) Carbon footprint per kilometre in the base scenario

Figure 5.6: Comparison of echelon contribution and carbon footprint

Figure 5.6b displays the different echelons and their corresponding environmental footprint, it can be concluded that the electrolyser is the dominant contributor regarding the GWP of the functional unit. Two assumptions need to be stated clearly in order to understand the dominant role of the electricity consumption of the electrolyser. Namely, the electricity consumption of the electrolyser itself and the carbon footprint assumed to be associated with the electricity.

1. **Electricity consumption electrolyser:** The electricity consumption of the electrolyser is calculated to be 9300000 MWh/ Mtonne Syngas based on the ISPT report [102]. This high number is due to *(i)* conversion taking place at elevated temperatures (700 ºC), *(ii)* an electrical efficiency of 75% (25% of electricity is lost according to the ISPT report), and *(iii)* the reaction takes place in the gas phase, which means that the vaporization of water consumes a lot of energy.
2. **CO_2-eq footprint of electricity:** The carbon footprint of electricity is based on the work of Silva Ortiz et al. 2020, wherein the supply stage, transformation stage and end-use stage of the current Dutch electricity mix are calculated. In this research, the allocation of each specific stage is used and an average Dutch electricity mix is calculated to be 373.21 g CO_2 / kWh, this value is in line with other academic literature [78][37].

For further research, it is recommended to look at the effect of only renewable energy on the objective criterion on the objective criterion.

However, it is important to notice that for this specific market penetration, the CO_2-eq footprint of the transport is almost negligible compared to the other echelons. This is in contradiction to the other market penetrations. Figure 5.6b illustrates that for this optimum an efficient transport versus footprint is reached. This metric indicates that despite the construction of a significant total footprint due to transport pathways [kg CO_2-eq due to transport], there is a correspondingly high carbon footprint [measured in CO_2-eq mass units]. Put differently, a minimal extent of transport pathways could achieve an equivalent total CO_2-eq footprint as the CO_2E SC infrastructure. This results in the distinctive peak observed in Figure 5.6b. It is therefore beneficial to have a high distance indicator since this means that there is only a relatively small amount of transport distance needed in order to configure the CO_2E SC infrastructure.

Figure 5.7 displays the distribution of topologies as a function of market penetration. It can be concluded that co-located topologies are preferred for lower market penetrations and that fully decentralized by product plays a significant role for higher market shares.

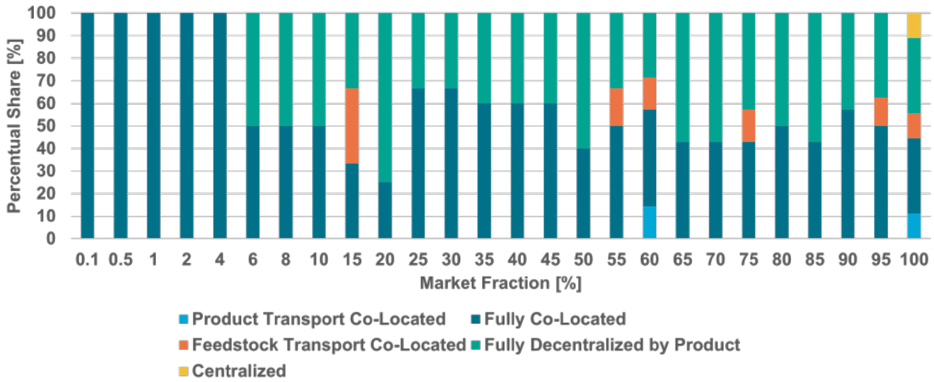


Figure 5.7: Distribution of topologies as a function of market penetration

For certain market fractions feedstock transport co-located is observed as well. Product transport co-located is observed at 60% and 100% market penetration and centralized is solemnly observed for the full 100% market penetration. Based on this a range of topologies is observed, however, the overall preference when a CO_2E SC infrastructure is minimised for its environmental impact is for fully co-located and fully decentralized by product.

As displayed in figure 3.14, it can be argued why there is a preference for this specific topology. Since the transport of syngas has a higher environmental impact compared to the transport of CO_2, it can be argued that it is less favourable to locate the electrolyser not within a 10-kilometre radius of the syngas demand position. In other words, it is environmentally beneficial to locate your electrolyser as close as possible to the syngas demand position. Additionally, the constructional footprint of the electrolyser is relatively high compared to other echelons in the CO_2E SC. Moreover, it's important to note that the CO_2-eq footprint of syngas is higher compared to the CO_2-eq footprint of CO_2 transport, given syngas's higher global warming potential. Therefore, it can be argued that a minimal amount of electrolysers is preferred for the total amount of syngas demand positions. In other words, if one electrolyser has the capacity to fulfil the demand of multiple syngas demand locations, it is environmentally beneficial. Therefore, the so-called "forking" which can be defined as two separate syngas streams exiting the electrolyser is expected. Hence, this is exactly what is observed for the fully co-located and fully decentralized by product topologies. Therefore, it can be argued why these two topologies are preferred when a CO_2E SC infrastructure is minimised regarding its environmental impact. This deeper understanding of the base case scenario paves the way to discuss the results of the verification scenarios mentioned in Chapter 4.

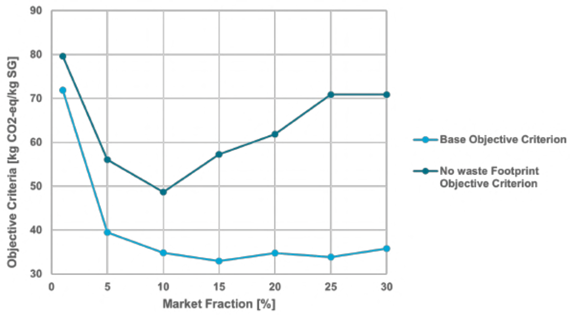
5.3. Results of other scenarios

This section will discuss the no waste scenario, minimal transport footprint, uniform CO_2 input and a single demand scenario in this subsequent order and their corresponding results.

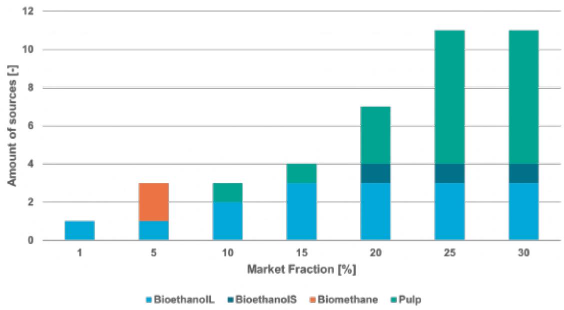
5.3.1. Results of no waste scenario

The no waste scenario shows limited (<30%) market penetration is possible and that there is an increased objective criterion, Bioethanol and Pulp & Paper are the main biogenic sources of choice to minimise the global warming potential of the CO_2E SC infrastructure.

As displayed in figure 5.8a, the scenario of no waste incinerators indicates that achieving a market satisfaction level of less than 30% market penetration is feasible, with an increased objective criterion for each penetration. Bioethanol and Pulp & Paper emerge as primary biogenic sources for mitigating the environmental impact of the CO_2E SC infrastructure.



(a) Objective criterion for the no waste incinerators scenario



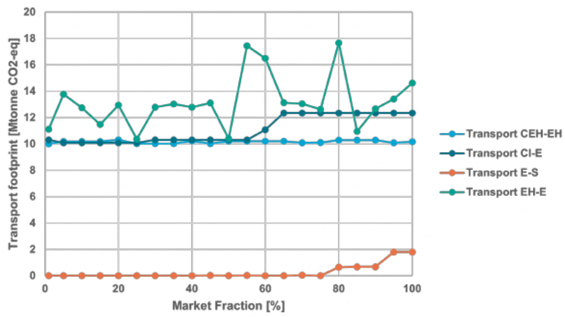
(b) Transport footprint for the no waste incinerators available scenario

Figure 5.8: Results obtained for the no waste incinerators available scenario

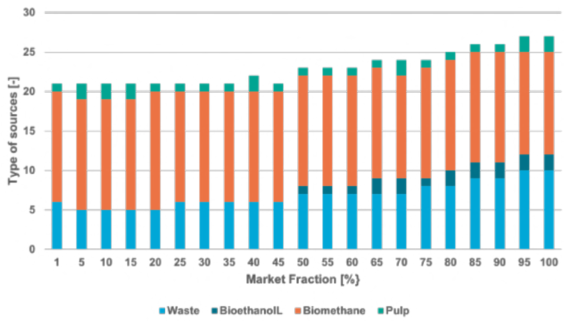
Figure 5.8 displays a diverse mix of sources and a main preference for Pulp & Paper for the higher market penetrations. For market penetrations higher than 25%, a plateau is reached as displayed in figure 5.8a, this plateau means that there is no feasible solution to the objective function since there is an insufficient supply of CO_2 for the system. In mathematical optimisations, this is referred to as the infeasible region. It represents the points where one or more constraints are violated in the problem, in this case, the CO_2 input is insufficient to satisfy the demand constraint in any CO_2E SC infrastructure configuration.

5.3.2. Results of minimal transport footprint scenario

Although the scenario of a minimal transport footprint of 10 Mtonne CO_2-eq is unrealistic, the results regarding source mix give new insights into tradeoffs regarding environmental impact minimisation. From the results obtained, it can be concluded that for this scenario it is beneficial to construct a minimal distance of transport and capture from multiple smaller CO_2 sources along this route. This scenario models the situation that for the CEH-EH, EH-E and CI-E transport routes a minimal transport footprint of 10 Mtonne CO_2-eq is required for every market fraction for which the results are displayed in figure 5.9.



(a) Transport footprint for the minimal transport footprint scenario



(b) Source mix for the minimal transport footprint scenario

Figure 5.9: Results obtained for the uniform CO_2 input scenario

Based on the results displayed in 5.9b a wide diversity and an increased amount of biogenic CO_2 sources can be observed, it is environmentally beneficial for the model to transport the CO_2 over a distance along which CO_2 is captured from small CO_2 sources. Additionally, there is a minimal value for the three constrained transport routes as displayed in 5.9a wherein the EH-E and CI-E for some market penetrations obtain higher values than the threshold of 10 Mtonne CO_2-eq.

Note needs to be taken into account that this scenario is highly unrealistic, especially for this high minimal transport value, however, it can be concluded that for additional transport pipelines, it is environmentally beneficial to capture from smaller and a diverse range of biogenic CO_2 sources. This minimal transport footprint, however, has a detrimental effect on the objective criterion since it is increased compared to the base case scenario, especially for lower market penetrations as displayed in figure 5.10.

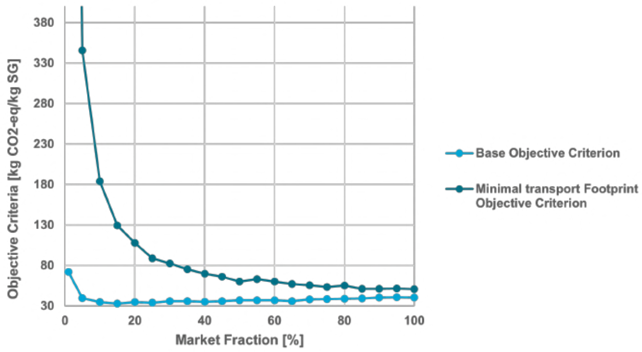


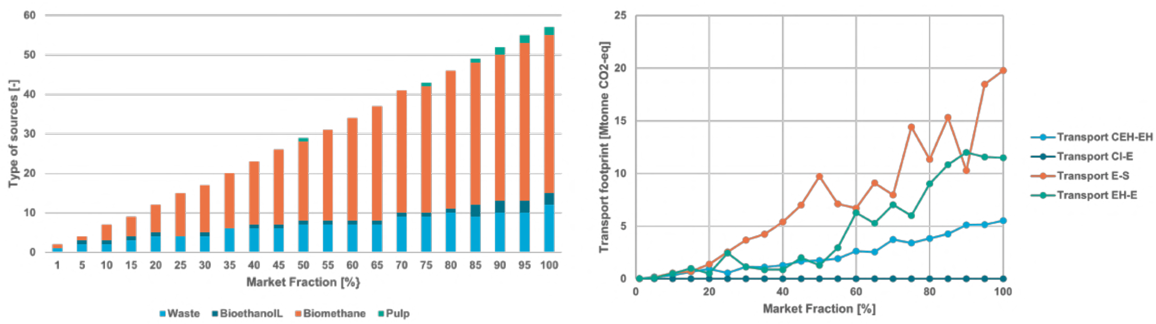
Figure 5.10: The objective criterion for the minimal transport footprint scenario

This graph shows this deviation from the base scenario for the lower market penetration values. The most significant deviation occurs at the lowest market penetration, suggesting that a minimal carbon footprint will result in an increased objective criterion, especially for lower market penetrations.

Although only a small portion of the syngas demand is met, it's worth noting that the supply can be sourced from nearby locations, as illustrated in Figure 5.5. However, despite this proximity, a considerable number of pipelines would still need to be installed. This installation requirement significantly amplifies the total CO_2-eq footprint of the specific CO_2E SC infrastructure configuration. This might be less of a problem for higher market penetrations since already a strong degree of interconnectedness is observed for the full 100% market penetration in the bottom right of figure B.2.

5.3.3. Results of uniform CO_2 input scenario

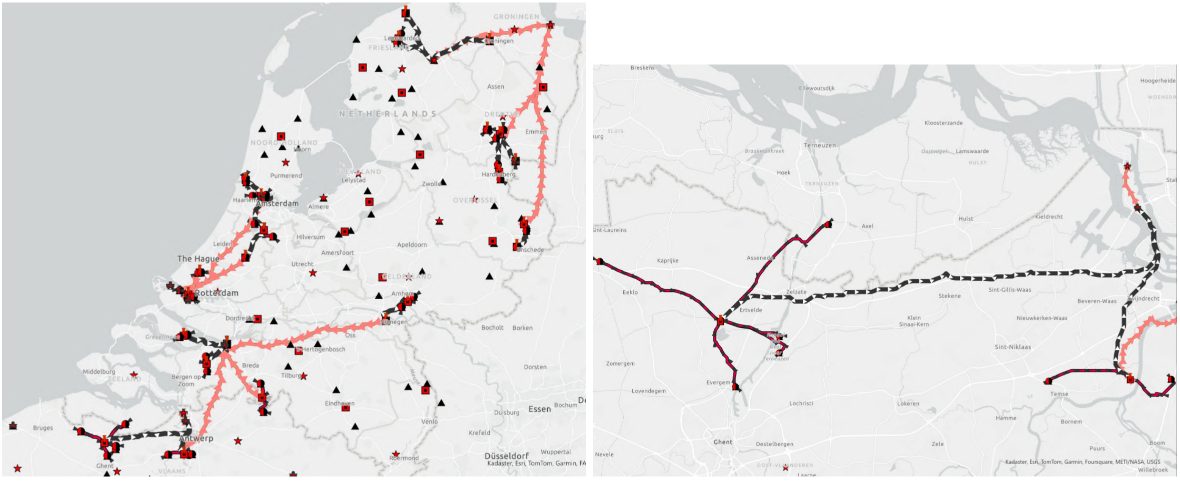
Based on the results obtained for a uniform CO_2 input, it can be concluded that there is a variety of sources used and that the EH-E transport route is beneficial in order to minimise the environmental footprint of the CO_2E SC infrastructure. The results most deviating from the base scenario are plotted in figure 5.11



(a) Source mix for the uniform CO_2 input scenario **(b)** Transport footprint for the uniform CO_2 input scenario

Figure 5.11: Results obtained for the uniform CO_2 input scenario

From these plots, it can be concluded that apart from waste incinerators it is beneficial to capture from biomethane and bioethanol plants too. The sharp increase of the EH-E and its relatively high value in comparison to other routes shows that especially for higher market penetrations the hubbing of CO_2 is environmentally friendly. A CO_2E SC infrastructure configuration for a 100% market penetration can be seen in figure 5.12 wherein note needs to be taken into account for the exclusive hubbing of CO_2 prior to conversion from multiple types of sources in the Antwerp area as displayed in figure 5.12b.



(a) CO_2E SC infrastructure for 100% market penetration **(b)** CO_2E SC infrastructure for zoomed in for the Antwerp area

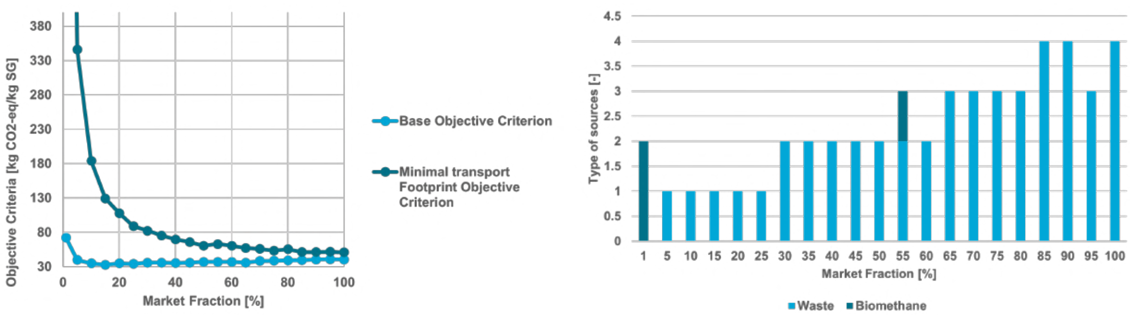
Figure 5.12: CO_2E SC infrastructure for 100% market penetration for uniform CO_2 input

These results clearly show the added value of using the exclusive hubs to minimise the environmental impact. Using this transport route is especially beneficial for this scenario of a uniform CO_2 input in the supply chain.

5.3.4. Results of a single demand scenario

The goal of the single demand scenario is to assess the least environmental impact of a CO_2E SC infrastructure when there is a single demand position located with only a limited amount of small biogenic CO_2 sources nearby, hence validating the choice of the Dynea demand position in Delfzijl. From the results obtained and displayed in figure 5.13 it can be observed that, for lower market penetration the objective criterion is always higher in this scenario compared to the base scenario. Subsequently, it can be concluded that the choice of preference mostly relies on waste incinerators and only for the 55% and 1% market penetration on biomethane. However, due to the limited supply of local biogenic CO_2 sources, the visualised CO_2E SC infrastructure is of interest to see.

Figure 5.14 displays the CO_2E SC infrastructure for a solemn syngas demand position in an isolated area for the market penetration values of 100%, 75%, 50% and 25% from left to right. Based on these visualisations it can be concluded that it is beneficial for this demand position to choose a waste incinerator(s) and hub these sources together. Subsequently, the syngas is produced not at the demand position but for every market penetration at the source or exclusive hub. It can therefore be observed



(a) Objective Criterion for a solemn demand from Dynea in Delfzijl **(b)** Source mix for a solemn demand from Dynea in Delfzijl

Figure 5.13: Results obtained for a solemn demand from Dynea in Delfzijl

from these results that the transport of syngas has a limited environmental impact in this configuration.

There is a distinct added value to prefer the capture from these relatively large waste incinerators, rather than capture from small local biomethane and bioethanol sources. This confirms that it is a beneficial configuration to capture the CO_2 from a relatively large source to minimise the constructional footprint of the capture unit per captured amount of CO_2. Now the results of the single-demand scenario have been discussed, it can be concluded that there is an increased objective criterion for lower market penetrations in this scenario.

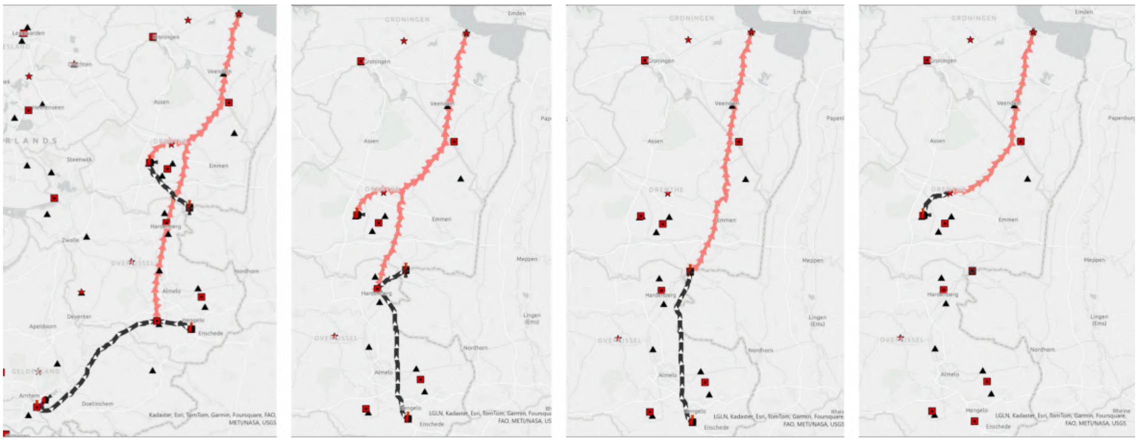


Figure 5.14: CO_2E SC infrastructure configurations for solemnly demand in Delfzijl, from left to right 100%, 75%, 50% and 25%.

5.4. Results of cost minimisation

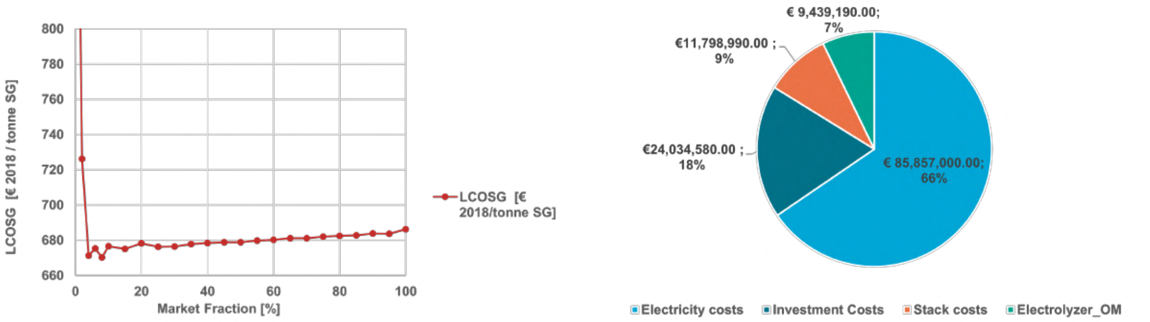
Based on the results obtained for the cost minimisation, it can be concluded that the Levelized Costs of Syngas (LCOSG) show a minimal value of 670 € per tonne of SG delivered to the demand position at a market penetration of 8%. This calculation reflects the spread-out costs over the lifetime of the equipment and operations, ensuring that capital expenditures, operational expenditures, and maintenance costs are all annualized, taking into account the time value of money. In this optimal configuration, it is preferred to configure the CO_2E SC infrastructure in a co-located and combined with a fully decentralized by-product topology. This optimal value can be converted into the units of €0.67 per kg. The main drivers regarding LCOSG are electricity costs, investment costs and stack costs respectively. An overview of the LCOSG and the split out per specific component of LCOSG can be observed in figure 5.15.

Apart from expressing the functional unit as a mass unit [kg syngas produced], conversion into other units can be of interest for the analysis of this CO_2E SC infrastructure. A common practice within LCA studies is to quantify the product by expressing it per unit of energy. Based on the research conducted by Wu et al. 2011 and corrected for the molar ratio of the syngas assumed, an LHV value of 120 MJ/kg and an HHV value of 142 MJ/kg are assumed [122] [35] [77]. Based on these figures, table 5.5 displays the objective criteria for both optimisations expressed per unit of energy.

Objective Criterion based on LHV	Objective Criterion based on HHV	Unit
0.006	0.005	[€/MJ]
1.55	1.31	[€/MWh]
0.274	0.232	[kg CO_2-eq/MJ]
76.20	64.40	[kg CO_2-eq/MWh]

Table 5.5: Objective Criterion based on LHV and HHV

The values displayed in this table can be put into perspective with additional literature to make a comparison. However, there are insufficient academic publications to truly validate and compare for this specific usecase. Therefore, a comparison is made to conventional syngas production routes. Accord-



(a) LCOSG as a function of market penetration

(b) LCOSG split out for the optimal value at 8% market penetration

Figure 5.15: A LCOSG analysis for a CO_2E SC infrastructure

ing to Sternberg et al. 2016, the GWP of SMR, reverse Water Gas Shift (rWGS) and Dry Reforming of Methane are respectively 2.27, 5.36 and 3.73 [kg CO_2-eq per kWh of syngas] [100]. Thus it can be concluded that the objective criterion is higher for both the LHV and HHV estimated case when compared to academic literature. Note needs to be taken into account that the study conducted by Sternberg et al. 2016 did not take into account the construction of the plant and in the system conducted within this research capture and transport are taken into account. A visual representation of the objective criterion expressed per energy unit of SG as a function of market penetration is given in figure B.6.

Based on the plot displayed in figure 5.15a it can be observed that there is a similar shape of the objective criterion proposed for the cost minimisation compared to the objective criterion for the environmental impact minimisation. Additionally, electricity consumption is one of the main drivers in costs just as for the environmental impact of the CO_2E SC infrastructure. Further analysis of the optimum observed at 8% can be found in figure 5.15.

The CO_2E SC infrastructure configurations for the 4%, 6%, and 8% are the exact same. The configuration for the 10% market penetration encompasses as well a configuration in the Botlek area. However, the key answer on why there is this specific minimum obtained at the 8% market penetration mark can be found in figure 5.18. In this figure, the LCOSG of transport and capture/compression are plotted as a function of market penetration. The figure suggests a decrease in LCOSG attributed to capture/compression and transportation, coinciding with the maximum syngas production capacity for the infrastructure at this market penetration. The reduced contribution of these factors to LCOSG becomes the decisive factor in the overall LCOSG. For this constant number of electrolysers and a linear increase in required electricity for syngas production.

The topology structure used for this specific optimum is a mix of fully co-located and fully decentralized by product. In the figure displayed, it can be clearly seen that there is capture and hubbing from sources prior to transport to the Antwerp area, where the the CO_2 entering is converted into syngas at the demand position itself (See figure 5.16).

From figure 5.17, it can be concluded that just as for the environmental impact minimisation, it is beneficial to configure in a fully co-located or fully decentralized by product topology in order to minimise the costs. For the higher market penetrations, some feedstock transport co-located and only for the 60% market penetration product transport co-located is observed. It is important to notice that for almost every topology regarding cost minimisation, it is preferred to produce the syngas within a 10-kilometre radius of the demand position. However, there are some distinct differences between the topology mix and the two different optimisation goals. This analogy to environmental and cost minimisation can be one of the main lessons learned regarding cost and environmental minimisation of a CO_2E SC infrastructure.

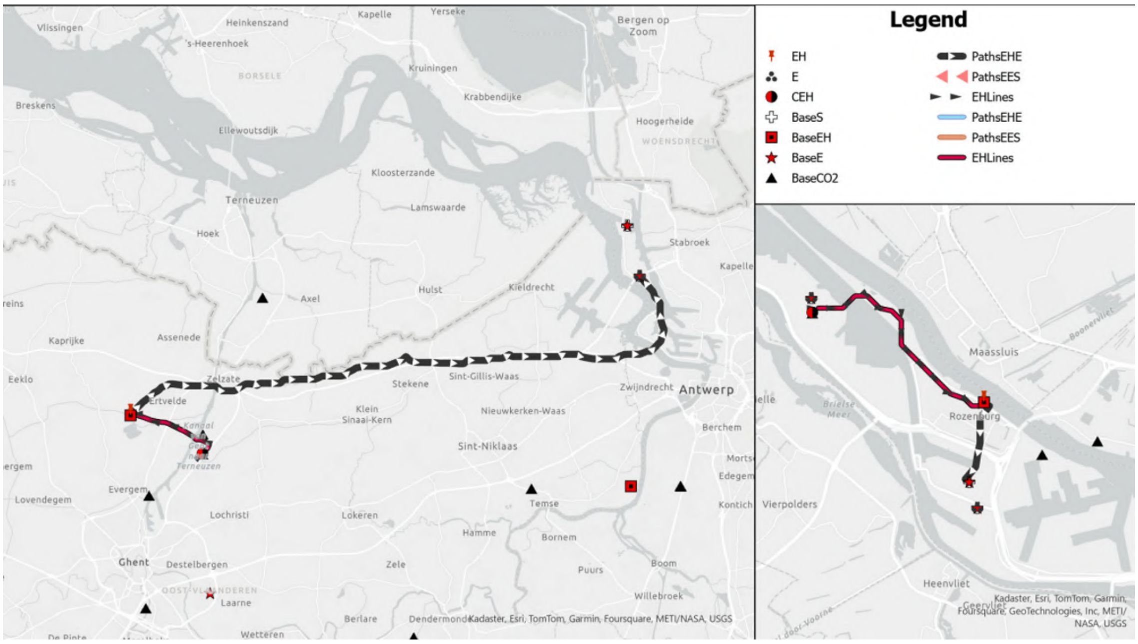


Figure 5.16: The CO_2E SC infrastructure configuration optimised at 8% market penetration

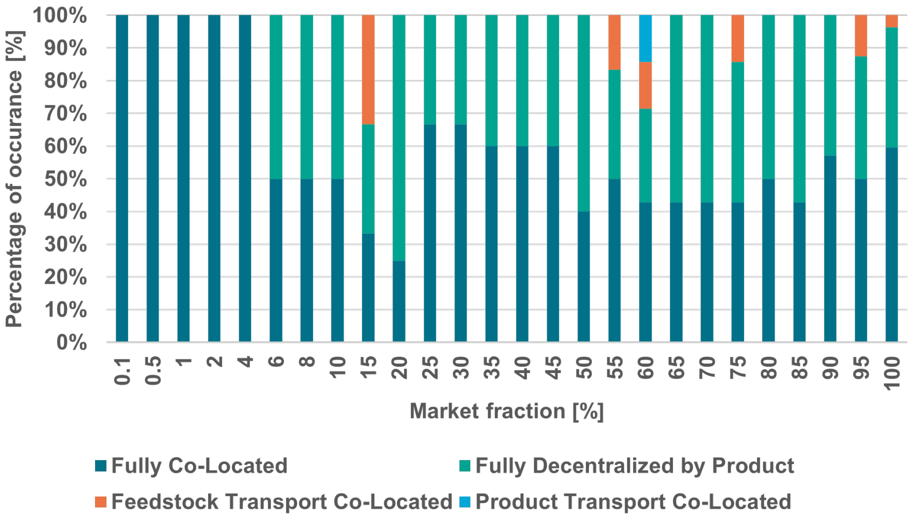


Figure 5.17: Distribution of topologies as a function of market penetration for the cost minimisation

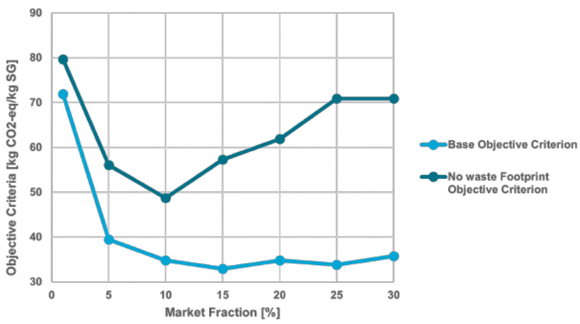


Figure 5.18: LCOSG of transport and capture & compression

6
Discussion

This chapter will provide a discussion of the results elaborated on in the previous chapter, it will summarize the lessons learned and the interpretation of the corresponding information. The lessons learned based on the research conducted can act as a first guideline for the Benelux authorities in further investigating a CO_2E SC Infrastructure. First of all, section 6.1 will give an overview of the similarities and differences between the two optimisation models. Second of all, section 6.2 will examine the lessons learned from this comparative analysis. Third of all, sections 6.3.1 and 6.3.2 will elaborate on the water consumption and materials used for the CO_2E SC infrastructure.

6.1. Comparitive Analysis: Environmental vs. Cost minimisation

Based on the results discussed in Chapter 5, it can be concluded that the main similarities for a CO_2E SC infrastructure minimised for CO_2-eq emissions and cost are *(i)* an overall preference of topology, *(ii)* a dominant role in electricity consumption and *(iii)* an optimum of the objective criterion for not full market penetration. The main differences can be identified in the *(iv)* topology preference at specific market penetrations, *(v)* location of CO_2E SC Infrastructure and *(vi)* share of contribution per SC echelon.

6.1.1. Similarites of environmental and cost minimisation

It is both for CO_2-eq and cost minimisation beneficial in general to configure the CO_2E SC infrastructure in a co-located or fully decentralized by product configuration. The rationale behind this lies in the costly nature of syngas transportation and its comparatively significant environmental footprint. Therefore, it would be beneficial for the authorities of the Benelux, when implementing a CO_2E SC infrastructure, to configure the infrastructure in one of these two topologies, or a combination thereof. An overview of the topology distribution as a function of market penetration is given in figure 6.1, in which the topology mix for CO_2-eq minimisation is given on the left and the topology mix for cost minimisation is given on the right. From this figure, it can be concluded that there are similarities. For lower market penetrations, it is beneficial from a cost perspective as from an environmental perspective to configure the CO_2E SC infrastructure in a co-located topology and for higher market penetration in combination with a fully decentralized by product. This is the first similarity identified.

Additionally, both CO_2-eq and cost minimisation show similarities in the major contribution of electricity consumption in the objective criteria. Depending on market penetration, every share of electricity is > 60% of the total costs or CO_2-eq emissions. This is a valuable conclusion to be drawn since this main driver can be investigated for further research. An overview of this split out and therefore share of the electricity consumption can be observed in figure 6.2.

The similarity in dominant electricity consumption's share to the total total CO_2-eq footprint and costs for both optimisation models is a second similarity identified.

Lastly, both objective criteria as a function of market penetration show a similar correlation and find that an optimum is found at relatively lower market penetrations (15% for CO_2-eq minimisation and 8% for cost minimisation respectively). Both objective criteria show a similar trend and volatility in the region of lower market penetrations satisfied [e.g. 5% up until 20%], however, with a quantitative analysis and visualisation in ArcGIS Pro both optima can be explained and understood as described

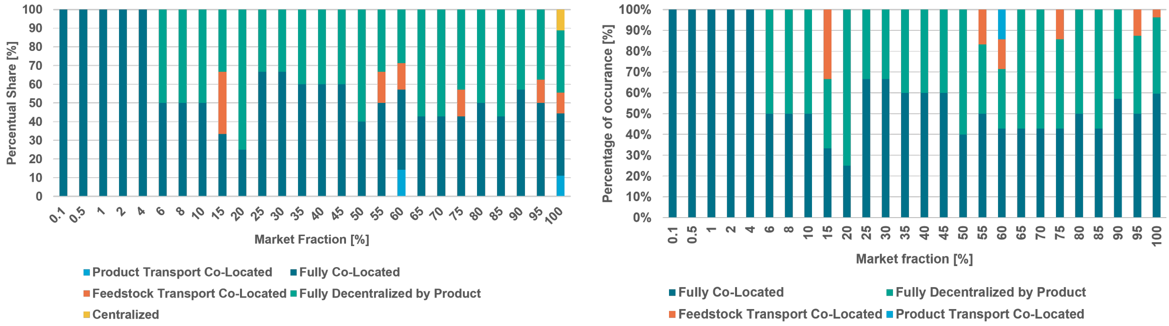


Figure 6.1: The CO_2-eq topology mix on the left, and the cost minimisation topology mix on the right

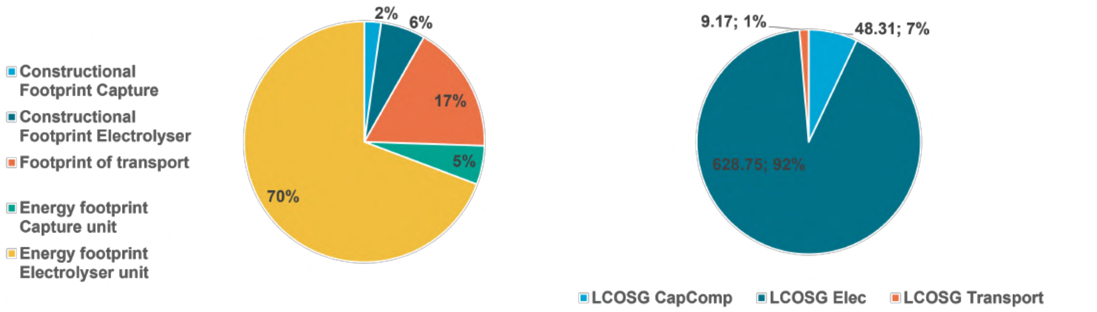


Figure 6.2: Split out of CO_2-eq emissions on the left and of the levelised costs on the right for a 100% market penetration

in Chapter 5. This correlation and optimum behaviour form the third similarity identified between both optimisation models and can be observed in figure 6.3.

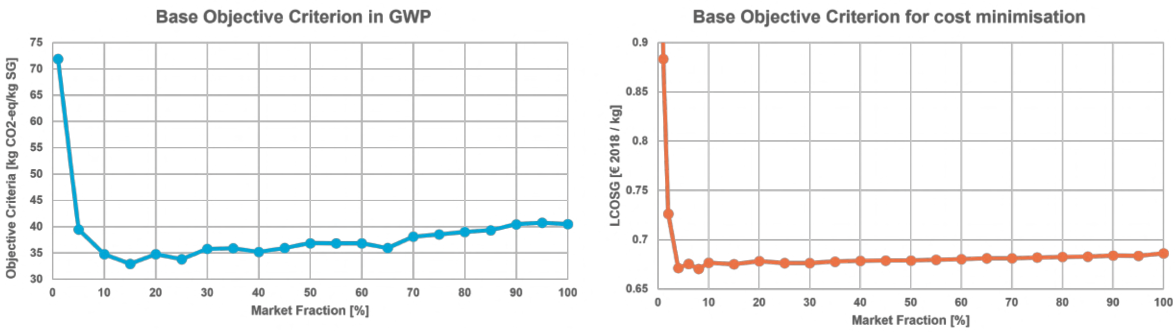


Figure 6.3: Objective criteria for minimised CO_2-eq footprint (left) and costs (right)

6.1.2. Differences of environmental and cost minimisation

Although it is overall beneficial to configure a CO_2E SC infrastructure in co-located and decentralized by product topology, distinct differences regarding exact topology can be identified especially for higher market penetration values. An example is given for both topology mixes at the 100% market penetration. Figure 6.4 displays the topology mix of the CO_2-eq minimisation on the left and the cost minimisation on the right for a full market fraction satisfied.

From these pie charts, it can be observed that there is a distinct difference in the mix of topologies optimal for the 100% market penetration for each objective. The CO_2-eq minimisation model prefers a centralized, product transport co-located and feedstock transport co-located topology in an equal share of each 11%. Additionally, the last two topologies are product transport co-located and fully co-located in which both have a share of 34%. For cost minimisation, it is more beneficial to configure the SC with a major focus on fully co-located (59%) and product transport co-located (36%). This difference in

Figure 6.4: The CO_2-eq topology mix on the left for 100%, and the cost minimisation topology mix on the right for 100%

CO_2E SC infrastructure configuration is therefore the first difference identified between the two.

Apart from different topology mixes beneficial for CO_2-eq and cost minimisation, the location of choice or specific configuration for each topology is different as well. An example of the differences in location is displayed in figure 6.5, in which the CO_2E SC infrastructure configuration for CO_2-eq minimisation is displayed on the left and for cost minimisation is displayed on the right. In this specific situation, transport of CO_2 can be seen from the source to an exclusive hub after which it is transported to the demand position in the Botlek.

By using this raster as the basis, ArcGIS Pro computes the distance accumulation and direction rasters from all the starting points. Then, ArcGIS Pro uses this output combined with all the end-points to find all the optimal paths between the different echelons. Simultaneously, the distance and average terrain factor of a path are calculated. The transport routes are averaged according to their terrain factor as explained in chapter 4. This can lead to unusual configurations as displayed in figure 6.5 on the left, in this configuration a pipeline is constructed in the densely populated area of Rozenburg. For additional research in this field, it is recommended to further investigate these kind of configurations and terrain factor in order to minimise these unusual routes.

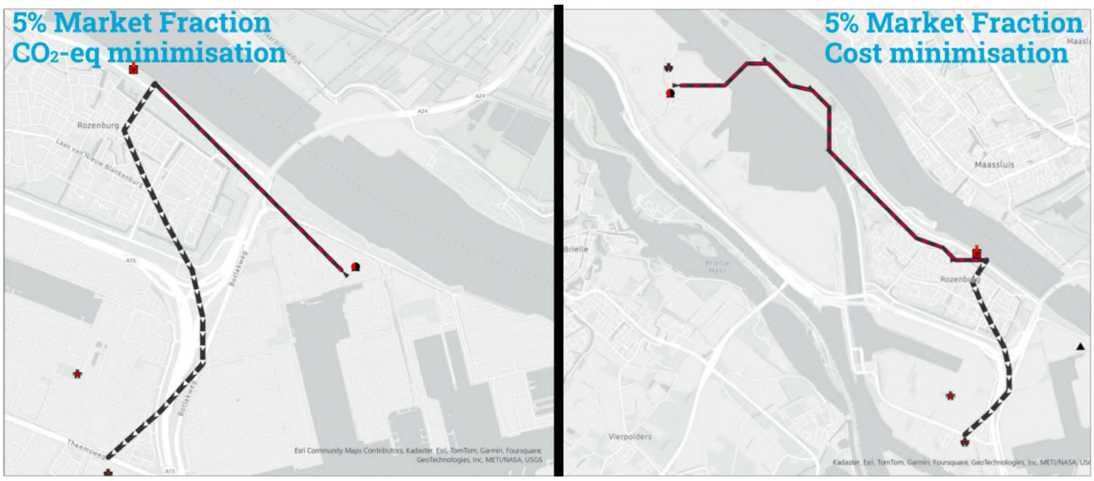


Figure 6.5: The CO_2-eq visualisation for 5% and the cost minimisation visualisation for 5%, wherein each share the same topology but different structure

Although both solutions are configured in the same topology (co-located), there is a distinct difference in the form of the exact CO_2E SC infrastructure. From the figure, it can be concluded that it is in terms of CO_2-eq emissions beneficial to capture the CO_2 from the waste incinerator and exclusively hub it near Rozenburg. From this exclusive hub, the CO_2 is transported to the syngas demand position (in this case LyondellBasell) at which it is converted into syngas. On the contrary, capturing from a local bioethanol plant is more cost-effective and beneficial, exclusively hub this captured CO_2 and then transporting it to the exact same syngas demand position. In other words, although the topology classification is the same, distinct differences can occur regarding the exact CO_2E SC configuration.

This forms the second difference identified between CO_2-eq and the cost minimisation of these CO_2E SC infrastructures.

Lastly, different shares of echelons contributing to CO_2-eq emissions or costs in the CO_2E SC infrastructure are identified especially for higher market penetrations. To illustrate this difference, figure 6.2 shows the contribution of each SC echelon at the 100% market penetration mark. On the left is the distribution of each echelon for minimal CO_2-eq emissions, on the right for minimised costs.

Based on the figures 6.2,6.6 and the overall trend in correlation to market penetration it can be concluded that for every market penetration, the levelised costs of transport are always smaller than 3% compared to the total levelised costs. However, regarding CO_2-eq footprint the transport can account for 17%. Therefore, it can be concluded that regarding environmental footprint, transport plays a more dominant role than compared to cost, this correlation to market penetration is displayed in figure 6.6. This forms the third difference identified.

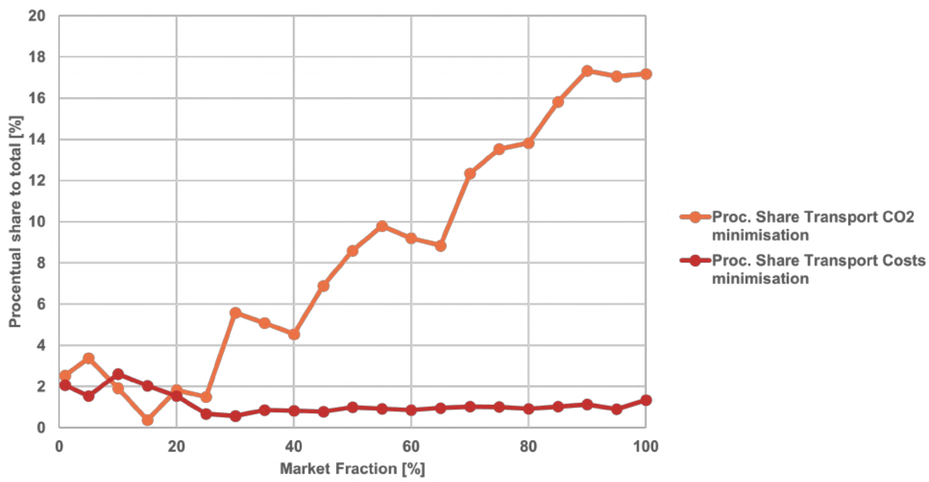


Figure 6.6: Percentual share of transport to the objective criteria as a function of market penetration

6.2. Insights gained for CO_2E SC infrastructure configurations

From the similarities and differences identified in the previous section, lessons can be learned and shaped into advice for the Benelux authorities. These lessons can act as a guideline for the responsible operator of this CO_2E SC infrastructure. As identified in the introduction, the Benelux authorities are identified as the problem owners of reaching the Green Deal goals, in which CO_2E SC infrastructures can play a key role. Therefore, the following can be used as a first insight into this guideline. The key takeaways are formulated as follows based on the discussed results:

1. It is advised to configure the CO_2E SC infrastructure in a co-located and fully decentralized by product configuration for not full market penetration in order to minimise the environmental impact regarding CO_2-eq emissions and costs.
2. Electricity consumption is the main driver in CO_2-eq footprint and costs, therefore, it is advised to maximise energy efficiency and conduct further research in the electricity consumption with a main focus on the electrolyser.
3. The share of transport's CO_2-eq footprint increases for increased market penetration, thus thorough research on the exact CO_2E SC infrastructure for each penetration and objective criteria is advised. Although certain CO_2E SC infrastructures can show the exact same topology classification, variation can occur regarding the exact pathways or location of the CO_2E SC infrastructure minimised for CO_2-eq footprint or total cost.
4. Transport contribution regarding CO_2-eq emissions is significantly increased for an increase in market penetration but constant regarding costs. This is a significant insight for the Benelux authorities, as the objective of this stakeholder is to achieve the Green Deal goals without the profit motives of a private company.

5. Given that co-located and fully decentralized by-product configurations are advantageous from both environmental and cost perspectives, close collaboration with stakeholders such as the chemical industry, power generation companies, and water suppliers is essential. An example can be found in the Botlek and Port of Antwerp areas, being high-density industrial zones, that require tight collaboration to enhance efficiency.
6. To complement this stakeholder management it is advised to the Benelux authorities to incentivise companies with taxation or subsidies in the direction of collaboration in the operation of this CO_2E SC. E.g. subsidise the installation of carbon capture units and increase taxes on CO_2 emissions, creating a motivational incentive.

Additional similarities and differences can be identified based on the results obtained, however, the ones mentioned and the corresponding insights are found most prominent.

Apart from these three main takeaways regarding the minimisation of CO_2-eq footprint and costs, an additional factor is the water consumption of a CO_2E SC infrastructure. This additional factor can be of interest to the Benelux authorities since it could be a bottleneck in the construction and operation of such a CO_2E SC Infrastructure. In addition, other factors need to be taken into account such as the criticality of materials used in the electrolyser. Therefore, the following section will briefly discuss these topics.

6.3. Additional environmental insights

This section will first estimate an order of magnitude regarding the water consumption, subsequently, it will zoom in on the criticality of the Rare Earth Elements (REEs) used. Both of these estimates are only focussed on the electrolyser echelon in the supply chain.

6.3.1. Results of water consumption

Based on the factor used to estimate the water consumption of the electrolyser as stated in Chapter 3, it can be concluded that for full market penetration around 3 Mtonne of water is needed per year.

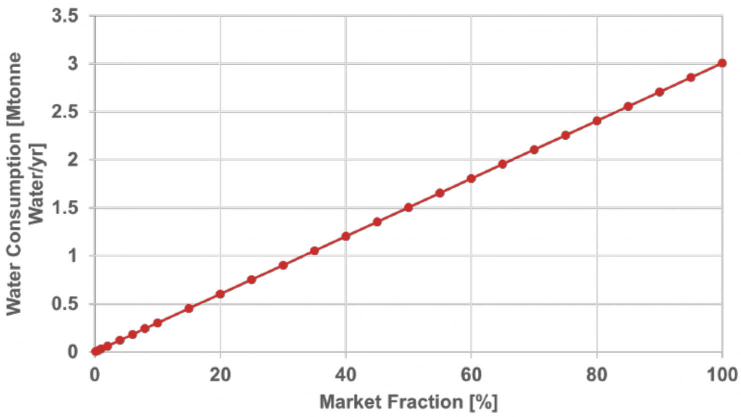


Figure 6.7: Water consumption as a function of market penetration

Note needs to be taken into account that this is only based on the stoichiometric coefficients present in the chemical reaction taking place at the electrolyser. It can be argued that there are additional direct and indirect water consumption streams present within the CO_2E SC infrastructure.

Based on the figures proposed by CBS in 2019, it is estimated that companies consumed around 386 million cubic meters of mains water for the year 2018 in The Netherlands [15].

386 million cubic meters would convert (assume a mass density of water of 1000 kg per cubic meter), into 386 Mtonne of water consumed per year in 2018. To put into perspective, a CO_2E SC infrastructure operating at a full 100% market penetration would correspond to 0.77% of this water consumption. For the optimum (market penetration at 15% or 0.24 Mtonne of water consumed per year), this would correspond to a 0.6% share in total industrial consumption.

These percentages of share by the CO_2E SC infrastructure are significant in the total Dutch water consumption, therefore, it is recommended to conduct further research in this field. Additional factors that are vital to assess regarding water consumption are its regional distribution since the availability of water might be limited.

6.3.2. Material evaluation

As described in Chapter 3, the Rare Earth Elements (REEs) used in the stack of the SOEC will be assessed based on the criteria of abundance, geographical distribution, CO_2-eq footprint and costs. Figure 6.8 displays the abundance, CO_2-eq footprint and costs of the REEs considered, from which it can be concluded that the main contributors are Zirconium and Yttrium in costs, Gadolinium, Yttrium and Cerium in CO_2-eq footprint, and Gadolinium and Yttrium are least abundant. A further elaboration on the values and their calculations can be found in table B.14 in Appendix B.

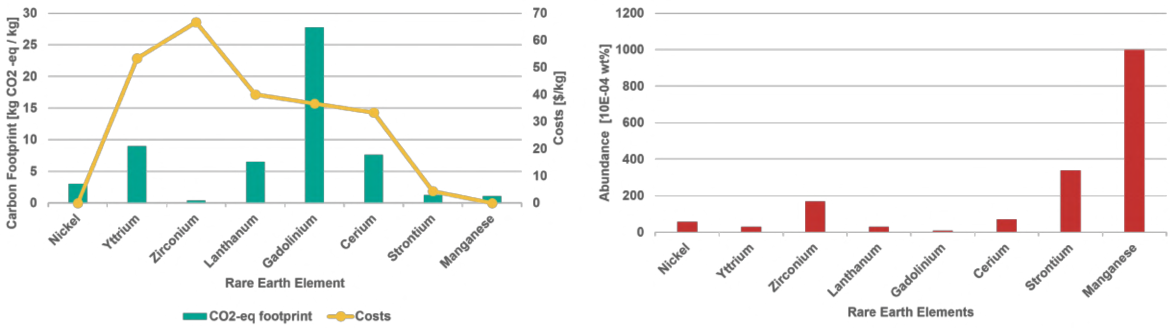


Figure 6.8: Overview of CO_2-eq footprint, cost and abundance of REEs normalized compared to iron

The last criterion identified in Chapter 3 is the geographical distribution of these REEs. From table B.13, it can be concluded that China is the main supplier of Yttrium, Lanthanum and Strontium. Since REEs mined from China need to be transported to the Benelux, an additional environmental impact will be present which will affect the environmental impact of the CO_2E SC infrastructure as well. Apart from the environmental impact it forms as well a dependency of supply which can become an additional risk.

This chapter discussed the similarities, and differences of the two optimisation models proposed which form the basis for the lessons learned. Additionally, a brief analysis was conducted regarding the water consumption and criticality of the materials used. Based on the research conducted the conclusions will be drawn in order to answer the research question proposed.

7 Conclusion

The goal of this thesis was to conduct research on the conceptual CO_2E supply chain infrastructure for biogenic CO_2 sources in the Benelux minimised for its environmental impact. The focus on CO_2-eq emissions aims to provide valuable insights for the Benelux authorities, who, as the problem owners, are responsible for achieving the Green Deal targets. This research question was answered by developing an optimisation model that minimised the Global Warming Potential (GWP) as an impact category of a Life Cycle Assessment (LCA) using a Mixed Integer Linear Problem (MILP) in General Algebraic Modeling System (GAMS) which was visualised in ArcGIS pro. Based on the results obtained, and the corresponding discussion, the following conclusions can be drawn to each subquestion.

Which CO_2-eq footprints contribute the most in a gate-to-gate system within a CO_2E SC infrastructure based on biogenic CO_2 sources?

It can be concluded that the CO_2-eq footprint due to the electricity consumption of the electrolyser is the biggest contributor to the total CO_2-eq emissions of the CO_2E SC infrastructure in a G2G system. With a minimum share of 70% with respect to total emissions, the electricity consumption of the electrolyser is dominant for every market penetration. For varying levels of market penetration, different shares of each echelon to the total CO_2-eq emissions were observed. Additionally, significant contributors to the CO_2-eq footprint within the CO_2E SC infrastructure include the constructional footprint of the electrolyser, the constructional footprint of the capture unit, and the footprint due to transport especially for higher market penetration, in that respective order.

How can the minimum environmental impact in a CO_2E supply chain infrastructure be explained and assessed using multiple metrics?

A minimum is obtained for 15% market penetration and a corresponding objective criterion of 32.92 kg CO_2-eq per kg syngas. The CO_2E SC infrastructure should be configured in a co-located topology for low market penetration and in a mix with fully decentralized by product for higher market penetrations. The optimum at 15% market penetration is observed since the distance indicator shows an optimal value, which suggests there is a maximum amount of GWP per distance covered by the transport routes. In addition to this, the water consumption of a CO_2E SC infrastructure would consume 3 Mtonne of water for 100% market penetration. This would correspond to a 0.77% share of the current water consumption of the Dutch industry.

What are the lessons learned based on the optimum obtained and the metrics used to assess a CO_2E SC infrastructure?

Lessons can be learned based on the four different scenarios proposed and when a CO_2-eq minimisation is compared to a cost minimisation. The similarities when a CO_2E SC infrastructure is minimised for CO_2-eq footprint and costs are in the form of *(i)* overall topology characteristics (co-located and fully decentralized by product), *(ii)* share of electricity consumption by electrolyser and *(iii)* an optimum for lower market penetration (15% and 8% respectively). Differences can be found in the mix of topologies for higher market penetrations and exact configurations/pathways of the CO_2E SC. When optimising for the global warming potential at 100% market fulfilment, the transport sector accounts for 17% of emissions, whereas in the case of a cost-minimised CO_2E SC infrastructure, its share is at a maximum of 3%. This percentage represents the relative share of transport emissions to the total CO_2-eq emissions and therefore forms a significant difference.

What is the optimal CO_2E supply chain infrastructure for biogenic CO_2 sources in the Benelux to minimise the environmental impact?

To minimise the environmental impact of a CO_2E SC infrastructure within the Benelux based on biogenic CO_2 sources, a focus should be put on co-located and fully decentralized by product topologies for a market penetration at 15% in order to deliver the functional of kg syngas for a CO_2-eq footprint of 32.92 kg. The main driver of this CO_2-eq footprint is the electricity consumption of the electrolyser with an 85% at this market penetration. Other echelons with a significant contribution to the CO_2-eq footprint are the constructional footprint of the electrolyser unit, the electricity consumption of the capture unit and for higher market penetration the transport footprint. Additional environmental footprints identified are water consumption and material use. For optimal market penetration, 0.24 Mtonne of water is consumed, and REEs can form additional environmental components of this CO_2E SC infrastructure.

8
Recommendations for further research

This chapter will discuss the recommendations for further research based on the assumptions made, model proposed and results obtained. The suggestions stated here can be interpreted as the next steps for gaining further insights regarding CO_2E SC infrastructures within the Benelux.

8.1. Assumptions:

It is recommended that further research is conducted regarding the assumptions made of the electrolyser, focussing on its electricity consumption, constructional footprint and the materials used for the stack. Since no large-scale application of CO_2E exists and only a limited number of academic publications mention the materials used for an electrolyser at this scale, further insight is advised to make a more accurate estimate regarding the environmental impact of the electrolyser.

Additionally, it is recommended that a more thorough analysis is made regarding the differences between natural gas transport and the transport in this specific use case which is CO_2 and syngas. Due to a lack of academic literature and for simplicity, it was assumed that all components transported could be treated equally to the transport of natural gas. This assumption should be investigated further since it is known that the permeation of especially hydrogen is relatively high compared to the other components. Subsequently, the transport of CO_2 in the supercritical state poses significant differences when compared to the transport of natural gas.

8.2. Model:

Expanding the proposed model for minimising environmental impact through factors such as a variable electricity carbon footprint and considering the size of capture units in relation to the amount of CO_2 captured would enhance research in this area. Additionally, incorporating the non-linear relationship between upscaling electrolysers e.g. material use in the stack would provide a more comprehensive understanding.

One can argue that as the number of stacks installed increases, the footprint per installed stack decreases, suggesting that upscaling becomes progressively easier after the initial stack. This leads to a non-linear relationship between the number of stacks and their corresponding footprints.

In the model proposed it is assumed that there is always electricity available generated from renewable energy sources such as wind and solar energy. However, due to their intermittent characteristics, it is unlikely that these type of sources can deliver at a constant rate for the CO_2-eq footprint assumed. Therefore, it is recommended to further investigate different CO_2-eq footprints of the electricity and corresponding storage technologies since they will have to be considered as well.

Additions can be implemented within the CO_2E SC Infrastructure's capture echelon to further augment its capacity, modelling a more realistic scenario. One can argue that the constructional footprint is proportional to the amount of CO_2 captured. Defining a difference in capture and compression units could be of added value as well.

8.3. Results:

Further research is recommended in the validation of the results obtained from the research proposed since an objective criterion of 32.92 kg CO_2-eq per kg syngas compares relatively high to alternative syngas production routes. It is advised to dive deeper into the orders of magnitude and the system considered in order to truly validate this system proposed to academic literature. Additionally, the validation of this model is complex since similar use cases wherein boundaries are clearly defined remain absent. Therefore, further validation of the results obtained should be investigated to reaffirm whether an objective criterion of 32.92 kg CO_2-eq per kg syngas is within line of alternative syngas production routes.

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A

Appendix A

This appendix contains the models proposed in GAMS

The following code is used for the CO_2-eq minimisation

```

*--------------------------------          0          --------------------------------*
*--------------------------------   DEFINE A MAX GAP OF   --------------------------------*
*-------------------------------- MINIMISATION FOR MODEL --------------------------------*

$eolCom #
$inlinecom /* */

option reslim = 29000;
option optCR=0.0275;
;


*--------------------------------          1          ----------------------------------*
*--------------------------------    DEFINE ALL SETS    ----------------------------------*
*--------------------------------   THAT WILL BE USED   ----------------------------------*
$title                  CO_2 FOOTPRINT MINIMISATION MODELLING BY B.L.P.Thio
$title                  MSc. THESIS SUSTAINABLE ENERGY TECHNOLOGY, TU DELFT


$OnFold
Sets
    c       "Set␣containing␣all␣the␣CO_2␣sources␣in␣the␣model,␣indexed␣by␣c_1␣..␣1573;"   /
        C1232,C1239,C1300,C82,C84,C240,C459,C517,C42,C1267,C1289,C298,C391,C1283,C1236,C1272,
        C1296,C40,C41,C1291,C161,C1237,C160,C455,C1271,C162,C163,C166,C1278,C43,C1250,C39,
        C1266,C1277,C1285,C273,C1294,C393,C1238,C514,C1235,C1246,C1295,C1253,C1255,C1297,
        C1282,C1298,C1299,C1242,C1262,C1265,C1292,C38,C1251,C1252,C1260,C1274,C1243,C1287,
        C1240,C1284,C1248,C1293,C1263,C1273,C1301,C1233,C1234,C1257,C1288,C1247,C1270,C164,
        C1244,C1245,C1140,C1259,C1275,C1254,C1256,C1286,C1302,C165,C1279,C1280,C1281,C1258,
        C1290,C1249,C1264,C1241,C1261,C1268,C1269,C237,C390,C432,C81,C83,C238,C519,C1054,C235
        ,C515,C516,C335,C469,C80,C239,C433,C460,C480,C1276,C209,C867,C1229,C1230,C1231/

    cci(c)  "Subset␣of␣Set␣C␣containing␣all␣the␣individual␣CO_2␣sources␣(cci)␣in␣the␣model␣
        which␣are␣not␣part␣of␣a␣25␣kilometer␣cluster,␣indexed␣by␣c"   /C1232,C1239,C1300,C82,
        C84,C240,C459,C517/

    ceh(c)   "Subset␣of␣Set␣C␣containing␣all␣the␣exclusive␣hub␣CO_2␣sources␣(ceh)␣which␣are␣
        part␣of␣a␣25␣kilometer␣cluster,␣indexed␣by␣c"    /C42,C1267,C1289,C298,C391,C1283,
        C1236,C1272,C1296,C40,C41,C1291,C161,C1237,C160,C455,C1271,C162,C163,C166,C1278,C43,
        C1250,C39,C1266,C1277,C1285,C273,C1294,C393,C1238,C514,C1235,C1246,C1295,C1253,C1255,
        C1297,C1282,C1298,C1299,C1242,C1262,C1265,C1292,C38,C1251,C1252,C1260,C1274,C1243,
        C1287,C1240,C1284,C1248,C1293,C1263,C1273,C1301,C1233,C1234,C1257,C1288,C1247,C1270,
        C164,C1244,C1245,C1140,C1259,C1275,C1254,C1256,C1286,C1302,C165,C1279,C1280,C1281,
        C1258,C1290,C1249,C1264,C1241,C1261,C1268,C1269,C237,C390,C432,C81,C83,C238,C519,
        C1054,C235,C515,C516,C335,C469,C80,C239,C433,C460,C480,C1276,C209,C867,C1229,C1230,
        C1231/
    eh       "Set␣EH␣-␣containing␣all␣the␣exclusive␣hub␣CO_2␣sources␣with␣dedicated␣label␣(eh
        )␣which␣are␣part␣of␣a␣25␣kilometer␣cluster,␣indexed␣by␣eh_1␣..␣481;"  /EH1,EH2,EH4,
```

```
        EH43,EH59,EH60,EH67,EH68,EH69,EH105,EH122,EH146,EH204,EH370,EH374,EH375,EH381,EH382,
        EH387,EH388,EH390,EH391,EH392,EH393,EH396,EH398,EH399,EH400,EH401,EH402,EH403,EH404,
        EH408,EH479,EH29,EH113,EH142,EH167,EH177,EH191,EH175/
    ci      "Set␣containing␣all␣the␣individual␣CO_2␣sources␣with␣dedicated␣label␣(CI)␣in␣the
        ␣model␣which␣are␣not␣part␣of␣a␣25␣kilometer␣cluster,␣indexed␣by␣ci_1␣..␣256;"   /
        CI225,CI226,CI227,CI17,CI18,CI36,CI106,CI123/
    e       "Set␣E␣-␣containing␣all␣the␣possible␣electrolyzer␣locations,␣build␣up␣of␣CO_2␣
        source␣locations,␣syngas␣demand␣points␣and␣intermediate␣hub␣locations,␣indexed␣by␣e_1
        ␣..␣1071;"    /E15,E20,E28,E31,E35,E38,E41,E46,E231,E232,E233,E234,E235,E236,E237,
        E238,E239,E240,E241,E242,E559,E560,E561,E591,E592,E594,E633,E649,E650,E657,E658,E659,
        E695,E712,E736,E794,E960,E964,E965,E971,E972,E977,E978,E980,E981,E982,E983,E986,E988,
        E989,E990,E991,E992,E993,E994,E998,E1069,E19,E30,E59,E60,E61,E62,E63,E64,E65,E66,E67,
        E68,E69,E351,E352,E370,E440,E457,E619,E703,E732,E757,E767,E781,E229,E765/
    s       "Set␣S␣-␣containing␣all␣the␣direct␣and␣indirect␣syngas␣demand␣locations␣in␣the␣
        system,␣indexed␣by␣s_1␣..␣54;"    /S15,S20,S28,S31,S35,S38,S41,S46,S19,S30/
;

Alias(E,EE);
$OffFold

$OnFold
$onText
Sets
   C        /C1*C1573/
   CCI(C)   /C1,C3,C8,C11,C12,C15,C21,C28,C32,C33,C37,C47,C61,C66,C68,C74,C82,C84,C87,C92,C94
       ,C96,C100,C104,C106,C108,C109,C142,C159,C173,C175,C186,C188,C224,C230,C240,C241,C248,
       C250,C251,C253,C256,C263,C265,C267,C272,C274,C275,C276,C278,C282,C284,C286,C287,C295,
       C299,C302,C309,C311,C312,C315,C316,C317,C318,C319,C321,C322,C323,C325,C329,C331,C333,
       C336,C341,C342,C348,C349,C350,C351,C352,C355,C356,C357,C358,C359,C360,C361,C362,C363,
       C364,C375,C387,C394,C400,C417,C421,C428,C429,C445,C446,C449,C452,C453,C456,C458,C459,
       C461,C465,C470,C472,C473,C474,C475,C479,C485,C492,C494,C495,C496,C503,C506,C512,C517,
       C520,C523,C526,C528,C533,C535,C549,C556,C581,C585,C587,C592,C593,C599,C602,C617,C630,
       C634,C637,C647,C664,C670,C674,C680,C685,C688,C703,C704,C712,C728,C734,C755,C760,C765,
       C773,C777,C781,C808,C813,C820,C822,C846,C856,C874,C878,C905,C909,C913,C923,C940,C942,
       C947,C950,C956,C960,C962,C974,C986,C991,C1000,C1002,C1004,C1007,C1026,C1046,C1053,
       C1063,C1069,C1070,C1074,C1082,C1085,C1086,C1098,C1100,C1110,C1122,C1126,C1129,C1145,
       C1149,C1157,C1163,C1166,C1167,C1173,C1190,C1195,C1196,C1197,C1198,C1199,C1200,C1205,
       C1207,C1209,C1210,C1217,C1220,C1226,C1228,C1232,C1239,C1300,C1304,C1308,C1309,C1310,
       C1321,C1332,C1333,C1345,C1360,C1361,C1363,C1370,C1374,C1377,C1380,C1401,C1412,C1414,
       C1429,C1435,C1439,C1456,C1457,C1476,C1507,C1508,C1522,C1533,C1565/
   CEH(C)   /C2*C1573/
   CI       /CI1*CI256/
   EH       /EH1*EH481/
   E        /E1*E1071/
   S        /S1*S54/
;
Alias(E,EE);
$offtext
$offFold

$onfold     #Definition of the looping set for different market fractions that need to be
    fulfilled by the model
Set         Count             "Looping␣set␣over␣the␣different␣market␣fractions,␣the␣number␣
    indicates␣the␣percentage␣of␣mCap__Costarket␣fulfilment" /Count1,Count5,Count10,Count15,
    Count20,Count25,Count30,Count35,Count40,Count45,Count50,Count55,Count60,Count65,Count70,
    Count75,Count80,Count85,Count90,Count95,Count100/;
;
$OffFold





$GDXIN "DistanceDataC2.gdx"

$onfold      #CO_2 location linking set - The parameter linking CO_2 sourcesand unclustered/
    individual CO_2 sources
Parameter    Link(CCI,CI)        "The␣parameter␣linking␣CO_2␣sourcesand␣unclustered/
    individual␣CO_2␣sources"
$load        Link
;
```

```
$offfold
$onFold     #Electrolyzer translation set - Sets that are used to translate subsets of C into individual CO_2 sources and exclusive hubs
Set         TSetCCI(CCI,CI)     "Set␣to␣translate␣set␣CCI␣into␣CI";
Set         TSetCEH(CEH,EH)     "Set␣to␣translate␣set␣CEH␣into␣EH";
$offFold


$GDXIN "TSetCEH.gdx"


$onfold      #CO_2 location linking set - The parameter linking CO_2 sourcesand unclustered/individual CO_2 sources
Parameter    Link2(CEH,EH)        "The␣parameter␣linking␣CO_2␣sourcesand␣unclustered/individual␣CO_2␣sources"
$load        Link2
;
$offfold



$GDXIN "TransportLinks.gdx"

$onfold #Exclusive Linking set definitions
TSetCCI(CCI,CI)  = yes$(Link(CCI,CI) eq 1);
TSetCEH(CEH,EH)  = yes$(Link2(CEH,EH) eq 1);
$offFold

*--------------------------------         2           --------------------------------*
*-------------------------------- IMPORT ALL GDX FILES --------------------------------*
*-------------------------------- NEEDED AS INPUT DATA --------------------------------*


$GDXIN "tc.gdx"

$onfold #Set with the different capture technologies
set         pex                 "Set␣containing␣all␣the␣capture␣technologies␣in␣the␣model␣specific␣for␣each␣CO_2␣source,␣TC_BioethanolL,BioethanolS,Waste,␣P&P␣and␣Biomethane;"
$load       pex
;
$offFold


*--------------------------------         2.1          --------------------------------*
*--------------------------------    IMPORT DISTANCES  --------------------------------*
$GDXIN      "Distances5.gdx"
Parameter   T__Dist                     "The␣parameter␣defining␣all␣distances␣that␣are␣present␣between␣the␣nodes␣in␣my␣model␣given␣in␣[km]";
$LOAD       T__Dist
$GDXIN


*--------------------------------         2.2          --------------------------------*
*--------------------------------    IMPORT EMISSIONS  --------------------------------*
$onfold
$GDXIN      "CO2_in.gdx"
Parameter   CO2_in(C,pex)           "The␣parameter␣defining␣all␣CO2␣emission␣orders␣of␣magnitude␣in␣the␣model␣[Mtonne␣CO2␣/␣yr]"
$LOAD       CO2_in
;
$OffFold
$GDXOUT


$onFold #Electrolyzer location linking sets - The electrolyzer can be placed at individual
Set         TSetCap(C,pex)      "Translation␣set␣of␣the␣CO_2␣sources␣to␣the␣right␣technology␣of␣capture␣(TC)";
$offFold


$onfold #Dynamic set definition of the CO_2 sources to the right technology of capture (TC)
```

```
             TSetCap(C,pex)  = yes$(CO2_in(C, pex) gt 0);
$offFold


*--------------------------------         2.3          --------------------------------*
*-------------------------------- IMPORT SYNGAS DEMAND --------------------------------*

$onfold
$GDXIN      "SG_Demand.gdx"
Parameter   SG_Demand(S)      "The␣parameter␣defining␣all␣CO2␣emission␣orders␣of␣magnitude␣in␣the␣model␣[Mtonne␣Syngas/yr]"
$LOAD       SG_Demand
;
$OffFold
$GDXOUT



*--------------------------------         2.4          --------------------------------*
*-------------------------------- VARY SYNGAS DEMAND FR--------------------------------*

$GDXIN       "SGFract2.gdx"
parameter    Market__Fr(Count)   "Parameter␣with␣the␣market␣fraction␣of␣the␣total␣demand␣in␣Europe␣that␣needs␣to␣be␣fulfilled␣[-]␣";
$LOAD        Market__Fr
;
$GDXOUT
$offfold


*--------------------------------         2.5          --------------------------------*
*-------------------------------- VARY SYNGAS DEMAND FR--------------------------------*

$GDXIN       "Capture_Eff.gdx"
parameter    x_conv(pex)   "Parameter␣with␣the␣market␣fraction␣of␣the␣total␣demand␣in␣Europe␣that␣needs␣to␣be␣fulfilled␣[-]␣";
$LOAD        x_conv
;
$GDXOUT
$offfold




*--------------------------------         3            --------------------------------*
*--------------------------------  DEFINE OPTION FILE  --------------------------------*
*-------------------------------- TO BE READ BY CPLEX  --------------------------------*

file fcpx "Cplex␣Option␣file␣for␣indicator␣Constraints␣and␣specifications␣regarding␣memory␣usage" / cplex.opt /;


*--------------------------------         4            --------------------------------*
*--------------------------------   DEFINE THE SCALARS --------------------------------*
*-------------------------------- FOR ALL COEFFICIENTS --------------------------------*


*GENERAL ELECTRICITY FOOTPRINT
Scalars CO2_FP_elec      The carbon footprint of electricity in 2040 in [Mtonne CO2-eq per MWh]  (based on 50:50 ratio PV wind)                  /0.0001       /     ;


*CAPTURE UNITS
Scalars Cap_conv         Average capture efficiency (same for all CO2 sources)                                                    /0.87         /
        E_CO2_cap        CO2 conversion factor for a carbon capture unit given in [MWh per Mtonne CO2 captured]                    /374444.44    /
        Con_Cap_CO2      Construction CO2 footprint of a capture unit given in BASED ON SIMAPRO [Mtonne CO2-eq per capture unit]   /0.279        /
        OM_Cap_CO2       O&M CO2 footprint of a capture unit given in BASED ON SIMAPRO [Mtonne CO2-eq per Mtonne CO2 captured]     /0.01116      /     ;
```

```
*COMPRESSOR UNITS
Scalars E_CO2_compr      CO2 conversion factor for a compressor unit used for biomethane and
    bioethanol [MWh per Mtonne CO2 compressed]         /111388.888   /
        Con_compr_CO2    Construction CO2 footprint of a compressor unit given in [Mtonne CO2
            -eq per compressor unit] based on Peng et al 2016  /0.10453      /
        OM_compr_CO2    O&M CO2 footprint of a compressor unit given in [Mtonne CO2-eq per
            compressor unit] based on Peng et al 2016            /4.1812E-3    /     ;






*ELECTROLYSER UNITS
Scalars Elec_conv        Inefficiency of electrolyser unit due to not full conversion of CO2
    into syngas [%]                                    /0.85         /
        E_CO2_elec       CO2 conversion factor for an electrolyser unit given in [MWh per
            Mtonne syngas produced]                               /9200000      /
        GWP_SG           Global warming potential of syngas (assumed CO2:H2 in 1:2 ratio)
                                                                  /4.5          /
        Con_Elect_CO2    Construction CO2 footprint of an electrolyser unit given in BASED ON
             SIMAPRO [Mtonne CO2-eq per electrolyser unit]     /0.75         /
        OM_Elect_CO2     O&M CO2 footprint of an electrolyser unit given in BASED ON SIMAPRO
            [Mtonne CO2-eq per Mtonne CO2 converted]           /0.03         /
        Conserv_Mass     The mass ratio to go from CO2 to syngas based on stochiometric
            coefficients                                            /0.58         /
        Mod__Flow        Syngas flow produced per module per year [Mtonne syngas per year]
                                                                 /0.0078       /     ;




Scalars Trans_conv       Leakage of CO2 during transport (assumed to be constant and
    independent over distance)                             /0.98         /     ;


*--------------------------------         5            --------------------------------*
*-------------------------------- DEFINE A NEW FUNCTION--------------------------------*
*-------------------------------- THAT DESCRIBES TRANS --------------------------------*
*--------------------------------  CARBON FOOTPRINT    --------------------------------*






Parameter   Mrk__Fulfill            "Input parameter regarding the flow of syngas that is 
    produced yearly [Mtonne syngas/year]";


*--------------------------------         6            --------------------------------*
*--------------------------------   DEFINE THE VARIA-  --------------------------------*
*-------------------------------- BLES THAT ARE USED   --------------------------------*

Positive Variables
                    x                        Amount of CO2 transported from source going
                        into system [Mtonne CO2 per year from source in Set C entering the
                        supply chain]
                    y                        Amount of syngas transported from the
                        electrolyser prior to transport and corresponding losses [Mtonne SG
                        per year from electrolyser in Set E leaving the electrolyser]
                    Source_Type              Variable to display to show which type of
                        source has been chosen to collect the emitted CO2 from
                    Total_Type               Variable to sum up the total amount of type of
                        CO2 sources used in the model to capture from  ;


```

```
Variable
                    z                              Total transportation footprint for source
                        to electrolyser
                    OF
                    ;


Binary variable     Alloc__Flow                    Binary variable dealing with the
    allocation of flows from source to destination for sets C and E that can take the values
    of 0 or 1;


$onfold
Integer Variable    Mod__Nr(E)                     "The␣number␣of␣modules␣installed␣per␣
    electrolyzer␣system␣␣[#number␣of␣modules]";
                    Mod__Nr.lo(E) = 0;
#                    Mod__Nr.up(E) = ;
$offfold

Variable            Trans_CI_E
                    Trans_CEH_EH
                    Trans_EH_E
                    Trans_E_S;

Variable            CO2Flow__Cap       "Variable␣with␣the␣amount␣of␣CO_2␣captured␣from␣each␣
    CO_2␣source␣in␣set␣C␣[Mtonne/yr]";

*--------------------------------         7           ---------------------------------*
*--------------------------------   DEFINE THE EQUATI- ---------------------------------*
*-------------------------------- ONS/OF. THAT WE USE  ---------------------------------*

Equations
     Footprint                     Define objective function total footprint of the the
         supply chain                                                   [Mtonne CO2-eq per
         year]
     Capt(C)                       Capture constraint that defines the maximum amount of CO2
          that can be captured at a specific location                [Mtonne CO2 captured at
         location C per year]
     Demand(S)                     Define the demand constraint at location S
                                                                                  [All SG
         demand should be satisfied OR looped over a certain fraction]
     eqCIE__Flow1(CI,E)            Indicator Constraint for the fixed capture unit
         constructional carbon footprint of C to E active when flow is > 0   [is 1 if there
         is flow]
     eqCIE__Flow0(CI,E)            Indicator Constraint for the fixed capture unit
         constructional carbon footprint of C to E active when flow is = 0   [is 0 if there
         is NO flow]
     Elect_E(E)                    Define the maximum amount of CO2 that can be converted
         into syngas at location E                                    [Max Mtonne SG produced
          at electrolyser site E in Mtonne SG per year]
     eq_ES_Trans0(E,S)             Indicator constraint for the constructional transport
         unit carbon footprint of C to E active when flow is >0        [is 1 if there is flow
         ]
     eq_ES_Trans1(E,S)             Indicator constraint for the constructional transport
         unit carbon footprint of C to E active when flow is =0        [is 0 if there is NO
         flow]
     eqMrk__Fulfill                Constraint looping the syngas demand from 1% to a full
         100% with a step function of 1 % at a time                   [%]
     eqElyzr__Mod                  Constraint limiting the maximum amount of syngas that can
          be produced at the electrolyser                           []
     eqCI                          Mass constraint for CO2 Flow from CI to directly the
         electrolyser E                                                 [Mtonne CO2 per yr]
     eqEH                          Mass constraint for the CO2 flow at an exclusive hub
                                                                        [Mtonne CO2 per yr]
     eqCIE                         Mass balance constraint that states conservation of mass
         from Idividual source to electrolyser                      [Mtonne CO2 per yr]
     eqEHE                         Mass balance constraint that states conservation of mass
         from Exclusive Hub to the Electrolyser                     [Mtonne CO2 per yr]
     eqES                          Mass balance constraint that states conservation of mass
         from Electrolyser to the syngas demand position            [Mtonne SG per yr]
     eqCEHEH__Flow1(CEH,EH)        Indicator constraint for whether there is flow from CEH
```

```
         to the exclusive hub                                        []
     eqCEHEH__Flow0(CEH,EH)         Indicator constraint for whether there is NO flow from
         CEH to the exclusive hub                                      []
     eqEHE__Flow1(EH,E)             Indicator constraint for whether there is flow from
         exclusive hub to the Electrolyser                                  []
     eqEHE__Flow0(EH,E)             Indicator constraint for whether there is NO flow from
         exclusive hub to the Electrolyser                             []
     Total_KmCI_E                   Distance constraint that calculates the total amount from
          individual CO2 source to the electrolyser                  [km]
     Total_KmCEH_EH                 Distance constraint that calculates the total amount from
          CO2 source to the exclusive hub                            [km]
     Total_KmEH_E                   Distance constraint that calculates the total amount from
          exclusive hub to the electrolyser                          [km]
     Total_KmE_S                    Distance constraint that calculates the total amount from
          electrolyser to the syngas demand location                 [km]
     eqSource_Type1                 Constraint that accounts for the first type of sources
         that require (individual ones)                                [is 1 if there is flow]
     eqSource_Type2                 Constraint that accounts for the second type of sources
         that require (individual ones)                              [is 0 if there is NO
         flow]
     eqTotal_Type                   Constraint that accounts for the total type of sources
         based on the sum of the previous constraints within set pex   []
     eqCCI__Flow1                   Constraint that will take binary variables depending on
         whether there is capture at a CO2 individual source         [is 1 if there is flow]
     eqCCI__Flow0                   Constraint that will take binary variables depending on
         whether there is capture at a CO2 individual source         [is 0 if there is NO
         flow]
     eqOF                           Equation regarding the functional unit that will divide
         the objective function over that specific market fraction   [kg CO2-eq per kg syngas
         ]
     eqTotal_Type1                  ;



Footprint ..        z   =e=         sum((CCI,CI), x(CCI,CI))* (1-Cap_conv)
                                                                            +

                                    sum((CCI,CEH), x(CCI,CEH))* (1-Cap_conv)

                                        +

                                    Trans_CI_E + Trans_CEH_EH + Trans_EH_E + Trans_E_S +
                                        GWP_SG * 0.02 *  sum((E,S), y(E,S))
                                                                +

                                    sum((CI,E), x(CI,E))      * E_CO2_cap * CO2_FP_elec

                                        +

                                    sum((CEH,EH), x(CEH,EH))  * E_CO2_cap * CO2_FP_elec

                                        +

                                    (sum((E,S), y(E,S)))    * E_CO2_elec *  CO2_FP_elec

                                        +

                                    sum((CCI,CI),Alloc__Flow(CCI,CI))   * Con_Cap_CO2

                                        +

                                    sum((CEH,EH),Alloc__Flow(CEH,EH))   * Con_Cap_CO2

                                        +

                                    sum((CEH,EH), x(CEH,EH))            * Cap_conv *
                                        OM_Cap_CO2

                                        +

                                    sum((CI,E), x(CI,E))                * Cap_conv *
```

```
                                        OM_Cap_CO2
                                        +
                                    sum(E, Mod__Nr(E))                 * Con_Elect_CO2
                                        +
                                    (sum((E,S), y(E,S))) * OM_Elect_CO2
                                        +
                                    eps*sum[(E,S), Alloc__Flow(E,S)]
                                        +
                                    eps*sum[(CI,E), Alloc__Flow(CI,E)]
                                        +
                                    eps*sum[(CEH,EH), Alloc__Flow(CEH,EH)]
                                        +
                                    eps*sum[(EH,E), Alloc__Flow(EH,E)]
                                        ;



*Constraints that will obtain binary values, depends on whether the model decides to capture
    carbon at  an emission location
eqCCI__Flow1(CCI,CI)..                x(CCI,CI)                         =g=     0
                                                                      ;
eqCCI__Flow0(CCI,CI) ..               x(CCI,CI)                         =e=     0
                                                                      ;

*Constraints that will obtain binary values, depends on whether the model decides to capture
    carbon at  an emission location
eqCIE__Flow1(CI,E)..                  x(CI,E)                           =g=     0
                                                                      ;
eqCIE__Flow0(CI,E) ..                 x(CI,E)                           =e=     0
                                                                      ;



*Constraints that will obtain binary values, depends on whether the model decides to capture
    carbon at  an emission location
eqCEHEH__Flow1(CEH,EH)..             x(CEH,EH)                          =g=     0
                                                                      ;
eqCEHEH__Flow0(CEH,EH) ..            x(CEH,EH)                          =e=     0
                                                                      ;


*Constraints that will obtain binary values, depends on whether the model decides to capture
    carbon at  an emission location
eqEHE__Flow1(EH,E)..                  x(EH,E)                           =g=     0
                                                                      ;
eqEHE__Flow0(EH,E) ..                 x(EH,E)                           =e=     0
                                                                      ;

*Constraints that will obtain binary values, depends on whether the model decides to
    transport syngas from electrolyser E to syngas demand location S
eq_ES_Trans1(E,S)..                  y(E,S)                             =g=     0
                                                                      ;
eq_ES_Trans0(E,S) ..                 y(E,S)                             =e=     0
                                                                      ;


*Maximum amount of CO2 that can be captured at the sources (C)
Capt(C)..                           sum[pex, CO2_In(C, pex) * x_conv(pex)$(TSetCap(C,pex))]
```

```
         =e=     CO2Flow__Cap(C)                            ;

*Maximum amount of CO2 that can be converted into syngas at location (E)
Elect_E(E)..                       sum(S, y(E,S))                      =e=     Conserv_Mass
     * Trans_conv*Elec_conv*sum(C, x(C,E))                   ;

*All syngas produced should be equal to the total demand
Demand(S)..                        sum(E, y(E,S))* Trans_conv          =l=     SG_Demand(S)
                                                             ;

*Constraint limiting the demand to the different fractions that are defined in the SG_Fract2
    .gdx file
eqMrk__Fulfill..                   sum[(E,S), y(E,S)]                  =e=     Mrk__Fulfill
                                                             ;

*Constraint limit the amount of syngas that can be produced by an electrolyser
eqElyzr__Mod(E)..                  Mod__Nr(E)*Mod__Flow                =g=     sum[(S),y(E,
    S)]                                                      ;



*New mass constraints due to extra step in the Supply Chain
eqCI(CCI)..                        sum[(CI), x(CCI,CI)$TSetCCI(CCI,CI)]
                                  =l=         CO2Flow__Cap(CCI)              ;

eqEH(CEH)..                        sum[(EH), x(CEH,EH)$TSetCEH(CEH,EH)]
                                  =l=         CO2Flow__Cap(CEH)              ;

eqCIE(CI)..                        sum[(CCI),x(CCI,CI)$TSetCCI(CCI,CI)]
                                  =e=         sum[(E), x(CI,E)]              ;

eqEHE(EH)..                        sum[(CEH),x(CEH,EH)$TSetCEH(CEH,EH)]
                                  =e=         sum[(E), x(EH,E)]              ;

eqES(E)..                          (sum[(EH), x(EH,E)*Conserv_Mass] + sum[(CI), x(CI,E)*
    Conserv_Mass])*Elec_conv =e=        sum[(S), y(E,S)]       ;





#Take the sum of all distances that are there
Total_KmCI_E..                     sum((CI,E), (T__Dist(CI,E))*  Alloc__Flow(CI,E))        *
     0.0326    =e=         Trans_CI_E                        ;

Total_KmCEH_EH..                   sum((CEH,EH), (T__Dist(CEH,EH))*  Alloc__Flow(CEH,EH))  *
     0.0326    =e=         Trans_CEH_EH                      ;

Total_KmEH_E..                     sum((EH,E), (T__Dist(EH,E)) *  Alloc__Flow(EH,E))       *
     0.0326    =e=         Trans_EH_E                        ;

Total_KmE_S..                      sum((E,S), (T__Dist(E,S))*  Alloc__Flow(E,S))           *
     0.0326    =e=         Trans_E_S                         ;



eqSource_Type1(CCI, pex)..         sum((CI), Alloc__Flow(CCI,CI))$  (sum((CI), Link(CCI,CI)
    $TSetCap(cci,pex)))     =e=     Source_Type(CCI, pex)     ;
eqSource_Type2(CEH, pex)..         sum((EH), Alloc__Flow(CEH,EH))$  (sum((EH), Link2(CEH,EH)
    $TSetCap(ceh,pex)))    =e=     Source_Type(CEH, pex)     ;

eqTotal_Type(pex)..                sum(CI, Source_Type(CI, pex)) +   sum(CEH, Source_Type(
    CEH, pex))                =e=     Total_Type(pex)          ;
eqTotal_Type1(pex)..               sum(EH, Source_Type(EH, pex)) +   sum(CEH, Source_Type(
    CEH, pex))                =e=     Total_Type(pex)          ;


eqOF ..                            OF
                                                                               =e=     z/
    Mrk__Fulfill           ;

```

```
*--------------------------------          8          ---------------------------------*
*--------------------------------   LOOP IN ORDER TO    ---------------------------------*
*-------------------------------- MAKE THE BINARY VAR.  ---------------------------------*
loop((CCI,CI),
    put fcpx 'indic␣' eqCCI__Flow1.tn(CCI,CI)         '$' Alloc__Flow.tn(CCI,CI) yes
         / 'indic␣' eqCCI__Flow0.tn(CCI,CI)           '$' Alloc__Flow.tn(CCI,CI) No / );

loop((CI,E),
    put fcpx 'indic␣' eqCIE__Flow1.tn(CI,E)           '$' Alloc__Flow.tn(CI,E) yes
         / 'indic␣' eqCIE__Flow0.tn(CI,E)             '$' Alloc__Flow.tn(CI,E) No / );

loop((CEH,EH),
    put fcpx 'indic␣' eqCEHEH__Flow1.tn(CEH,EH)       '$' Alloc__Flow.tn(CEH,EH) yes
         / 'indic␣' eqCEHEH__Flow0.tn(CEH,EH)         '$' Alloc__Flow.tn(CEH,EH) No / );

loop((EH,E),
    put fcpx 'indic␣' eqEHE__Flow1.tn(EH,E)           '$' Alloc__Flow.tn(EH,E) yes
         / 'indic␣' eqEHE__Flow0.tn(EH,E)             '$' Alloc__Flow.tn(EH,E) No / );


loop((E,S),
   put fcpx 'indic␣' eq_ES_Trans1.tn(E,S)             '$' Alloc__Flow.tn(E,S) yes
        / 'indic␣' eq_ES_Trans0.tn(E,S)               '$' Alloc__Flow.tn(E,S) No / );




put fcpx "parallelmode␣=␣1"/
"threads␣␣=␣0"/
putclose fcpx;

putclose fcpx


*--------------------------------         9          ---------------------------------*
*--------------------------------  DEFINE THE PARAMETERS---------------------------------*
*-------------------------------- FOR THE OPTIMUM FRACT.---------------------------------*


$onfold #Defintion of output parameters
Parameters    OptGap             "Parameter␣storing␣the␣optimality␣gap␣in␣an␣output␣gdx␣file␣
    [-]"
              CO2FlowCCI         "Output␣parameter␣of␣CO_2␣flow␣from␣C␣to␣CI"
              CO2FlowCEH         "Output␣parameter␣of␣CO_2␣flow␣from␣C␣to␣EH"
              CO2FlowCIE         "Output␣parameter␣of␣CO_2␣flow␣from␣CI␣to␣E"
              CO2FlowEHE         "Output␣parameter␣of␣CO_2␣flow␣from␣EH␣to␣E"
              CO2FlowEEE         "Output␣parameter␣of␣CO_2␣flow␣from␣E␣to␣EE"
              CO2FlowEES         "Output␣parameter␣of␣CO_2␣flow␣from␣EE␣to␣S"
              z2                 "Output␣parameter␣for␣the␣objective␣function␣value"
              OF2                "Output␣of␣the␣functional␣unit␣that␣we␣want␣to␣minimise␣[kg␣
                 CO2-eq/kg␣SG]"
              Source_Type2       "Output␣for␣the␣different␣type␣of␣output␣units␣within␣CCI␣and
                 ␣[BioethanolL,␣BioethanolS,␣Biomethane,␣Pulp,␣Waste"
              Source_Type3       "Output␣for␣the␣different␣type␣of␣output␣units␣within␣CEH␣and
                 ␣[BioethanolL,␣BioethanolS,␣Biomethane,␣Pulp,␣Waste"
              Total_Type2        "Output␣for␣the␣TOTAL␣per␣type␣of␣output␣units␣[BioethanolL,␣
                 BioethanolS,␣Biomethane,␣Pulp,␣Waste"
              Trans_CI_E2        "Output␣variable␣to␣store␣the␣distance␣from␣CI-E␣in␣[km]"
              Trans_CEH_EH2      "Output␣variable␣to␣store␣the␣distance␣from␣CEH-EH␣in␣[km]"
              Trans_EH_E2        "Output␣variable␣to␣store␣the␣distance␣from␣EH-E␣in␣[km]"
              Trans_E_S2         "Output␣variable␣to␣store␣the␣distance␣from␣E-S␣in␣[km]" ;
$offFold


*--------------------------------          10          ---------------------------------*
*--------------------------------  MINIMSE OVER FRACT.  ---------------------------------*
*-------------------------------- EXPORT .GDX WITH VALUES---------------------------------*

model transport /all/ ;
transport.optfile =1;

```

```
loop(count,
    Mrk__Fulfill = sum[(s),SG_Demand(S)]*Market__Fr(Count);

        Solve transport using MIP minimizing OF ;
;
# This is for running the model with a range of different market fulfilments
            CO2FlowCCI(count,CCI,CI)$(x.l(CCI,CI)  gt 0.000001)      =   x.l(CCI,CI)
                           ;
            CO2FlowCEH(count,CEH,EH)$(x.l(CEH,EH)  gt 0.000001)      =   x.l(CEH,EH)
                           ;
            CO2FlowCIE(count,CI,E)  $(x.l(CI,E)    gt 0.000001)      =   x.l(CI, E)
                            ;
            CO2FlowEHE(count,EH,E)  $(x.l(EH,E)    gt 0.000001)      =   x.l(EH, E)
                            ;
            CO2FlowEES(count,E,S)   $(y.l(E,S)     gt 0.000001)      =   y.l(E,S)
                              ;
            CO2FlowEEE(count,E,EE)$(x.l(E,EE) gt 0.000001)           =   x.l(E,EE)
                             ;
            z2(count)                                                =   z.l
                                   ;
            OF2(count)                                               =   OF.l
                                  ;
            Total_Type2(count,pex)                                   =   Total_Type.l(pex)
                     ;
            Source_Type2(count,CCI,pex)                              =   Source_Type.l(CCI,
                pex) ;
            Source_Type3(count,CEH,pex)                              =   Source_Type.l(CEH,
                pex) ;
            Trans_CI_E2(count)                                       =   Trans_CI_E.l
                          ;
            Trans_CEH_EH2(count)                                     =   Trans_CEH_EH.l
                        ;
            Trans_EH_E2(count)                                       =   Trans_EH_E.l
                          ;
            Trans_E_S2(count)                                        =   Trans_E_S.l
                           ;



execute_unload "GDXOutput_Results.gdx",
CO2FlowCCI,CO2FlowCEH, CO2FlowCIE,CO2FlowEHE CO2FlowEEE, CO2FlowEES,z2,OF2,  Total_Type2,
    Source_Type2,Source_Type3, Trans_CI_E2, Trans_CEH_EH2,Trans_EH_E2,Trans_E_S2 ;
);

*---------------------------------           11          ---------------------------------*
*---------------------------------  DISPLAY THE DIFFERENT ---------------------------------*
*--------------------------------- VALUES IN PROCESS LOG  ---------------------------------*


display  Trans_CI_E.l
         Trans_CEH_EH.l
         Trans_EH_E.l
         Trans_E_S.l
         x.l,x.m
         y.l,y.m
         Alloc__Flow.l
         Source_Type.l
         Total_Type.l                                                                   ;
```

The following code is used for the cost minimisation

```
$eolCom #
$inlinecom /* */

option reslim = 21600;
option optCR=0.002;
Option MIP = GUROBI;
$ontext
$OnFold #Set / Subset definition of total model
Sets
   C        /C68,C311,C82,C84,C240,C459,C363,C92,C94,C96,C100,C104,C253,C256,C263,C265,C267,
       C272,C295,C449,C74,C224,C37,C159,C299,C309,C394,C230,C312,C315,C316,C317,C318,C319,
```

```
        C417,C421,C456,C458,C47,C61,C173,C175,C186,C188,C302,C400,C323,C325,C329,C331,C333,
        C428,C429,C241,C336,C461,C3,C8,C11,C12,C108,C109,C282,C465,C250,C251,C66,C142,C286,C1,
        C106,C274,C275,C276,C278,C375,C452,C453,C248,C357,C358,C359,C360,C361,C445,C321,C322,
        C87,C341,C342,C348,C349,C350,C351,C352,C355,C356,C364,C15,C21,C28,C32,C33,C284,C407,
        C410,C415,C211,C412,C468,C214,C215,C212,C216,C310,C213,C411,C67,C408,C414,C406,C409,
        C413,C237,C390,C432,C81,C83,C238,C235,C335,C80,C239,C433,C460,C480,C447,C105,C99,C102,
        C308,C262,C1023,C365,C95,C145,C148,C153,C144,C154,C155,C293,C34,C150,C291,C97,C35,C292
        ,C103,C146,C149,C156,C101,C36,C294,C371,C98,C269,C270,C271,C198,C403,C252,C366,C290,
        C372,C261,C257,C259,C147,C289,C368,C255,C374,C268,C370,C264,C450,C448,C451,C464,C93,
        C266,C152,C373,C107,C157,C254,C367,C258,C151,C388,C369,C392,C70,C73,C69,C75,C76,C72,
        C77,C71,C220,C222,C217,C221,C225,C219,C226,C227,C228,C223,C296,C297,C389,C201,C207,C65
        ,C63,C204,C205,C208,C203,C206,C313,C314,C231,C232,C416,C233,C418,C419,C420,C320,C187,
        C46,C185,C305,C218,C399,C45,C171,C194,C196,C197,C52,C59,C168,C178,C177,C179,C189,C190,
        C191,C192,C169,C60,C176,C172,C182,C183,C51,C54,C397,C181,C58,C48,C55,C158,C174,C457,
        C193,C195,C50,C62,C199,C260,C167,C200,C301,C334,C304,C401,C402,C467,C300,C398,C396,
        C395,C49,C466,C170,C56,C184,C53,C44,C236,C180,C57,C303,C79,C324,C234,C422,C426,C78,
        C332,C328,C423,C326,C327,C330,C430,C427,C405,C431,C424,C425,C110,C114,C143,C6,C113,C10
        ,C5,C376,C2,C111,C112,C1201,C9,C279,C280,C4,C7,C281,C209,C42,C298,C391,C40,C41,C161,
        C160,C455,C162,C163,C166,C43,C39,C273,C393,C38,C164,C165,C138,C139,C140,C141,C383,C137
        ,C386,C277,C288,C247,C249,C379,C443,C444,C90,C88,C86,C243,C337,C435,C436,C462,C340,
        C346,C343,C344,C345,C353,C354,C347,C244,C339,C441,C442,C245,C91,C242,C437,C338,C85,C89
        ,C202,C246,C434,C438,C439,C440,C24,C31,C119,C136,C127,C128,C131,C18,C20,C22,C13,C19,
        C134,C121,C122,C123,C130,C132,C27,C129,C463,C14,C133,C29,C16,C30,C126,C378,C377,C454,
        C115,C25,C23,C118,C124,C125,C135,C116,C117,C283,C285,C17,C26/
    CCI(C)   /C68,C311,C82,C84,C240,C459,C363,C92,C94,C96,C100,C104,C253,C256,C263,C265,C267,
        C272,C295,C449,C74,C224,C37,C159,C299,C309,C394,C230,C312,C315,C316,C317,C318,C319,
        C417,C421,C456,C458,C47,C61,C173,C175,C186,C188,C302,C400,C323,C325,C329,C331,C333,
        C428,C429,C241,C336,C461,C3,C8,C11,C12,C108,C109,C282,C465,C250,C251,C66,C142,C286,C1,
        C106,C274,C275,C276,C278,C375,C452,C453,C248,C357,C358,C359,C360,C361,C445,C321,C322,
        C87,C341,C342,C348,C349,C350,C351,C352,C355,C356,C364,C15,C21,C28,C32,C33,C284/
    CEH(C)   /C407,C410,C415,C211,C412,C468,C214,C215,C212,C216,C310,C213,C411,C67,C408,C414,
        C406,C409,C413,C237,C390,C432,C81,C83,C238,C235,C335,C80,C239,C433,C460,C480,C447,C105
        ,C99,C102,C308,C262,C1023,C365,C95,C145,C148,C153,C144,C154,C155,C293,C34,C150,C291,
        C97,C35,C292,C103,C146,C149,C156,C101,C36,C294,C371,C98,C269,C270,C271,C198,C403,C252,
        C366,C290,C372,C261,C257,C259,C147,C289,C368,C255,C374,C268,C370,C264,C450,C448,C451,
        C464,C93,C266,C152,C373,C107,C157,C254,C367,C258,C151,C388,C369,C392,C70,C73,C69,C75,
        C76,C72,C77,C71,C220,C222,C217,C221,C225,C219,C226,C227,C228,C223,C296,C297,C389,C201,
        C207,C65,C63,C204,C205,C208,C203,C206,C313,C314,C231,C232,C416,C233,C418,C419,C420,
        C320,C187,C46,C185,C305,C218,C399,C45,C171,C194,C196,C197,C52,C59,C168,C178,C177,C179,
        C189,C190,C191,C192,C169,C60,C176,C172,C182,C183,C51,C54,C397,C181,C58,C48,C55,C158,
        C174,C457,C193,C195,C50,C62,C199,C260,C167,C200,C301,C334,C304,C401,C402,C467,C300,
        C398,C396,C395,C49,C466,C170,C56,C184,C53,C44,C236,C180,C57,C303,C79,C324,C234,C422,
        C426,C78,C332,C328,C423,C326,C327,C330,C430,C427,C405,C431,C424,C425,C110,C114,C143,C6
        ,C113,C10,C5,C376,C2,C111,C112,C1201,C9,C279,C280,C4,C7,C281,C209,C42,C298,C391,C40,
        C41,C161,C160,C455,C162,C163,C166,C43,C39,C273,C393,C38,C164,C165,C138,C139,C140,C141,
        C383,C137,C386,C277,C288,C247,C249,C379,C443,C444,C90,C88,C86,C243,C337,C435,C436,C462
        ,C340,C346,C343,C344,C345,C353,C354,C347,C244,C339,C441,C442,C245,C91,C242,C437,C338,
        C85,C89,C202,C246,C434,C438,C439,C440,C24,C31,C119,C136,C127,C128,C131,C18,C20,C22,C13
        ,C19,C134,C121,C122,C123,C130,C132,C27,C129,C463,C14,C133,C29,C16,C30,C126,C378,C377,
        C454,C115,C25,C23,C118,C124,C125,C135,C116,C117,C283,C285,C17,C26/
    CI       /CI15,CI59,CI17,CI18,CI36,CI106,CI89,CI20,CI21,CI22,CI23,CI24,CI41,CI42,CI43,CI44
        ,CI45,CI46,CI55,CI101,CI16,CI34,CI11,CI29,CI56,CI58,CI93,CI35,CI60,CI61,CI62,CI63,CI64
        ,CI65,CI95,CI96,CI104,CI105,CI12,CI13,CI30,CI31,CI32,CI33,CI57,CI94,CI68,CI69,CI70,
        CI71,CI72,CI97,CI98,CI37,CI73,CI107,CI2,CI3,CI4,CI5,CI26,CI27,CI51,CI108,CI39,CI40,
        CI14,CI28,CI53,CI1,CI25,CI47,CI48,CI49,CI50,CI91,CI102,CI103,CI38,CI83,CI84,CI85,CI86,
        CI87,CI99,CI66,CI67,CI19,CI74,CI75,CI76,CI77,CI78,CI79,CI80,CI81,CI82,CI90,CI6,CI7,CI8
        ,CI9,CI10,CI52/
    EH       /EH66,EH13,EH128,EH89,EH212,EH353,EH20,EH102,EH222,EH238,EH181,EH399,EH215,EH39,
        EH468,EH183,EH121,EH126,EH113,EH164,EH133,EH29,EH104,EH176,EH377,EH141,EH6,EH467,EH79,
        EH105,EH68,EH373,EH115,EH217,EH175,EH106,EH75,EH402,EH45,EH72,EH199,EH25,EH156,EH123,
        EH210,EH12,EH194,EH146,EH227,EH197,EH369,EH90,EH142,EH252,EH10,EH96,EH88,EH57,EH94,
        EH278,EH218,EH148,EH185,EH125,EH184,EH195,EH110,EH158,EH32,EH171,EH462,EH463,EH91,
        EH155,EH119,EH209,EH62,EH161,EH53,EH461,EH117,EH85,EH38,EH80,EH114,EH459,EH173,EH101,
        EH151,EH378,EH124,EH385,EH100,EH386,EH77,EH112,EH139,EH153,EH47,EH120,EH87,EH92,EH69,
        EH82,EH418,EH144,EH130,EH310,EH76,EH134,EH312,EH73,EH337,EH49,EH147,EH84,EH56,EH395,
        EH16,EH143,EH67,EH129,EH340,EH23,EH188,EH165,EH116,EH464,EH182,EH111,EH457,EH179,EH65,
        EH127,EH30,EH22,EH108,EH168,EH36,EH465,EH177,EH162,EH24,EH187,EH419,EH132,EH460,EH103,
        EH137,EH135,EH387,EH189,EH136,EH296,EH21,EH131,EH446,EH326,EH41,EH86,EH145,EH17,EH44,
        EH19,EH70,EH191,EH169,EH172,EH159,EH54,EH93,EH167,EH11,EH97,EH174,EH152,EH219,EH74,
        EH405,EH306,EH63,EH61,EH224,EH206,EH149,EH214,EH2,EH59,EH98,EH163,EH150,EH27,EH60,EH15
        ,EH469,EH447,EH160,EH364,EH178,EH226,EH203,EH71,EH42,EH14,EH359,EH18,EH458,EH43,EH107,
```

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        EH95,EH48,EH83,EH64,EH58,EH434,EH466,EH122,EH28,EH52,EH1,EH5,EH157,EH207,EH154,EH78,
        EH55,EH420,EH118,EH286,EH109,EH50,EH225,EH198,EH322,EH429,EH46,EH81,EH180,EH51,EH138,
        EH140,EH190,EH318/
    E        /E349,E393,E351,E352,E370,E440,E423,E354,E355,E356,E357,E358,E375,E376,E377,E378,
        E379,E380,E389,E435,E350,E368,E345,E363,E390,E392,E427,E369,E394,E395,E396,E397,E398,
        E399,E429,E430,E438,E439,E346,E347,E364,E365,E366,E367,E391,E428,E402,E403,E404,E405,
        E406,E431,E432,E371,E407,E441,E336,E337,E338,E339,E360,E361,E385,E442,E373,E374,E348,
        E362,E387,E335,E359,E381,E382,E383,E384,E425,E436,E437,E372,E417,E418,E419,E420,E421,
        E433,E400,E401,E353,E408,E409,E410,E411,E412,E413,E414,E415,E416,E424,E340,E341,E342,
        E343,E344,E386,E13,E37,E47,E50,E19,E30,E5,E6,E7,E10,E11,E14,E16,E21,E23,E24,E27,E29,
        E39,E42,E44,E12,E36,E52,E2,E26,E40,E51,E54,E3,E18,E33,E22,E43,E48,E49,E15,E20,E28,E31,
        E35,E38,E41,E46,E1,E9,E17,E25,E45,E53,E4,E8,E32,E34,E55,E56,E57,E58,E74,E75,E76,E77,
        E78,E59,E60,E61,E62,E63,E64,E65,E66,E67,E68,E69,E70,E71,E72,E73,E87,E88,E79,E80,E81,
        E82,E83,E84,E85,E86,E105,E106,E107,E108,E109,E110,E111,E112,E113,E114,E115,E116,E117,
        E118,E119,E120,E121,E122,E123,E124,E125,E126,E127,E135,E136,E137,E138,E139,E140,E141,
        E89,E90,E91,E92,E93,E94,E95,E96,E97,E98,E99,E100,E101,E102,E103,E104,E128,E129,E130,
        E131,E132,E133,E134,E148,E149,E150,E165,E166,E167,E142,E143,E144,E145,E146,E147,E151,
        E152,E153,E154,E155,E156,E157,E158,E159,E160,E161,E162,E163,E164,E180,E181,E168,E169,
        E170,E171,E172,E173,E174,E175,E176,E177,E178,E179,E187,E188,E189,E190,E191,E192,E193,
        E200,E201,E202,E182,E183,E184,E185,E186,E194,E195,E196,E197,E198,E199,E216,E217,E218,
        E203,E204,E205,E206,E207,E208,E209,E210,E211,E212,E213,E214,E215,E222,E223,E224,E225,
        E226,E227,E228,E243,E219,E220,E221,E229,E230,E231,E232,E233,E234,E235,E236,E237,E238,
        E239,E240,E241,E242,E244,E245,E249,E250,E251,E252,E253,E254,E246,E247,E248,E255,E256,
        E257,E258,E259,E260,E261,E262,E263,E264,E273,E274,E275,E265,E266,E267,E268,E269,E270,
        E271,E272,E283,E284,E285,E286,E287,E276,E288,E289,E290,E291,E292,E293,E294,E277,E278,
        E279,E280,E281,E282,E295,E296,E297,E298,E299,E300,E301,E302,E303,E304,E305,E306,E307,
        E308,E309,E310,E311,E312,E313,E314,E315,E316,E317,E318,E319,E320,E321,E322,E323,E324,
        E325,E326,E327,E328,E329,E330,E331,E332,E333,E334/
    S        /S13,S37,S47,S50,S19,S30,S5,S6,S7,S10,S11,S14,S16,S21,S23,S24,S27,S29,S39,S42,S44
        ,S12,S36,S52,S2,S26,S40,S51,S54,S3,S18,S33,S22,S43,S48,S49,S15,S20,S28,S31,S35,S38,S41
        ,S46,S1,S9,S17,S25,S45,S53,S4,S8,S32,S34/
;
Alias(E,EE);
$OffFold
$offtext

$OnFold  #Set / Subset definition of BENELUX model
Sets
     c        "Set␣containing␣all␣the␣CO_2␣sources␣in␣the␣model,␣indexed␣by␣c_1␣..␣1573;"   /
         C1232,C1239,C1300,C82,C84,C240,C459,C517,C42,C1267,C1289,C298,C391,C1283,C1236,C1272,
         C1296,C40,C41,C1291,C161,C1237,C160,C455,C1271,C162,C163,C166,C1278,C43,C1250,C39,
         C1266,C1277,C1285,C273,C1294,C393,C1238,C514,C1235,C1246,C1295,C1253,C1255,C1297,
         C1282,C1298,C1299,C1242,C1262,C1265,C1292,C38,C1251,C1252,C1260,C1274,C1243,C1287,
         C1240,C1284,C1248,C1293,C1263,C1273,C1301,C1233,C1234,C1257,C1288,C1247,C1270,C164,
         C1244,C1245,C1140,C1259,C1275,C1254,C1256,C1286,C1302,C165,C1279,C1280,C1281,C1258,
         C1290,C1249,C1264,C1241,C1261,C1268,C1269,C237,C390,C432,C81,C83,C238,C519,C1054,C235
         ,C515,C516,C335,C469,C80,C239,C433,C460,C480,C1276,C209,C867,C1229,C1230,C1231/

     cci(c)   "Subset␣of␣Set␣C␣containing␣all␣the␣individual␣CO_2␣sources␣(cci)␣in␣the␣model␣
         which␣are␣not␣part␣of␣a␣25␣kilometer␣cluster,␣indexed␣by␣c"   /C1232,C1239,C1300,C82,
         C84,C240,C459,C517/

     ceh(c)   "Subset␣of␣Set␣C␣containing␣all␣the␣exclusive␣hub␣CO_2␣sources␣(ceh)␣which␣are␣
         part␣of␣a␣25␣kilometer␣cluster,␣indexed␣by␣c"    /C42,C1267,C1289,C298,C391,C1283,
         C1236,C1272,C1296,C40,C41,C1291,C161,C1237,C160,C455,C1271,C162,C163,C166,C1278,C43,
         C1250,C39,C1266,C1277,C1285,C273,C1294,C393,C1238,C514,C1235,C1246,C1295,C1253,C1255,
         C1297,C1282,C1298,C1299,C1242,C1262,C1265,C1292,C38,C1251,C1252,C1260,C1274,C1243,
         C1287,C1240,C1284,C1248,C1293,C1263,C1273,C1301,C1233,C1234,C1257,C1288,C1247,C1270,
         C164,C1244,C1245,C1140,C1259,C1275,C1254,C1256,C1286,C1302,C165,C1279,C1280,C1281,
         C1258,C1290,C1249,C1264,C1241,C1261,C1268,C1269,C237,C390,C432,C81,C83,C238,C519,
         C1054,C235,C515,C516,C335,C469,C80,C239,C433,C460,C480,C1276,C209,C867,C1229,C1230,
         C1231/
     eh        "Set␣EH␣-␣containing␣all␣the␣exclusive␣hub␣CO_2␣sources␣with␣dedicated␣label␣(eh
         )␣which␣are␣part␣of␣a␣25␣kilometer␣cluster,␣indexed␣by␣eh_1␣..␣481;"  /EH1,EH2,EH4,
         EH43,EH59,EH60,EH67,EH68,EH69,EH105,EH122,EH146,EH204,EH370,EH374,EH375,EH381,EH382,
         EH387,EH388,EH390,EH391,EH392,EH393,EH396,EH398,EH399,EH400,EH401,EH402,EH403,EH404,
         EH408,EH479,EH29,EH113,EH142,EH167,EH177,EH191,EH175/
     ci        "Set␣containing␣all␣the␣individual␣CO_2␣sources␣with␣dedicated␣label␣(CI)␣in␣the
         ␣model␣which␣are␣not␣part␣of␣a␣25␣kilometer␣cluster,␣indexed␣by␣ci_1␣..␣256;"   /
         CI225,CI226,CI227,CI17,CI18,CI36,CI106,CI123/
     e         "Set␣E␣-␣containing␣all␣the␣possible␣electrolyzer␣locations,␣build␣up␣of␣CO_2␣
```

```
        source␣locations,␣syngas␣demand␣points␣and␣intermediate␣hub␣locations,␣indexed␣by␣e_1
        ␣..␣1071;"    /E15,E20,E28,E31,E35,E38,E41,E46,E231,E232,E233,E234,E235,E236,E237,
        E238,E239,E240,E241,E242,E559,E560,E561,E591,E592,E594,E633,E649,E650,E657,E658,E659,
        E695,E712,E736,E794,E960,E964,E965,E971,E972,E977,E978,E980,E981,E982,E983,E986,E988,
        E989,E990,E991,E992,E993,E994,E998,E1069,E19,E30,E59,E60,E61,E62,E63,E64,E65,E66,E67,
        E68,E69,E351,E352,E370,E440,E457,E619,E703,E732,E757,E767,E781,E229,E765/
    s        "Set␣S␣-␣containing␣all␣the␣direct␣and␣indirect␣syngas␣demand␣locations␣in␣the␣
        system,␣indexed␣by␣s_1␣..␣54;"    /S15,S20,S28,S31,S35,S38,S41,S46,S19,S30/
;

Alias(E,EE);
$OffFold

$GDXIN "TransportLinks.gdx"
$onFold #Electrolyzer translation set - Sets that are used to translate subets of C into
    individual CO_2 sources and exclusive hub
Set          TSetCCI(CCI,CI)     "Set␣to␣translate␣set␣CCI␣into␣CI";
$load         TSetCCI
;
Set          TSetCEH(CEH,EH)     "Set␣to␣translate␣set␣CEH␣into␣EH";
$load         TSetCEH
;
$gdxOut
$offFold

$GDXIN "SyngasDemand.gdx"
$onfold #Demand parameters in the model
Parameter   SG__Demand(S)          "Syngas␣demand␣at␣end-use␣location␣s,␣[Mtonne␣syngas]"
$load         SG__Demand
;
$gdxOut
$offFold

$GDXIN "CaptureData.gdx"
$onfold #Set with the different capture technologies, expenditures set and CO_2 input data
    and capture technology
set          tc                  "Set␣containing␣all␣the␣capture␣technologies␣in␣the␣model␣
    specific␣for␣each␣CO_2␣source,␣TC_BioethanolL,BioethanolS,Waste,␣P&P␣and␣Biomethane;"
$load         tc
;

set          pex                  "Set␣containing␣the␣expenditures␣of␣gas␣transport␣(CO_2␣and␣
    syngas)␣and␣capture,pex_opex,␣capex;"
$load         pex
;
Set pexOC(pex) /OPEX,CAPEX/;

Parameter   CO2__In(C, TC)         "The␣CO_2␣emitted␣by␣the␣different␣sources␣in␣set␣C␣with␣
    the␣specific␣capture␣technology␣used␣in␣set␣TC␣[Mtonne/year]"
$load         CO2__In
;
$GDXOUT
$offFold

$onfold #Dynamic set definition of the CO_2 sources to the right technology of capture (TC)
Set          TSetCap(C,TC)       "Translation␣set␣of␣the␣CO_2␣sources␣to␣the␣right␣technology␣
    of␣capture␣(TC)"
             TSetComp(C)          "Translation␣set␣of␣the␣CO_2␣sources␣to␣high␣purity␣
                 compression"
             TCC                  "Total␣capture␣and␣compression␣set␣containing␣all␣the␣
                 technologies␣with␣their␣capture␣";

             TSetCap(C,TC)  = yes$(CO2__In(C, TC) gt 0 and (CO2__In(C, "Pulp") or CO2__In(C, "
                 Waste")));
             TSetComp(C)  = yes$sum(TC,(CO2__In(C, TC) gt 0 and not (CO2__In(C, "Pulp") or
                 CO2__In(C, "Waste"))));
             TCC(C,TC)= yes$(CO2__In(C, TC) gt 0);

$offFold

$GDXIN "Distances.gdx"
```

```
$OnFold #load the distances of all the paths into the model for Constraints
Parameter   T__Dist             "The␣transport␣distances␣of␣all␣parts␣of␣the␣SC␣over␣sets␣CI,EH,E,S␣[km]";
$load        T__Dist
;
$GDXOUT
$OffFold

$OnFold #Scalar Constraints regarding conversion of CO_2 to syngas
Scalar      SG__Conv            "A␣scalar␣with␣the␣conversion␣factor␣to␣transform␣CO_2␣flow␣into␣syngas␣flow␣[(Mtonne␣Syngas/year)/(Mtonne␣CO_2/year)]␣or␣[-]␣Based␣on␣van␣Berkel␣2023␣(Next␣Level␣Solid␣Oxide␣Electrolysis)"    /0.58/;
Scalar      Water__Conv          "A␣scalar␣with␣the␣conversion␣factor␣to␣transform␣␣syngas␣flow␣into␣water␣[(Mtonne␣Syngas/year)/(Mtonne␣water/year)]␣or␣[-]␣Based␣on␣Detz␣2023" /0.862068966/;
$OffFold

file gurobi "Cplex␣Option␣file␣for␣indicator␣Constraints␣and␣specifications␣regarding␣memory␣usage" / gurobi.opt /;
$onFold #Load General information formulation data regarding the piecewise linearization of gas transport
Set
    q        'breakpoints' /q1*q6/
    p        'segments' /p1*p5/
    pq(p,q)  'mapping'
    b        'number␣of␣binary␣variables' /b1,b2,b3/
    b01      'number␣with␣the␣binary␣variables' /0,1/
    fc       'Set␣that␣contains␣the␣piece-wise␣linear␣(PWL)␣data,␣both␣about␣the␣Flow␣and␣Costs' /Flow, Cost/
;

# Calculate mapping between breakpoints and segments
pq(p,q) = ord(p)=ord(q) or ord(p)=ord(q)-1;

positive variable   Lambda     'interpolation␣for␣the␣piecewise␣linearization␣[-]';
Binary Variable     Delta       'segment␣encoding␣for␣the␣piecewiselinearization␣[-]';

Set                 incident    "Boolean␣incidence␣matrix,␣that␣indicatates␣if␣breakpoint␣q␣is␣part␣of␣segment␣p␣that␣has␣␣binary␣digit␣b␣equal␣to␣b01";
Set                 notincident "Opposite␣of␣the␣boolean␣incidence␣matrix␣defined␣above";

Table gray(p,b) 'Gray␣encoding␣of␣segments'
        b1  b2  b3
    p1   0   0   0
    p2   0   0   1
    p3   0   1   1
    p4   0   1   0
    p5   1   1   0
;
$offFold

$GDXIN "PWL_Trans45Elec.gdx"
$onFold #Load the pwl distance data and filter out the unneccesairy parts
Parameter         T__PWLTot                  "Parameter␣containing␣all␣the␣PWL␣data␣of␣all␣the␣paths␣for␣each␣transport␣segment"
$load             T__PWLTot
;
$gdxOut

Parameter        T__PWL              "Parameter␣containing␣(filtered/only␣the␣relevant)␣PWL␣data␣of␣all␣the␣paths␣for␣each␣transport␣segment";
    T__PWL(fc, ci,e,q)          =       T__PWLTot(fc, ci,e,q)$(T__PWLTot(fc, ci,e,q) ne Na);
    T__PWL(fc, eh,e,q)          =       T__PWLTot(fc, eh,e,q)$(T__PWLTot(fc, eh,e,q) ne Na);
    T__PWL(fc, ceh,eh,q)        =       T__PWLTot(fc, ceh,eh,q)$(T__PWLTot(fc, ceh,eh,q) ne Na);
    T__PWL(fc, e,s,q)           =       T__PWLTot(fc, e,s,q)$(T__PWLTot(fc, e,s,q) ne Na);

Set PWL_Breakpoint "Dynamic␣set␣responsible␣for␣keeping␣track␣how␣many␣pieces␣a␣PWL_Breakpoint␣cost␣function␣has" ;
    PWL_Breakpoint(ceh,eh,q)    $(sum((fc), T__PWLTot(fc,ceh,eh,q)) ne na and TSetCEH(CEH,EH)) = yes;
```

```
    PWL_Breakpoint(ci,e,q)       $(sum((fc), T__PWLTot(fc,ci,e,q))    ne na) = yes;
    PWL_Breakpoint(eh,e,q)       $(sum((fc), T__PWLTot(fc,eh,e,q))    ne na) = yes;
    PWL_Breakpoint(e,s,q)        $(sum((fc), T__PWLTot(fc,e,s,q))     ne na) = yes;

Set PWL_Flow "Set␣that␣keeps␣track␣of␣the␣transport␣parts␣of␣which␣a␣PWL_Breakpoint␣cost␣function␣exists";
    PWL_Flow(CEH,EH)            =       (sum((q),PWL_Breakpoint(CEH,EH,q)));
    PWL_Flow(CI,E)              =       (sum((q),PWL_Breakpoint(ci,e,q)));
    PWL_Flow(EH,E)              =       (sum((q),PWL_Breakpoint(eh,e,q)));
    PWL_Flow(E,S)               =       (sum((q),PWL_Breakpoint(e,s,q)));
$OffFold

$onFold #Decision variables regarding CO2Flow and syngas flow
Variable   CO2Flow   "Decision␣variable␣that␣designates␣the␣amount␣of␣CO_2␣flow␣transported␣from␣source␣to␣destination␣[Mtonne/yr]";
Variable   SGFlow    "Decision␣variable␣that␣designates␣the␣amount␣of␣syngas␣flow␣transported␣from␣electrolyzer␣to␣syngas␣demand␣location␣[Mtonne/yr]";
$OffFold

$onfold #Mass balance equations regarding capture of impure sources
Positive variable   Cap__Cost     "Variable␣capture␣cost␣of␣CO_2␣over␣the␣set␣C,␣TC␣and␣PEX␣[EUR2018]";
Binary Variable     Scont         "Semi␣continuous␣binary␣variable␣for␣the␣minimum␣capture␣fraction␣of␣CO2␣at␣inpure␣CO_2␣sources";
$offFold

$GDXIN "PWL_Comp45Elec.gdx"
$onFold #Load the pwl distance data and filter out the unneccesairy parts
Parameter         Tot__PWLCC       "Parameter␣containing␣all␣the␣piecewise␣linearization␣of␣all␣the␣capture␣and␣compression␣segments"
$load             Tot__PWLCC
;
$gdxOut

Parameter        C__PWL           "Parameter␣containg␣the␣piecewise␣linearization␣of␣capture␣and␣compression␣for␣each␣caputure␣technology␣";
    C__PWL(TC,fc,q)         =           Tot__PWLCC(TC,fc,q)$(Tot__PWLCC(TC,fc,q) ne Na);

Set PWL_CC "Dynamic␣set␣responsible␣for␣keeping␣track␣how␣many␣pieces␣a␣capture␣or␣compression␣cost␣function␣has" ;
    PWL_CC(TC,q)            $(sum((fc), Tot__PWLCC(TC, fc,q)) ne na ) = yes;
$offFold

$onFold #Compression cost equations
Positive Variable    CO2Flow__Cap       "Variable␣with␣the␣amount␣of␣CO_2␣captured␣from␣each␣CO_2␣source␣in␣set␣C␣[Mtonne/yr]";
Positive Variable      Cap__FR(C)                "The␣fraction␣of␣CO_2␣that␣is␣captured␣from␣waste␣and␣pulp␣and␣paper";
Scalars       UpFrac                     "Upper␣fraction␣of␣CO_2␣captured␣at␣the␣source" /1/
              LowFrac                    "Lower␣fraction␣of␣CO_2␣captured␣at␣the␣source" /0.75/;

Positive variable   LambdaCC             'interpolation␣for␣the␣piecewise␣linearization␣[-]';
Binary Variable     DeltaCC              'segment␣encoding␣for␣the␣piecewiselinearization␣[-]';

Set                 incidentCC           "Boolean␣incidence␣matrix,␣that␣indicatates␣if␣breakpoint␣q␣is␣part␣of␣segment␣p␣that␣has␣␣binary␣digit␣b␣equal␣to␣b01";
Set                 notincidentCC        "Opposite␣of␣the␣boolean␣incidence␣matrix␣defined␣above";

    incidentCC(C,b,'1',q)        =       sum(pq(p,q),gray(p,b));
    incidentCC(C,b,'0',q)        =       sum(pq(p,q),1-gray(p,b));
    notincidentCC(C,b,b01,q)     =       not incidentCC(C,b,b01,q);

Equations
    eqX__CC               'Equation␣to␣calculate␣the␣CO2␣flow'
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    eqY__CC               'Equation to calculate the annualized cost of that segment taking into conderation the terrain factor'
    eqCC__link0(TC, C,b)  'The link between delta (segment) and lamda the (interpolation)'
    eqCC__link1(TC, C,b)  'The link between delta (segment) and lamda the (interpolation)'
    eqLambda__sumCC       'Equation of the sum of the interpolated parts'
    eqCO2__In              "MASS Constraint about the CO_2 that is captured and entering the supply chain"
    eqMinCapture           "Equations responsible for creating a semi continuous variable out of Cap__Fr by constraining it to a min and max fraction"
    eqMaxCapture           "Equations responsible for creating a semi continuous variable out of Cap__Fr by constraining it to a min and max fraction"
;

    eqCO2__In(C)              ..       sum(TC, CO2__In(C, TC)) * Cap__Fr(C)               =e=        CO2Flow__Cap(C);
    eqX__CC(C)                ..       CO2Flow__Cap(C)         =e=      sum((TC, q), LambdaCC(TC, C,q)$[TCC(C,TC)]*C__PWL(TC, "Flow",q));
    eqY__CC(C)                ..       Cap__Cost(C,"TOTAL")    =e=      sum((TC, q), LambdaCC(TC, C,q)$[TCC(C,TC)]*C__PWL(TC, "Cost",q));
    eqCC__link0(TC, C,b)      ..       sum(notincidentCC(C,b,'0',q),LambdaCC(TC, C,q))    =l=        DeltaCC(TC, C,b);
    eqCC__link1(TC, C,b)      ..       sum(notincidentCC(C,b,'1',q),LambdaCC(TC, C,q))    =l=        1-DeltaCC(TC, C,b);
    eqLambda__sumCC(TC, C)  ..       sum((q), LambdaCC(TC, C,q)$PWL_CC(TC,q))            =e=        1;
    eqMinCapture(C)     $sum(TC,TSetCap(C,TC))  ..  Cap__Fr(C)                          =g=        LowFrac*Scont(C);
    eqMaxCapture(C)     $sum(TC, TSetCap(C,TC)) ..  Cap__Fr(C)                          =l=        UpFrac *Scont(C);
    Cap__FR.up(C)                                                                        =           1;
$offfold

$onfold #Total capture cost equation
Equation    eqCap__Tot            "COST Constraint calculating the total capture cost of CO_2 in the designed supply chain [EUR2018]";
Positive Variable   Cap__Tot     "Variable designating the total cost of CO_2 capture in the designed supply chain ";
             eqCap__Tot           ..      sum[(C), Cap__Cost(C,"TOTAL")  ]      =e=         Cap__Tot;
$offfold

Variable   T__Cost     "Variable dealing with the transport cost from source to destination for sets CI,EH,E,S over the set PEX [EUR2018]";
$onFold #CEHEH cost equations
    incident(CEH,EH,b,'1',q)         =       sum(pq(p,q),gray(p,b));
    incident(CEH,EH,b,'0',q)         =       sum(pq(p,q),1-gray(p,b));
    notincident(CEH,EH,b,b01,q)      =       not incident(CEH,EH,b,b01,q);

Equations
    eqX__CEH              'Equation to calculate the CO2 flow'
    eqY__CEH              'Equation to calculate the annualized cost of that segment taking into conderation the terrain factor'
    eqCEH__link0(CEH,EH,b)  'The link between delta (segment) and lamda the (interpolation)'
    eqCEH__link1(CEH,EH,b)  'The link between delta (segment) and lamda the (interpolation)'
    eqLambda__sumCEH      'Equation of the sum of the interpolated parts';

    eqX__CEH(CEH,EH)$PWL_Flow(CEH,EH)   ..       CO2Flow(CEH,EH)            =e=      sum((q), Lambda(CEH,EH,q)*T__PWL("Flow", ceh,eh,q) );
    eqY__CEH(CEH,EH)$PWL_Flow(CEH,EH)   ..       T__Cost(CEH,EH, "TOTAL")   =e=      sum((q), Lambda(CEH,EH,q)*T__PWL("Cost", ceh,eh,q));
    eqCEH__link0(CEH,EH,b)                ..       sum(notincident(CEH,EH,b,'0',q),Lambda(CEH, EH,q))      =l=     delta(CEH,EH,b);
    eqCEH__link1(CEH,EH,b)                ..       sum(notincident(CEH,EH,b,'1',q),Lambda(CEH, EH,q))      =l=     1-delta(CEH,EH,b);
    eqLambda__sumCEH(CEH,EH)$PWL_Flow(CEH,EH)  ..sum((q), Lambda(CEH,EH,q)$(PWL_Breakpoint( CEH,EH,q)))  =e=     1;
    CO2Flow.up(CEH,EH)                         = smax(q,T__PWL("Flow",CEH,EH,q));

Positive Variable   CEH__Tot    "Variable for the total transport cost of transporting CO_2 from the source (CEH) to the exclusive hub (EH) [EUR2018]";
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Equation    eqCEH__Tot          "COST␣Constraint␣for␣the␣total␣transport␣cost␣of␣transporting␣CO_2␣from␣the␣source␣(CEH)␣to␣␣electrolyzer␣location␣(EH)␣in␣the␣designed␣supply␣chain␣[EUR2018]";
             eqCEH__Tot          ..         sum[(CEH,EH), T__Cost(CEH,EH,"TOTAL")$PWL_Flow(CEH,EH)]      =e=     CEH__Tot;
$offFold

$onFold #CIE cost equations
    incident(CI,E,b,'1',q)      =       sum(pq(p,q),gray(p,b));
    incident(CI,E,b,'0',q)      =       sum(pq(p,q),1-gray(p,b));
    notincident(CI,E,b,b01,q)   =       not incident(CI,E,b,b01,q);

Equations
    eqX__CIE               'Equation␣to␣calculate␣the␣CO2␣flow'
    eqY__CIE               'Equation␣to␣calculate␣the␣annualized␣cost␣of␣that␣segment␣taking␣into␣conderation␣the␣terrain␣factor'
    eqCIE__link0(CI,E,b)   'The␣link␣between␣delta␣(segment)␣and␣lamda␣the␣(interpolation)'
    eqCIE__link1(CI,E,b)   'The␣link␣between␣delta␣(segment)␣and␣lamda␣the␣(interpolation)'
    eqLambda__sumCIE       'Equation␣of␣the␣sum␣of␣the␣interpolated␣parts';

    eqX__CIE(CI,E)$PWL_Flow(CI,E)        ..  CO2Flow(CI,E)               =e=     sum((q),Lambda(CI,E,q)*T__PWL("Flow",CI,E, q));
    eqY__CIE(CI,E)$PWL_Flow(CI,E)        ..  T__Cost(CI,E, "TOTAL")      =e=     sum((q),Lambda(CI,E,q)*T__PWL("Cost",CI,E, q));
    eqCIE__link0(CI,E,b)                 ..  sum(notincident(CI,E,b,'0',q),Lambda(CI,E,q))     =l=     delta(CI,E,b);
    eqCIE__link1(CI,E,b)                 ..  sum(notincident(CI,E,b,'1',q),Lambda(CI,E,q))     =l=     1-delta(CI,E,b);
    eqLambda__sumCIE(CI,E)$PWL_Flow(CI,E) ..sum((q), Lambda(CI,E,q)$(PWL_Breakpoint(ci,e,q)))   =e=     1;
    CO2Flow.up(CI,E)                          =smax(q,T__PWL("Flow",CI,E,q));

Positive Variable   CIE__Tot    "Variable␣for␣the␣total␣transport␣cost␣of␣transporting␣CO_2␣from␣the␣exclusive␣hub␣(CI)␣to␣electrolyzer␣location␣(E)␣[EUR2018]";
Equation    eqCIE__Tot          "COST␣Constraint␣for␣the␣total␣transport␣cost␣of␣transporting␣CO_2␣from␣the␣source␣(CI)␣to␣␣electrolyzer␣location␣(E)␣in␣the␣designed␣supply␣chain␣[EUR2018]";
             eqCIE__Tot          ..         sum[(CI,E), T__Cost(CI,E,"TOTAL")$PWL_Flow(CI,E)]      =e=     CIE__Tot;
$offFold

$onFold #EHE cost equations
    incident(EH,E,b,'1',q)      =       sum(pq(p,q),gray(p,b));
    incident(EH,E,b,'0',q)      =       sum(pq(p,q),1-gray(p,b));
    notincident(EH,E,b,b01,q)   =       not incident(EH,E,b,b01,q);

Equations
    eqX__EHE               'Equation␣to␣calculate␣the␣CO2␣flow'
    eqY__EHE               'Equation␣to␣calculate␣the␣annualized␣cost␣of␣that␣segment␣taking␣into␣conderation␣the␣terrain␣factor'
    eqEHE__link0(EH,E,b)   'The␣link␣between␣delta␣(segment)␣and␣lamda␣the␣(interpolation)'
    eqEHE__link1(EH,E,b)   'The␣link␣between␣delta␣(segment)␣and␣lamda␣the␣(interpolation)'
    eqLambda__sumEHE       'Equation␣of␣the␣sum␣of␣the␣interpolated␣parts';

    eqX__EHE(EH,E)$PWL_Flow(EH,E)       ..  CO2Flow(EH,E)               =e=         sum((q),Lambda(EH,E,q)*T__PWL("Flow",EH,E,q));
    eqY__EHE(EH,E)$PWL_Flow(EH,E)       ..  T__Cost(EH,E, "TOTAL")      =e=         sum((q),Lambda(EH,E,q)*T__PWL("Cost",EH,E,q));
    eqEHE__link0(EH,E,b)                ..  sum(notincident(EH,E,b,'0',q),Lambda(EH,E,q))      =l=     delta(EH,E,b);
    eqEHE__link1(EH,E,b)                ..  sum(notincident(EH,E,b,'1',q),Lambda(EH,E,q))      =l=     1-delta(EH,E,b);
    eqLambda__sumEHE(EH,E)$PWL_Flow(EH,E)..sum((q), Lambda(EH,E,q)$(PWL_Breakpoint(eh,e,q)))    =e=     1;
    CO2Flow.up(EH,E)                         =smax(q,T__PWL("Flow",EH,E,q));

Positive Variable   EHE__Tot    "Variable␣for␣the␣total␣transport␣cost␣of␣transporting␣CO_2␣from␣the␣exclusive␣hub␣(EH)␣to␣electrolyzer␣location␣(E)␣[EUR2018]";
Equation    eqEHE__Tot          "COST␣Constraint␣for␣the␣total␣transport␣cost␣of␣transporting␣CO_2␣from␣the␣source␣(EH)␣to␣␣electrolyzer␣location␣(E)␣in␣the␣designed␣supply␣chain␣[EUR2018]";
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              eqEHE__Tot         ..        sum[(EH,E), T__Cost(EH,E,"TOTAL")$PWL_Flow(EH,E) ]        =e=     EHE__Tot;
$offFold

$onFold #Formulate the pwlinearization of syngas transport and calculate the costs
    incident(E,S,b,'1',q)       =      sum(pq(p,q),gray(p,b));
    incident(E,S,b,'0',q)       =      sum(pq(p,q),1-gray(p,b));
    notincident(E,S,b,b01,q)    =      not incident(E,S,b,b01,q);

Equations
    eqX__ES             'Equation␣to␣calculate␣the␣MtonneKm␣value,␣that␣corresponds␣to␣a␣diameter␣value'
    eqY__ES             'Equation␣to␣calculate␣the␣annualized␣cost␣of␣that␣segment␣taking␣into␣conderation␣the␣terrain␣factor'
    eqES__link0(E,S,b)  'The␣link␣between␣delta␣(segment)␣and␣lamda␣the␣(interpolation)'
    eqES__link1(E,S,b)  'The␣link␣between␣delta␣(segment)␣and␣lamda␣the␣(interpolation)'
    eqLambda__sumES     'Equation␣of␣the␣sum␣of␣the␣interpolated␣parts';

    eqX__ES(E,S)$PWL_Flow(E,S)       ..   SGFlow(E,S)              =e=         sum((q),Lambda(E,S,q)*T__PWL("Flow",e,s,q));
    eqY__ES(E,S)$PWL_Flow(E,S)       ..   T__Cost(E,S, "TOTAL")    =e=         sum((q),Lambda(E,S,q)*T__PWL("Cost",e,s,q));
    eqES__link0(E,S,b)               ..   sum(notincident(E,S,b,'0',q),Lambda(E,S,q))        =l=  delta(E,S,b);
    eqES__link1(E,S,b)               ..   sum(notincident(E,S,b,'1',q),Lambda(E,S,q))        =l=  1-delta(E,S,b);
    eqLambda__sumES(E,S)$PWL_Flow(E,S)..  sum((q), Lambda(E,S,q)$(PWL_Breakpoint(e,s,q)))        =e=  1;
    SGFlow.up(E,S)                   =    smax(q,T__PWL("Flow",e,s,q));

Positive Variable   ES__Tot    "Variable␣for␣the␣total␣transport␣cost␣of␣transporting␣CO_2␣from␣the␣exclusive␣hub␣(CI)␣to␣electrolyzer␣location␣(E)␣[EUR2018]";
Equation    eqES__Tot          "COST␣Constraint␣for␣the␣total␣transport␣cost␣of␣transporting␣CO_2␣from␣the␣source␣(CI)␣to␣␣electrolyzer␣location␣(E)␣in␣the␣designed␣supply␣chain␣[EUR2018]";
              eqES__Tot          ..       sum[(E,S), T__Cost(E,S,"TOTAL")$PWL_Flow(E,S) ]        =e=     ES__Tot;
$offFold

$onFold #Mass balance at the CO_2 sources of CO_2 capture
Equation    eqCI                "MASS␣Constraint␣CO_2␣flow␣of␣capture␣at␣the␣individual␣source␣should␣be␣equal␣to␣the␣amount␣of␣CO_2␣captured␣at␣that␣source";
              eqCI(CCI)            ..       sum[(CI), CO2Flow(CCI,CI)$TSetCCI(CCI,CI)]        =e=     CO2Flow__Cap(CCI);

Equation    eqEH                "MASS␣Constraint␣CO_2␣flow␣of␣capture␣at␣the␣sources␣that␣are␣part␣of␣an␣exclusive␣hub␣should␣be␣equal␣to␣the␣amount␣of␣CO_2␣captured␣at␣that␣source";
              eqEH(CEH)            ..       sum[(EH),CO2Flow(CEH,EH)$TSetCEH(CEH,EH)]        =e=     CO2Flow__Cap(CEH);
$offfold

$onFold #Formulated equations of Carbon balances
Equation    eqCIE               "MASS␣Constraint␣CO_2␣at␣the␣individual␣source␣transported␣to␣the␣electrolyzer␣location";
              eqCIE(CI)            ..       sum[(CCI),CO2Flow(CCI,CI)$TSetCCI(CCI,CI)]        =e=     sum[(E), CO2Flow(CI,E)];

Equation    eqEHE               "MASS␣Constraint␣CO_2␣at␣the␣exclusive␣hub␣transported␣to␣the␣electrolyzer␣location";
              eqEHE(EH)            ..       sum[(CEH),CO2Flow(CEH,EH)$TSetCEH(CEH,EH)]        /*NL*/
              =e=     sum[(E), CO2Flow(EH,E)];

Equation    eqES                "MASS␣Constraint␣syngas␣at␣the␣electrolyzer␣transported␣to␣the␣demand␣location";
              eqES(E)              ..       sum[(EH), CO2Flow(EH,E)*SG__Conv] /*NL*/
              +sum[(CI), CO2Flow(CI,E)*SG__Conv] /*NL*/
              =e=     sum[(S), SGFlow(E,S)];
$offfold

$onFold #Formulated equations for the Electrolyzer
```

```
Integer Variable    Mod__Nr(E) "The␣number␣of␣modules␣installed␣per␣electrolyzer␣system␣␣[#number␣of␣modules]";
             Mod__Nr.lo(E) = 0;

Scalars
            E__cost              "Electricity␣cost␣[EUR2018/MWh]"   /45/
            Elyzr__Hfeed         "Electrolyzer␣electricity␣consumption␣for␣heating␣the␣feed␣stream␣(CO_2␣coming␣in␣the␣plant)␣[MWh/tonne␣syngas]"   /0.2/
            Elyzr__Hair          "Electrolyzer␣electricity␣consumption␣for␣heating␣the␣air␣stream␣[MWh/tonne␣syngas]"  /0.4/
            Elyzr__SGcomp        "Electrolyzer␣electricity␣consumption␣for␣compression␣of␣syngas␣[MWh/tonne␣syngas]"   /0.4/
            Elyzr__Turbine       "Electrolyzer␣electricity␣recovery␣due␣to␣running␣a␣steam␣turbine␣[MWh/tonne␣syngas]" /0/
            Elyzr__Conversion    "Electrolyzer␣electricity␣consumption␣for␣the␣conversion␣into␣syngas␣[MWh/tonne␣syngas]"  /7.1/
            Elyzr__Air           "Electrolyzer␣electricity␣consumption␣for␣the␣compression␣of␣air␣[MWh/tonne␣syngas]"  /0.1/
            Elyzr__Steam         "Electrolyzer␣electricity␣consumption␣for␣the␣steam␣required␣for␣the␣high␣temperature␣solid␣oxide␣electrolyzer␣[MWh/tonne␣syngas]"  /1/
            Elyzr__Pre           "The␣CO_2␣pre-treatment␣cost␣within␣the␣electrolyzer␣system␣[EUR2018/Mtonne␣syngas]"
            Elyzr__Conv          "The␣cost␣of␣converting␣CO_2␣into␣syngas␣within␣the␣electrolyzer␣system␣[EUR2018/Mtonne␣syngas]"
            Elyzr__Post          "The␣syngas␣post␣conversion␣treatment␣costs␣of␣the␣electrolyzer␣system␣[EUR2018/Mtonne␣syngas]"
            Elyzr__Heat          "The␣heating␣cost␣of␣the␣electrolyzer␣system␣[EUR2018/Mtonne␣syngas]"
            Mod__Flow            "Syngas␣flow␣produced␣per␣module␣per␣year␣[Mtonne␣syngas/year]"   /0.0078260870/
            LR                   "The␣cost␣improvements␣due␣to␣learning␣about␣the␣cost␣of␣the␣electrolysis␣plant␣in␣a␣2040␣scenario" /1/
            BaseMod__Cost        "Cost␣of␣the␣standard␣module␣[EUR2018/module]" /10924992/;
            Elyzr__Pre           =      E__cost*(Elyzr__Air)*1000000;
            Elyzr__Conv          =      E__cost*(Elyzr__Conversion)*1000000;
            Elyzr__Post          =      E__cost*(Elyzr__SGcomp)*1000000;
            Elyzr__Heat          =      E__cost*(Elyzr__Hfeed+Elyzr__Hair+Elyzr__Turbine+Elyzr__Steam)*1000000;

Set
    qe       'breakpoints' /q1*q9/
    pe       'segments' /p1*p8/
    peqe(pe,qe) 'mapping'
    mc      'Set␣that␣contains␣the␣piece-wise␣linear␣(PWL)␣data,␣both␣about␣the␣Modules␣and␣Costs' /Module, Cost/
;
Table graye(pe,b) 'Gray␣encoding␣of␣segments'
        b1   b2  b3
    p1   0    0   0
    p2   0    0   1
    p3   0    1   1
    p4   0    1   0
    p5   1    1   0
    p6   1    1   1
    p7   1    0   1
    p8   1    0   0
;

peqe(pe,qe) = ord(pe)=ord(qe) or ord(pe)=ord(qe)-1;

Positive Variable Mod__Cost;
Positive variable   LambdaEle           'interpolation␣for␣the␣piecewise␣linearization␣[-]';
Binary Variable     DeltaEle            'segment␣encoding␣for␣the␣piecewiselinearization␣[-]';

Set                 incidentEle          "Boolean␣incidence␣matrix,␣that␣indicatates␣if␣breakpoint␣q␣is␣part␣of␣segment␣p␣that␣has␣␣binary␣digit␣b␣equal␣to␣b01";
Set                 notincidentEle       "Opposite␣of␣the␣boolean␣incidence␣matrix␣defined␣above";

    incidentEle(E,b,'1',qe)        =       sum(peqe(pe,qe),graye(pe,b));
```

```
    incidentEle(E,b,'0',qe)         =       sum(peqe(pe,qe),1-graye(pe,b));
    notincidentEle(E,b,b01,qe)      =       not incidentEle(E,b,b01,qe);
$offFold

$GDXIN "PWL_Ele.gdx"
$onFold #Load the pwl electorlyzer data
Parameter         Tot__PWLElectrolyzer       "Parameter␣containing␣all␣the␣piecewise␣linearization␣of␣the␣electrolzyer␣investment␣cost"
$load             Tot__PWLElectrolyzer
$offFold #Load the pwl electorlyzer data
$gdxOut

$onFold #PWL electorlyzer data
Equations
    eqX__Ele                'Equation␣to␣map␣the␣number␣of␣electrolyzers␣to␣the␣costs'
    eqY__Ele                'Equation␣to␣calculate␣the␣bare␣investment␣cost␣of␣the␣number␣of␣modules␣slected␣by␣the␣Mod__Nr␣'
    eqEle__link0(E,b)       'The␣link␣between␣delta␣(segment)␣and␣lamda␣the␣(interpolation)'
    eqEle__link1(E,b)       'The␣link␣between␣delta␣(segment)␣and␣lamda␣the␣(interpolation)'
    eqLambda__sumEle        'Equation␣of␣the␣sum␣of␣the␣interpolated␣parts';

    eqX__Ele(E)               ..       Mod__Nr(E)           =e=     sum((qe), LambdaEle(E,qe)*Tot__PWLElectrolyzer("Module",qe));
    eqY__Ele(E)               ..       Mod__Cost(E)         =e=     sum((qe), LambdaEle(E,qe)*Tot__PWLElectrolyzer("Cost",qe))*LR;
    eqEle__link0(E,b)         ..       sum(notincidentEle(E,b,'0',qe),LambdaEle(E,qe))    =l= DeltaEle(E,b);
    eqEle__link1(E,b)         ..       sum(notincidentEle(E,b,'1',qe),LambdaEle(E,qe))    =l= 1-DeltaEle(E,b);
    eqLambda__sumEle(E)       ..       sum((qe), LambdaEle(E, qe))                        =e= 1;
$offFold

$onFold #Electrolyzer capex and opex equations
Equation    eqElyzr__Mod          "Constraint␣regarding␣the␣number␣of␣electrolyzer␣modules";
             eqElyzr__Mod(E)       ..      Mod__Nr(E)*Mod__Flow        =g=     sum[(S),SGFlow(E,S)];

Positive variable   Elyzr__Cost "Variable␣regarding␣the␣electrolyzer␣cost␣dependent␣on␣set␣E␣and␣expenditure␣set␣PEX";

Equation    eqElyzr__Elect        "Equation␣regarding␣the␣electrolyzer␣OPEX␣for␣the␣electrolyzers␣at␣location␣E";
Positive variable Elyzr__Elect "Variable␣regarding␣the␣electrolyzer␣cost␣dependent␣on␣set␣E␣and␣OPEX␣expenditure␣[EUR2018/year]";
             eqElyzr__Elect(E)     ..      sum[(S),SGFlow(E,S)]*(Elyzr__Pre+Elyzr__Conv+Elyzr__Post+Elyzr__Heat)      =e=     Elyzr__Elect(E);

Scalar      OM__Use            'Percentage␣OM␣cost␣as␣function␣of␣the␣CAPEX␣[%]' /4/;
Scalar      Capex__FrStack      "Percentage␣of␣the␣CAPEX␣which␣is␣attributed␣to␣the␣stack␣[%]" /20/;
Scalar      CRF__Plant          'CRF␣based␣on␣20␣yr␣and␣8%␣[-]' /0.10185/;

Positive variable Elyzr__OM;
Equation    eqElyzr__OM        "Equation␣regarding␣the␣electrolyzer␣CAPEX␣for␣the␣electrolyzers␣at␣location␣E␣and␣OPEX␣expenditure␣[EUR2018/year]";
             eqElyzr__OM(E)    ..      (Mod__Cost(E)*((100 - Capex__FrStack)/100))*(OM__Use/100)       =e=     Elyzr__OM(E);


Equation    eqElyzr__CAPEX       "Equation␣regarding␣the␣electrolyzer␣CAPEX␣for␣the␣electrolyzers␣at␣location␣E";
             eqElyzr__CAPEX(E)    ..      Mod__Cost(E) *CRF__Plant*((100 - Capex__FrStack)/100)        =e=     Elyzr__Cost(E, "CAPEX");

Positive variable Elyzr__Stack  "Replacement␣cost␣of␣the␣electrolyzer␣stack␣dependent␣on␣set␣E␣and␣OPEX␣expenditure␣[EUR2018/year]";
Scalar      LT__Stack           "The␣lifetime␣of␣the␣electrolyzer␣stack␣40000h␣or␣5␣[year]" /5/;
Equation    eqElyzr__Stack       "Equation␣regarding␣the␣electrolyzer␣CAPEX␣for␣the␣electrolyzers␣at␣location␣E";
```

```
             eqElyzr__Stack(E)    ..      (BaseMod__Cost*LR*Mod__Nr(E) *(Capex__FrStack/100)) /LT__Stack        =e=     Elyzr__Stack(E);

Equation    eqElyzr__OPEX       "Equation␣regarding␣the␣electrolyzer␣CAPEX␣for␣the␣electrolyzers␣at␣location␣E";
             eqElyzr__OPEX(E)     ..      Elyzr__Stack(E)+Elyzr__OM(E)+Elyzr__Elect(E) =e= Elyzr__Cost(E, "OPEX");

Positive variable   Elyzr__Tot  "Total␣electrolyzer␣cost␣in␣[EUR2018/yr]";
Equation    eqElyzr__Tot         "Constraint␣regarding␣the␣total␣electrolyzer␣cost␣[EUR2018]";
             eqElyzr__Tot          ..      Elyzr__Tot       =e=       sum[(E,pex), Elyzr__Cost(E,pex)];
$offfold

$onFold #Market demand fulfilment Constraint
Equation    eqDemand__Flow      "Constraint␣regarding␣the␣syngas␣demand␣fulfillment␣at␣syngas␣demand␣location␣S";
 eqDemand__Flow(S)   ..      sum[(E), SGFlow(E,S)]       =l=     SG__Demand(S);

Equation eqMax__Flow "Constraint␣regarding␣the␣maximum␣syngas␣demand␣production␣at␣the␣electrolyzer␣E";
    eqMax__Flow(E) ..       sum[(S), SGFlow(E,S)]        =l=     1;

Parameter   Mrk__Fulfill        "Input␣parameter␣regarding␣the␣flow␣of␣syngas␣that␣is␣produced␣yearly␣[Mtonne␣syngas/year]";

Equation    eqMrk__Fulfill      "Constraint␣regarding␣the␣total␣yearly␣market␣fulfilment";
             eqMrk__Fulfill      ..      sum[(E,S), SGFlow(E,S)]       =e=     Mrk__Fulfill;
$offfold

$onFold #Objective functions
Positive Variable  TotSC__Cost "Total␣cost␣of␣the␣supply␣chain␣elements␣capture,␣CO_2␣transport,␣CO_2␣conversion␣and␣syngas␣transport␣[EUR2018/year]";
Equation    eqTot               "Constraint␣for␣the␣total␣supply␣chain␣cost␣including:␣capture,␣CO_2␣transport,␣CO_2␣conversion␣and␣syngas␣transport";
             eqTot               ..      CIE__Tot+EHE__Tot+ES__Tot+CEH__Tot+Cap__Tot+Elyzr__Tot     =e=     TotSC__Cost;

Variable    LCOSG               "Objective␣variable␣for␣the␣levelized␣cost␣of␣syngas␣production␣[EUR2018/tonne]";
Equation    eqLCOSG             "Objective␣function␣for␣the␣levelized␣cost␣of␣syngas␣production";
             eqLCOSG             ..      TotSC__Cost/Mrk__Fulfill/ 1000000        =e= LCOSG;
$offfold

$GDXIN "SGFract2.gdx"
$onFold  #Definition of the looping set for different market fractions that need to be fulfilled by the model
Set         Count               "Looping␣set␣over␣the␣different␣market␣fractions,␣the␣number␣indicates␣the␣percentage␣of␣market␣fulfilment"
/Count01,Count05,Count1,Count2,Count4,Count6,Count8,Count10,Count15,Count20,Count25,Count30,Count35,Count40,Count45,Count50,Count55,Count60,Count65,Count70,Count75, Count80,Count85,Count90,Count95,Count100/;




Parameter   Market__Fr(Count)   "Parameter␣with␣the␣market␣fraction␣of␣the␣total␣demand␣in␣Europe␣that␣needs␣to␣be␣fulfilled␣[-]␣";
$load        Market__Fr
;
$GDXOUT
$offfold

Model       SC                  "Compile␣the␣supply␣chain␣configuration␣model" /all/ ;
$onFold #Formatting of the option file
put gurobi 'threads␣=8'/
"scaleflag␣=2"/
putclose gurobi;
```

```
SC.optfile = 1;
$offfold

$onFold #Defintion of output parameters
Parameters
            #Model characteristics and objective function
           LCOSG_OF           "Output␣parameter␣for␣the␣objective␣function␣value"
            OptInd              "Indicator␣for␣the␣model␣status␣at␣the␣end␣of␣the␣solve␣"
            OptEst             "Best␣posible␣within␣the␣bounds"
            OptGap             "Parameter␣storing␣the␣optimality␣gap␣in␣an␣output␣gdx␣file␣[-]"
            LC_Mrk__Fulfill     "Lead␣constraint␣regarding␣the␣market␣fullfillment"

            # CO2 LCOSG contribution
            LCOSG_Transport     "Contribution␣of␣transport␣to␣the␣levilized␣cost␣of␣syngas"
            LCOSG_CapComp       "Contribution␣of␣capture␣and␣compression␣to␣the␣levilized␣cost␣of␣syngas"
            LCOSG_Electrolyzer  "Contribution␣of␣conversion␣to␣the␣levilized␣cost␣of␣syngas"

            # CO_2 Flow outputs
            CO2FlowCaptured    "Output␣parameter␣of␣CO_2␣flow␣captured␣at␣source␣C"
            CO2FlowCCI         "Output␣parameter␣of␣CO_2␣flow␣from␣C␣to␣CI"
            CO2FlowCEH         "Output␣parameter␣of␣CO_2␣flow␣from␣C␣to␣EH"
            CO2FlowCIE         "Output␣parameter␣of␣CO_2␣flow␣from␣CI␣to␣E"
            CO2FlowEHE         "Output␣parameter␣of␣CO_2␣flow␣from␣EH␣to␣E"
            CO2FlowEEE         "Output␣parameter␣of␣CO_2␣flow␣from␣E␣to␣EE"
            SGFlowEES          "Output␣parameter␣of␣CO_2␣flow␣from␣EE␣to␣S"

            #Supply chain echalon costs
            Transport_ES__Tot           "Total␣annualized␣syngas␣transport␣cost␣from␣E␣to␣S"
            Transport_CEH__Tot          "Total␣annualized␣CO_2␣transport␣cost␣from␣CEH␣to␣EH"
            Transport_EHE__Tot          "Total␣annualized␣CO_2␣transport␣cost␣from␣EH␣to␣E"
            Transport_CIE__Tot          "Total␣annualized␣CO_2␣transport␣cost␣from␣CI␣to␣E"
            Transport_Tot               "Total␣annualized␣transport␣cost"
            Conversion_Elyzr__Tot       "Total␣annualized␣Electrolyzer␣cost"
            Capture_Cap__Tot            "Total␣annualized␣CO_2␣capture␣cost␣at␣source␣C"
            All_TotSC__Cost             "Total␣annualized␣cost␣of␣the␣SC"

            #Supply chain echalon percentages
            Percent_ES__Tot             "Percentage␣of␣cost␣to␣transport␣from␣E␣to␣S"
            Percent_CEH__Tot            "Percentage␣of␣cost␣to␣transport␣from␣C␣to␣EH"
            Percent_EHE__Tot            "Percentage␣of␣cost␣to␣transport␣from␣EH␣to␣E"
            Percent_CIE__Tot            "Percentage␣of␣cost␣to␣transport␣from␣CI␣to␣E"
            Percent_Elyzr__Tot          "Percentage␣of␣cost␣to␣convert␣CO_2"
            Percent_Cap__Tot            "Percentage␣of␣cost␣to␣capture␣CO_2"

            #Electrolyzer costs
            Conversion_Elyzr__Stack     "Cost␣of␣replacing␣the␣electrolyzer␣stack␣at␣each␣electrolyzer␣site"
            Conversion_Elyzr__OM        "Operation␣and␣maintainance␣cost␣at␣each␣electrolyzer␣site"
            Conversion_Elyzr__Elect     "Electricity␣cost␣at␣each␣electrolyzer␣site"
            Conversion_Elyzr__Cost      "Annualized␣investment␣cost␣at␣each␣electrolyzer␣site"

            #Electrolyzer percentages
            Percent_Elyzr__Stack     "Percentage␣of␣cost␣of␣replacing␣the␣electrolyzer␣stack␣at␣each␣electrolyzer␣site"
            Percent_Elyzr__OM        "Percentage␣of␣operation␣and␣maintainance␣cost␣at␣each␣electrolyzer␣site"
            Percent_Elyzr__Elect     "Percentage␣of␣electricity␣cost␣at␣each␣electrolyzer␣site"
            Percent_Elyzr__Cost      "Percentage␣of␣annualized␣investment␣cost␣at␣each␣electrolyzer␣site"

            #Transport cost per segment
            Capture__Cost              "The␣capture␣cost␣per␣induvidual␣source"
            Seg_T__Cost                "Total␣annualized␣␣transport␣cost␣per␣segment"
            Elyzr__Elect_I             "The␣electricity␣cost␣per␣electrolyzer␣E␣"
            Elyzr__OM_I                "The␣operations␣and␣maintainance␣cost␣per␣electrolyzer␣E"
```

```
            Elyzr__Stack_I              "The␣cost␣of␣the␣stack␣per␣electrolyzer␣E"
            Elyzr__Cost_I               "The␣investment␣cost␣of␣the␣electrolyzer␣E"

            #Other outputs
            Cap_Fraction                "Fraction␣of␣CO_2␣Captured␣at␣source␣C"
            IN_CO2Flow__Cap             "CO_2␣Input␣into␣the␣system"

            #Electrolyzer Flows
            Water__Cons                 "The␣stochiometric␣water␣consumption␣at␣electrolyzer␣location␣E"
            Syngas__Prod                "Syngas␣produced␣at␣electrolyzer␣location␣E"
            CO_2__Cons                  "CO_2␣consumed␣at␣electrolyzer␣location␣E"
            Electricity__Cons           "Electricity␣consumed␣at␣electrolyzer␣location␣E"
            Elyzr_Mod__Nr               "Nr␣of␣electrolzyers␣at␣the␣electrolyzer␣location␣E"

            #Total Consumptions
            Tot_CO2Flow                  "Total␣CO_2␣consumption␣of␣the␣system␣[MTonne/yr]"
            Tot_SGFlow                   "Total␣Syngas␣production␣consumption␣of␣the␣system␣[MTonne/yr]"
            Tot_WaterFlow                "Total␣water␣consumption␣of␣the␣system␣[MTonne/yr]"
            Tot_Electricity              "Electricity␣consumption␣of␣the␣system␣[TWh/yr]"

            #Cost for the modules induvidual and total
            Module_Cost                  "The␣cost␣payed␣for␣placing␣a␣set␣of␣modules␣dependent␣on␣Mod__NR␣[EUR2018]"
            ModUnit_Cost                 "The␣cost␣payed␣for␣placing␣a␣single␣module␣at␣electrolzyer␣location␣E␣[EUR2018/module]";
$offFold

$onFold #Loop over the different market fullfillment requirements
loop(count,
    Mrk__Fulfill = sum[(s),SG__Demand(S)]*(Market__Fr(Count)/100);

$onFold  #Scaling of the variables in the model
            SC.scaleopt                      =   1       ;
            eqX__CC.scale(C)                 =   0.005   ;
            eqX__CEH.scale(CEH,EH)           =   0.005   ;
            eqX__CIE.scale(CI,E)             =   0.005   ;
            eqX__EHE.scale(EH,E)             =   0.005   ;
            eqX__ES.scale(E,S)               =   0.005   ;

            eqY__CC.scale(C)                 =   100000. ;
            eqY__CEH.scale(CEH,EH)           =   10000.  ;
            eqY__CIE.scale(CI,E)             =   10000.  ;
            eqY__EHE.scale(EH,E)             =   10000.  ;
            eqY__ES.scale(E,S)               =   10000.  ;
            eqY__Ele.scale(E)                =   1000000.;

            eqCap__Tot.scale                 =   10000   ;
            eqCEH__Tot.scale                 =   10000   ;
            eqCIE__Tot.scale                 =   10000   ;
            eqEHE__Tot.scale                 =   10000   ;
            eqES__Tot.scale                  =   10000   ;
            eqTot.scale                      =   10      ;

            eqCIE.scale(CI)                  =   0.05    ;
            eqCI.scale(CCI)                  =   0.05    ;
            eqEHE.scale(EH)                  =   0.05    ;
            eqEH.scale(CEH)                  =   0.05    ;
            eqES.scale(E)                    =   0.05    ;

            eqElyzr__Elect.scale(E)          =   100000. ;
            eqElyzr__OM.scale(E)             =   100000. ;
            eqElyzr__CAPEX.scale(E)          =   100000. ;
            eqElyzr__Stack.scale(E)          =   100000. ;
            eqElyzr__OPEX.scale(E)           =   100000. ;
            eqElyzr__Tot.scale               =   10000.  ;

            eqDemand__Flow.scale(S)          =   0.05    ;
            eqMax__Flow.scale(E)             =   0.05    ;
            eqMrk__Fulfill.scale             =   10      ;
```

```
            eqLCOSG.scale                   =   100     ;
$offfold

            Solve SC using mip min LCOSG;

$onFold  #Writing of the outputs of the model
            OptInd(Count) = SC.modelstat;

            if (OptInd(Count) ne 10,
                #Model characteristics and objective function
                LCOSG_OF(Count)          =       LCOSG.l;
                OptEst(Count)            =       SC.objEst;
                OptGap(Count)            =       ((SC.objVal/SC.objEst)-1)*100;
                LC_Mrk__Fulfill(Count)   =       Mrk__Fulfill;

                # CO_2 Flow outputs
                CO2FlowCaptured(Count, C)                                 =  CO2Flow__Cap.l(C);
                CO2FlowCCI( CCI,CI)$(CO2Flow.l(CCI,CI) gt 0.000001) = CO2Flow.l(CCI,CI);
                CO2FlowCEH( CEH,EH)$(CO2Flow.l(CEH,EH) gt 0.000001)  = CO2Flow.l(CEH,EH);
                CO2FlowCIE( CI,E)$(CO2Flow.l(CI,E) gt 0.000001) = CO2Flow.l(CI,E);
                CO2FlowEHE( EH,E)$(CO2Flow.l(EH,E) gt 0.000001) = CO2Flow.l(EH,E);
                CO2FlowEEE( E,EE)$(CO2Flow.l(E,EE) gt 0.000001)  = CO2Flow.l(E,EE);
                SGFlowEES( EE,S)$(SGFlow.l(EE,S) gt 0.000001)= SGFlow.l(EE,S);

                #Capture fraction
                Cap_Fraction(count,C)                   =    Cap__FR.l(C);

                #Transport cost in the supply chain
                Transport_ES__Tot(Count)                =    ES__Tot.l;
                Transport_CEH__Tot(Count)               =    CEH__Tot.l;
                Transport_EHE__Tot(Count)               =    EHE__Tot.l;
                Transport_CIE__Tot(Count)               =    CIE__Tot.l;
                Transport_Tot(Count)                    =    CIE__Tot.l+EHE__Tot.l+CEH__Tot.l+ES__Tot.l;

                #Supply chain echolon costs [absolute]
                Conversion_Elyzr__Tot(Count)            =    Elyzr__Tot.l;
                Capture_Cap__Tot(Count)                 =    Cap__Tot.l;
                All_TotSC__Cost(Count)                  =    TotSC__Cost.l;

                #Supply chain echalon costs [as funciton of the syngas proudction]
                LCOSG_Transport(Count)                  =    (CIE__Tot.l+EHE__Tot.l+CEH__Tot.l+ES__Tot.l)/Mrk__Fulfill/ 1000000;
                LCOSG_CapComp(Count)                    =    Cap__Tot.l/Mrk__Fulfill/ 1000000;
                LCOSG_Electrolyzer(Count)               =    Elyzr__Tot.l/Mrk__Fulfill/1000000;

                #Supply chain echalon percentages
                Percent_ES__Tot(Count)                  =    ES__Tot.l/TotSC__Cost.l*100;
                Percent_CEH__Tot(Count)                 =    CEH__Tot.l/TotSC__Cost.l*100;
                Percent_EHE__Tot(Count)                 =    EHE__Tot.l/TotSC__Cost.l*100;
                Percent_CIE__Tot(Count)                 =    CIE__Tot.l/TotSC__Cost.l*100;
                Percent_Elyzr__Tot(Count)               =    Elyzr__Tot.l/TotSC__Cost.l*100;
                Percent_Cap__Tot(Count)                 =    Cap__Tot.l/TotSC__Cost.l*100;

                #TOTAL electrolyzer costs
                Conversion_Elyzr__Stack(Count)          =    sum[(E),Elyzr__Stack.l(E)];
                Conversion_Elyzr__OM(Count)             =    sum[(E),Elyzr__OM.l(E)];
                Conversion_Elyzr__Elect(Count)          =    sum[(E),Elyzr__Elect.l(E)];
                Conversion_Elyzr__Cost(Count)           =    sum[(E),Elyzr__Cost.l(E, "CAPEX")];

                #Electrolyzer percentages
                Percent_Elyzr__Stack(Count)             =     sum[(E),Elyzr__Stack.l(E)]/Elyzr__Tot.l*100;
                Percent_Elyzr__OM(Count)                =     sum[(E),Elyzr__OM.l(E)]/Elyzr__Tot.l*100;
                Percent_Elyzr__Elect(Count)             =     sum[(E),Elyzr__Elect.l(E)]/Elyzr__Tot.l*100;
                Percent_Elyzr__Cost(Count)              =     sum[(E),Elyzr__Cost.l(E, "CAPEX")]/Elyzr__Tot.l*100;
```

```

                #Caputre Cost per induvidual source
                Capture__Cost(count, C)                =    Cap__Cost.l(C,"TOTAL");

                #Transport cost per segment
                Seg_T__Cost(Count,E,S, "TOTAL")        =    T__Cost.l(E,S, "TOTAL");
                Seg_T__Cost(Count,CEH,EH, "TOTAL")     =    T__Cost.l(CEH,EH, "TOTAL");
                Seg_T__Cost(Count,CI,E, "TOTAL")       =    T__Cost.l(CI,E, "TOTAL");
                Seg_T__Cost(Count, EH,E, "TOTAL")      =    T__Cost.l(EH,E, "TOTAL");

                #Conversion per induvidual electrolyzer
                Elyzr__Stack_I(count, E)                =   Elyzr__Stack.l(E);
                Elyzr__OM_I(count, E)                   =   Elyzr__OM.l(E);
                Elyzr__Elect_I(count, E)                =   Elyzr__Elect.l(E);
                Elyzr__Cost_I(count, E)                 =   Elyzr__Cost.l(E, "CAPEX");

                #Capture Flows
                IN_CO2Flow__Cap(Count,C)               =    CO2Flow__Cap.l(C);

                #Electrolyzer Flows
                Water__Cons(Count,E)                   =    sum[(S),SGFlow.l(E,S)] / Water__Conv;
                Syngas__Prod(Count,E)                  =    sum[(S),SGFlow.l(E,S)];
                CO_2__Cons(Count,E)                    =    sum[(EH), CO2Flow.l(EH,E)]+sum[(CI), CO2Flow.l(CI,E)];
                Electricity__Cons(Count,E)             =    Elyzr__Elect.l(E)/E__cost;
                Elyzr_Mod__Nr(Count,E)                 =    Mod__Nr.l(E);

                #Total Consumptions
                Tot_CO2Flow(Count)                     =    sum[(C),CO2Flow__Cap.l(C)];
                Tot_SGFlow(Count)                      =    Mrk__Fulfill;
                Tot_WaterFlow(Count)                   =    sum[(E,S),SGFlow.l(E,S)] / Water__Conv;
                Tot_Electricity(Count)                 =    sum[(E), Elyzr__Elect.l(E)/E__cost]/1000000;

                #Cost for the modules induvidual and total
                Module_Cost(Count,E)                         =    Mod__Cost.l(E);
                ModUnit_Cost(Count,E)$(Mod__nr.l(E) ne 0) = Mod__Cost.l(E)/Mod__nr.l(E);;
            else
                LCOSG_OF(Count)         =       NA;);
$offfold

execute_unload "Solutions.gdx"
LCOSG_OF,OptInd, OptEst, OptGap,LC_Mrk__Fulfill,
LCOSG_Transport, LCOSG_CapComp, LCOSG_Electrolyzer, CO2FlowCaptured, CO2FlowCCI, CO2FlowCEH,
    CO2FlowCIE, CO2FlowEHE,CO2FlowEEE,SGFlowEES,Cap_Fraction,Transport_ES__Tot,
    Transport_CEH__Tot,Transport_EHE__Tot,Transport_CIE__Tot,Transport_Tot,
    Conversion_Elyzr__Tot,Capture_Cap__Tot,All_TotSC__Cost,Percent_ES__Tot,Percent_CEH__Tot,
    Percent_EHE__Tot,Percent_CIE__Tot,Percent_Elyzr__Tot,Percent_Cap__Tot,
    Conversion_Elyzr__Stack,Conversion_Elyzr__OM,Conversion_Elyzr__Elect,
    Conversion_Elyzr__Cost,Percent_Elyzr__Stack,Percent_Elyzr__OM,Percent_Elyzr__Elect,
    Percent_Elyzr__Cost,Capture__Cost,Seg_T__Cost,Elyzr__Stack_I,Elyzr__OM_I,Elyzr__Elect_I,
    Elyzr__Cost_I,IN_CO2Flow__Cap,Water__Cons,Syngas__Prod,CO_2__Cons, Electricity__Cons,
    Elyzr_Mod__Nr,Tot_CO2Flow,Tot_SGFlow, Tot_WaterFlow,Tot_Electricity,Module_Cost,
    ModUnit_Cost;
);

execute_unload "PWL_BaseOutput.gdx",C,CI,EH,E, S;
;
$offfold
```

B

Appendix B

This appendix contains all tables used

Table B.1: Specifications for SOEC System [102]

Specification	Magnitude	Unit
Conversion	7.1	kWh/kg product
Compression	0.5	kWh/kg product
e-heaters	0.6	kWh/kg product
AC/DC (97%)	0.2	kWh/kg product
Total	8.4	kWh/kg product
System efficiency	92	LHV (%)
Total Investment Costs (TIC)	1200	€/kW
Plant capacity	110	tonne syngas/hour
Inflow rate	190	tonne CO2/hour
Syngas ratio	02:01	Ratio H2:CO
CO2 purity	99.99	%
CO2 temperature	30	°C
CO2 pressure	30	barg
Electrolyser size	900	MW
Operation size	8000	hrs/year
Syngas temperature	30	°C
Syngas pressure	30	barg
Enriched air	30	vol% O2
Single pass conversion of CO2 to syngas	85	%
Electricity consumption Stack	786	MW
Electricity consumption Other	124	MW
Electricity consumption System	910	MW
Enthalpy steam generation	107	MW

Table B.2: CO_2 Capture and Transport Parameters

Symbol	Magnitude	Description	Reference	Unit
m_1	Model	Mass flow of CO_2 emitted at site	(Bin Ye 2019), (Anand B. Rao 2006)	[Mtonne CO_2]
$\alpha_{1,j}$	90	Efficiency of carbon capture unit (Avg)	(Cormos 2014), (Faruque 2012)	[%]
$\alpha_{1.1}$	95	Efficiency of carbon capture unit (Bioethanol)		[%]
$\alpha_{1.2}$	95	Efficiency of carbon capture unit (Biomethane)	(Menin 2022)	[%]
$\alpha_{1.3}$	80	Efficiency of carbon capture unit (Pulp/Paper)	(Sagues 2020), (Möllersten 2004)	[%]
$\alpha_{1.4}$	85	Efficiency of carbon capture unit (Waste incin.)	(Haaf 2020)	[%]
$m2$	Model	Mass flow of CO_2 lost during transport		[Mtonne CO_2]
α_2	98	Leakage efficiency of infrastructure	(A. Alvarez 2011), (B. Jackson 2014)	[%]
$m3$	Model	Mass flow of CO_2 lost due to not full conversion		[Mtonne CO_2]
α_3	85	Electrical efficiency of ind. scale electrolyser	(ISPT report, 2023)	[%]
$m4$	Model	Mass flow of syngas lost due to leakage		[Mtonne CO_2]
α_4	98	Leakage efficiency of infrastructure	(A. Alvarez 2011), (B. Jackson 2014)	[%]
$E4$	3.00×10^{-6}	Energy consumed for CO_2 capture site	(CE Delft, 2020)	[Mtonne CO_2 per MWh]
β_4	345000.00	CO_2 conversion factor for carbon capture unit	(Xiangping Zhang 2014)	[MWh per Mtonne CO_2]
$E5$	3.26×10^{-2}	Energy consumed for CO_2 transport	(CE Delft, 2020)	[Mtonne CO_2 per MWh]
β_5	0.98	CO_2 conversion factor for pump/compressors	(T. Rochelle 2009)	[Mtonne CO_2-eq/km/Mtonne transported]
$E6$	3.00×10^{-6}	Carbon footprint of electricity	(CE Delft, 2020)	[Mtonne CO_2 per MWh]
β_6	9300000.00	CO_2 conversion factor for electrolyser	(ISPT)	[MWh per Mtonne syngas]
$E7$	3.00×10^{-6}	Energy consumed for syngas transport	(CE Delft, 2020)	[Mtonne CO_2 per MWh]
β_7	0.98	CO_2 conversion factor for pump/compressors	(T. Rochelle 2009)	[MWh per Mtonne CO_2]
GWP_{H2}	5.8	GWP of Hydrogen gas	(Warwick 2022)	[-]
GWP_{CO}	1.9	GWP of CO gas	(Raman P 2013)	[-]
GWP_{syngas}	4.5	GWP of syngas (2:1 ratio)	(ISPT)	[-]

Table B.3: Cell Specifications [102]

Description	Magnitude	Symbol
Cell voltage	1.3	V
Cell area	800	cm^2
Current density	1.5	A/cm^2
Cell power	1560	W
Amount of Cells	60	#
Total cell area per stack	48000	cm^2
Stack current	1200	A
Stack Voltage	78	V
Stack Power	93.6	kW

Table B.4: Material Specifications for Electrode Composition [111] [31] [128]

Material	Magnitude	Unit	Molecular Formula	Critical Material
Ceria	1.29	g/kW	CeO_2	Yes
Lanthanum oxide	12.67	g/kW	La_2O_3	Yes
Gadolinium oxide	0.34	g/kW	Gd_2O_3	Yes
Yttria	15.49	g/kW	Y_2O_3	Yes
Strontium Carbonate	2.07	g/kW	$SrCO_3$	No
Nickel Cermet	114.56	g/kW	Nickel+Ceramic component	No
Zirconia	95.36	g/kW	ZrO_2	No
Manganese	18.93	g/kW	Mn	No
Nickel	132.00	g/kW	Ni	No
Lanthanum	3.22	g/kW	La	Yes

Table B.5: System Specifications [102]

Description	Magnitude	Symbol	Reference
Stacks per hot-box	16	#	ISPT
Hot-Box Power	1498	kW	ISPT
Total Voltage stacks in series	1248	V	ISPT
Hot-Box per repeating module	6	#	ISPT
Module	9	MW	ISPT

Table B.6: Detailed Materials and Distribution for the Project

Materials	Amount	Unit	Distribution	Comment	Reference
Capture unit	–	–	–	–	–
Idemat2022 Fe360	317	ton	Undefined	Steel for absorber, stripper, and piping/small equipment	Koorneef 2008
Autoclaved aerated concrete block	1,440	kg	Undefined	–	Koorneef 2008
Transport, freight train (EU)	9.5	tkm	Undefined	Transport of corresponding materials	Koorneef 2008
Transport unit	–	–	–	–	–
Idemat2023 Transport, pipeline, natural gas	150	tkm	Undefined	Transport unit for SG and CO2	Assumption
Electrolyser unit	–	–	–	–	–
Idemat2022 Fe360	84,600	kg	–	–	ISPT
Idemat2022 15Cr3	219,600	kg	–	–	ISPT
Idemat2022 Al99	37,800	kg	–	–	ISPT
Idemat2022 Al99	3,500	kg	–	–	ISPT
Idemat2023 Ni 99.6	1,800	kg	–	–	ISPT
Idemat2022 Fe360	84,600	kg	–	–	ISPT
Process water	1,404	kg	–	–	ISPT
Idemat2022 Manganese	170	kg	–	–	Thesis Stijn Yska
Idemat2023 Nickel (primary)	1,188	kg	–	–	Thesis Stijn Yska

Table B.7: Material Usage Data for an Electrolyser unit

Materials/Assemblies	Amount	Unit	Comment	Ref.1	Ref.2	Ref.3
Idemat2022 Fe360	84600	kg	Reinforcing Steel for construction	(C. Strazza 2010)	(M. Pehnt 2001)	(V. Karakoussis 2000)
Idemat2022 15Cr3	219600	kg	Chromium steel from Port of Rotterdam	(C. Strazza 2010)	(M. Pehnt 2001)	(V. Karakoussis 2000)
Idemat2022 Al99	37800	kg	Aluminium used to make oxide	(C. Strazza 2010)	(M. Pehnt 2001)	(V. Karakoussis 2000)
Idemat2022 Al99	3500	kg	Aluminium silica for insulation	(C. Strazza 2010)	(M. Pehnt 2001)	(V. Karakoussis 2000)
Idemat2022 Ni99.6	1800	kg	Nickel	(C. Strazza 2010)	(M. Pehnt 2001)	(V. Karakoussis 2000)
Idemat2022 Fe360	84600	kg	Sheet rolling steel	(C. Strazza 2010)	(M. Pehnt 2001)	(V. Karakoussis 2000)
Process water	1404	kg	Water used during construction process	(C. Strazza 2010)	(M. Pehnt 2001)	(V. Karakoussis 2000)
Idemat2022 Manganese	170	kg	Manganese used for electrode	(C. Strazza 2010)	(M. Pehnt 2001)	(V. Karakoussis 2000)
Idemat2023 Nickel (primary)	1188	kg	Nickel used for electrode	(C. Strazza 2010)	(M. Pehnt 2001)	(V. Karakoussis 2000)

Table B.8: Material Usage Data for a capture unit

Materials/Assemblies	Amount	Unit	Comment	Ref.1
Idemat2022 Fe360	317	Tonne	Steel for absorber stripper and small equipment	(Koornneef 2008)
Autocalved concrete blocks	1440	kg	Concrete needed for construction	(Koornneef 2008)
Transport, freight	9.5	tkm	Transport footprint of all components	(Koornneef 2008)

Raw Materials	Cell composition	Reference(s)
Nickel (Ni), Yttrium (Y), Zirconium (Zr), Lanthanum (LA), Strontium (Sr), Manganese (Mn)	*Ni-YSZ|YSZ|YSZ-LSM* **YSZ**: Yttria Stabilised Zirconia **LSM**: Lanthanum Strontium Manganite **Yttria**: Y_2O_3 **Zirconia**: ZrO_2 **Manganite**: MnO	(Lu et al, 2020) (Yun Zheng et al., 2017) (Choe et al., 20222) (Andika et al., 2018) (Redissi & Bouallou, 2013) (W. Li et al., 2013)
Lanthanum, Strontium, Vanadium, Yttrium, Zirconium, Platinum	*SV|YSZ|Pt* **LSV**: Lanthanum-doped Strontium Vanadate **Vanadate**: VO_4	(Yun Zheng et al., 2017) (Zhang et al., 2019)
Palladium, Cerium, Zirconium, Yttrium, Lanthanum, Strontium, Manganese, Ferrite	*Pd,CZY,LSCM-YSZ|YSZ|LSF-YSZ* **CZY**: Ceria Zirconia Yttria **LSCM**: Lanthanum Strontium Ceria **Manganite** **LSF**: Lanthanum Strontium Ferrite **Ceria**: CeO_2	(Yun Zheng et al., 2017)
Strontium, Ferrite, Manganese, Samarium, Ceriuim, Lanthanum, Gadolinium	*SFM-SDC|LSGM|SFM-SDC* **SFM**: Strontium Ferrite Manganite **SDC**: Strontium Doped Ceria **LSGM**: Strontium Doped Lanthanum Gadolinium	(Yao Wang et al., 2017)
Nickel, Yttrium, Strontium, Zirconium, Scandium, Lanthanum, Manganese	*Ni-YSZ|ScSZ|LSM-ScSZ* **ScSZ**: Scandia Stabilised Zirconia **Scandia**: Sc_2O_3	(Yao Wang et al., 2017)
Nickel, Yttrium, Strontium, Zirconium, Lanthanum, Cobalt, Ferrite, Gadolinium	*Ni-YSZ|YSZ|LSCF-CGO* **LSCF**: Strontium Iron Doped Lanthanum Cobalt **CGO**: Ceria Doped Gadolinium	(Yun Zheng et al., 2017)(X. Chen et al., 2015)
Nickel, Yttrium, Strontium, Zirconium, Lanthanum, Cobalt, Ferrite	*Ni-ScSZ|ScSZ-CGO|LSCF-CGO*	(D. Y. Lee et alk., 2020)
New: 8YSZ-8mol% Yttria-doped stabilized zirconia, Nickel, Yttrium, Zirconium	*Ni-8YSZ|8YSZ|LSCF-CGO*	(Schreiber et alk., 2020) (Nechache & Hody, 2021)(Reytier et alk., 2015) (Ebbehoj, 2015)
Nickel, Yttrium, Strontium, Zirconium, Lanthanum, Ferrite, Gadolinium, Cerium	*Ni-YSZ|YSZ|(Sr,Co)(La,Fe)-GCO*	(L.Wang et al., 2019)

Figure B.1: Material evaluation for SOEC electrodes

Unit	CO_2 [kg CO_2-eq]	Reference	CO_2 [kg CO_2-eq]	Reference	Average [kg CO_2-eq]
Nickel	8.82	Idemat 2022	6.5	Nusss 2014	7.66
Yttrium	29.9	Idemat 2022	15.1	Nusss 2014	22.5
Zirconium	0.9	Perks 2022	1.1	Nusss 2014	1
Lanthanum	21.8	Idemat 2022	11	Nusss 2014	16.4
Gadolinium	92.2	Idemat 2022	46.6	Nusss 2014	69.4
Cerium	25.3	Idemat 2022	12.9	Nusss 2014	19.1
Strontium	–	Nusss 2014	–	Nusss 2014	3.2
Manganese	4.52	Farjana 2019	1	Nusss 2014	2.76

Table B.9: Comparison of CO_2 Footprint of Rare Earth Elements

Table B.10: Impact Category Data

Impact Category	Abbreviation	Description	Unit
Global Warming potential	GWP	Measures greenhouse gas emissions	kg CO_2-eq
Stratospheric ozone depletion	SOP	Assesses potential for ozone layer damage	kg CFC11-eq
Ionizing radiation	IR	Evaluates radiation exposure risk	kBq Co60-eq
Ozone formation, human health	OF - HH	Assesses ground-level ozone effects on human health	kg NO_x-eq
Fine particulate matter formation	FP	Measures formation of small airborne particles	kg PM2.5-eq
Ozone formation, Terrestrial ecosystems	OF - TE	Assesses ground-level ozone effects on land ecosystems	kg NO_x-eq
Terrestrial ecotoxicity	TE	Evaluates toxicity impact on land ecosystems	kgS SO_2-eq
Freshwater ecotoxicity	FE	Measures toxicity impact on freshwater ecosystems	kg P -eq
Marine ecotoxicity	ME	Measures toxicity impact on marine ecosystems	kg N eq
human carcinogenic toxicity	HCT	Evaluates cancer risks to humans	kg 1.4-DCB
Human non-carcinogenic toxicity	HNCT	Assesses non-cancer health risks to humans	kg 1.4-DCB
Land use	LU	Quantifies land area required	kg 1.4-DCB
Mineral resource scarcity	MRS	Measures depletion of mineral resources	kg 1.4-DCB
Fossil resource scarcity	FRS	Measures depletion of fossil fuel resources	kg 1.4-DCB
water consumption	WC	Evaluates water resource usage	m^2a crop-eq

Table B.11: Impact Category Data

Impact category	Nickel	Yttrium	Zirconium	Lanthanium	Gadolinium	Cerium	Strontium	Manganese	Unit
Global Warming potential	8.82	29.9	NA	21.8	92.2	25.3	NA	NA	kg CO_2-eq
Stratospheric ozone depletion	3.54E-08	7.87E-06	NA	5.74E-06	2.43E-05	6.66E-06	NA	NA	kg CFC11-eq
Ionizing radiation	0.001190	0.052	NA	0.038	0.161	0.044	NA	NA	kBq Co_{60}-eq
Ozone formation, human health	0.013300	0.0561	NA	0.0409	0.174	0.0475	NA	NA	kg No_x-eq
Fine particulate matter formation	0.268	0.0508	NA	0.037	0.157	0.043	NA	NA	kg PM2.5-eq
Ozone formation, Terrestrial ecosystems	0.0214	0.0567	NA	0.0414	0.176	0.048	NA	NA	kg NO_x-eq
Terrestrial ecotoxicity	0.924	0.165	NA	0.12	0.51	0.139	NA	NA	kgS SO_2-eq
Freshwater ecotoxicity	8.95E-08	1.77E-05	NA	1.29E-05	5.45E-05	1.50E-05	NA	NA	kg P -eq
Marine ecotoxicity	2.17E-07	5.44E-05	NA	3.95E-05	1.67E-04	4.61E-05	NA	NA	kg N eq
human carcinogenic toxicity	0.0045	21.8	NA	15.9	67.6	18.5	NA	NA	kg 1.4-DCB
Human non-carcinogenic toxicity	0.00015	0.00732	NA	0.00539	0.0222	0.00622	NA	NA	kg 1.4-DCB
Land use	0.0921	92.3	NA	67.3	286	75.1	NA	NA	kg 1.4-DCB
Mineral resource scarcity	0.000202	0.39	NA	0.284	1.21	0.33	NA	NA	kg 1.4-DCB
Fossil resource scarcity	0.0654	106	NA	77.1	327	89.4	NA	NA	kg 1.4-DCB
water consumption	0.00111	0.0139	NA	0.0114	0.0329	0.0124	NA	NA	m^2a crop-eq
mineral resource	1.91	7.75E-04	NA	5.80E-04	2.28E-03	6.61E-04	NA	NA	kg Cu-eq
fossil resource	3.46	8.35	NA	6.1	21.9	7.07	NA	NA	kg oi-eq
water consumption	3.96E-06	1.86E-05	NA	1.86E-05	1.86E-05	1.85E-05	NA	NA	m^3

Fraction [%]	Capture units	Electrolyser units	Total Transport [Mtonne CO_2-eq]	Objective criterion
1	1	1	0.0468845	71.9068
5	1	1	0.1717016	39.4621
10	1	1	0.1717016	34.8008
15	1	1	0.0468845	32.924
20	2	2	0.3264286	34.7678
25	2	2	0.3264286	33.8422
30	2	3	1.5419916	35.7686
35	2	4	1.6463316	
40	2	4	1.6463316	35.1905
45	3	4	2.8668409	35.9229
50	3	5	4.0824019	36.8706
55	5	4	5.111111	36.8493
60	5	5	5.239911	36.8588
65	5	4	5.320981	35.9424
70	5	5	8.486084	38.1151
75	6	6	10.08154	38.5536
80	7	7	11.109946	39.0262
85	7	5	13.621364	39.3079
90	6	8	16.261946	40.4642
95	8	7	17.021403	40.7657
100	7	8	17.906733	40.4698

Table B.12: Total overview for the base case scenario

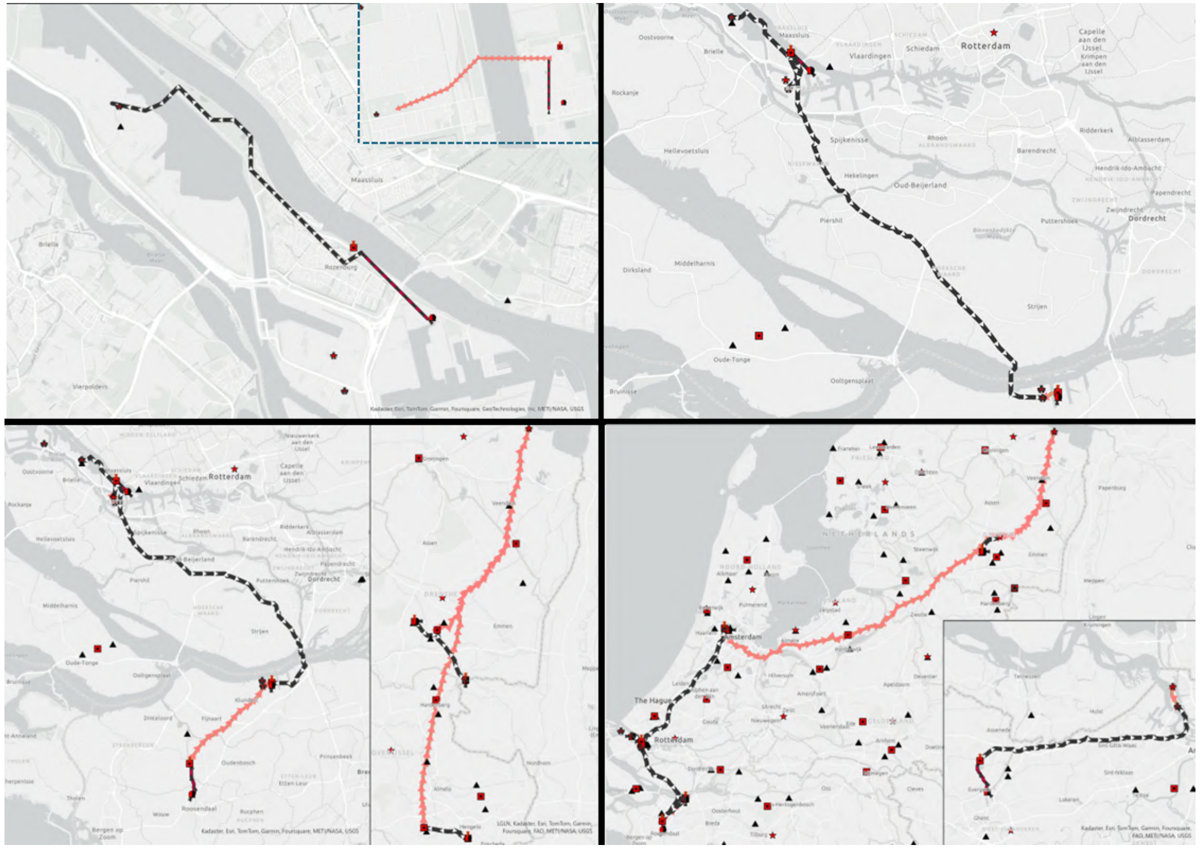

Figure B.2: Visualisation of base case scenario in ArcGIS pro for 25%, 50%, 75% and 100% market penetration.

Unit	Distribution [-]	Reference
Nickel	USA, China, EU	Nakajima 2018 [74]
Yttrium	China, Vietnam, Brazil	Choudhary 2022 [19]
Zirconium	Australia, South Africa	Perks 2019 [82]
Lanthanum	China, Canada	Dushyantha 2020 [28]
Gadolinium	USA, China	Dushyantha 2020 [28]
Cerium	South-Africa	Dushyantha 2020 [28]
Strontium	China, USA	Wang 2020 [114]
Manganese	Worldwide	Herndon 2011 [43]

Table B.13: Distribution of rare earth elements worldwide

	Nickel	Yttrium	Zirconium	Lanthanum	Gadolinium	Cerium	Strontium	Manganese	Unit
Abundance	58	29	170	29	8	70	340	1000	10^{-4} wt%
Geographical occurrence	USA, China, EU	China, Vietnam, Brazil	Australia, South Africa	China, Canada	USA, China	South Africa	China, USA	Worldwide	[-]
CO_2-eq footprint	3.06	9.00	0.40	6.56	27.76	7.64	1.28	1.10	[-]
Costs	0.01	53.33	66.67	40.00	36.67	33.33	4.35	0.01	[-]

Table B.14: Comparison of various elements.

Symbol	Description
C	Supply set – all the CO_2 sources in the model; consisting of 119 sources
CI	All the individual CO_2 sources which are not part of a 25-kilometer cluster; consisting of 8 sources
CCI	Subset – All the individual CO_2 sources (cci) in the model that are not part of a 25-kilometer cluster; consisting of 8 sources
CEH	Subset – All the exclusive hub CO_2 sources (ceh) which are part of a 25-kilometer cluster; consisting of 111 sources
EH	All the exclusive hub CO_2 sources which are part of a 25-kilometer cluster; consisting of 41 sources
E	All the possible electrolysis plant locations, consisting of CO_2 source locations, syngas demand points, and intermediate hub locations; consisting of 83 positions
S	All the direct and indirect syngas demand locations in the system; consisting of 10 positions
TSetCCI	Subset – Links the CO_2 sources CCI to CI; indexed by cci, ci
TSetCEH	Subset – Links the CO_2 sources CEH to exclusive hub EH; indexed by ceh, eh

Table B.15: Description of sets and subsets used in the model

Description	Symbol	Magnitude	Unit	Reference 1:	Reference 2:
Mass flow of CO2 emitted at site	m_1	Model	[Mtonne CO_2 emitted/year]		
Efficiency of carbon capture unit (OVERALL)	$\alpha_{1,j}$	90	[%]	(Bin Ye 2019)	(Anand B. Rao 2006)
Efficiency of carbon capture unit (BIOETHANOL)	$\alpha_{1,1}$	95	[%]	(Cormos 2014)	(Faruque 2012)
Efficiency of carbon capture unit (BIOMETHANE)	$\alpha_{1,2}$	95	[%]	(Menin 2022)	
Efficiency of carbon capture unit (PULP AND PAPER)	$\alpha_{1,3}$	80	[%]	(Sagues 2020)	(Möllersten 2004)
Efficiency of carbon capture unit (WASTE INCINERATION)	$\alpha_{1,4}$	85	[%]	(Haaf 2020)	
Mass flow of CO2 lost during transport	m_2	Model	[Mtonne CO_2 transported/year]		
Leakage efficiency of infrastructure	α_2	98	[%]	(A. Alvarez 2011)	(B. Jackson 2014)
Mass flow of CO2 lost due to not full conversion	m_3	Model	[Mtonne CO_2 entering CO_2E/year]		
efficiency of industrial scale electrolyser	α_3	85	[%]	(ISPT report, 2023)	
Mass flow of syngas lost due to leakage	m_4	Model	[Mtonne syngas transported/year]		
Leakage efficiency of infrastructure	α_4	98	[%]	(A. Alvarez 2011)	(B. Jackson 2014)
Energy consumed for CO2 capture site	E_4	0.000003	[Mtonne CO_2 - eq / MWh]	(Silva Ortiz 2020)	
CO2 conversion factor for carbon capture unit	β_4	345000.0	[MWh / Mtonne CO_2 captured]	(Xiangping Zhang 2014)	
Energy consumed for CO2 transport	E_5	0.000003	[Mtonne CO_2 - eq / MWh]	(Silva Ortiz 2020)	
CO2 conversion factor for pump/compressors	β_5	0.9839	[MWh/Mton CO_2]	(T. Rochelle 2009)	
Carbon footprint of electricity	E_6	0.000003	[Mtonne CO_2 - eq / MWh]	(Silva Ortiz 2020)	
CO2 conversion factor for electrolyzer	β_6	9300000.0000	[MWh/Mtonne SG Produced]	(ISPT)	
Energy consumed for syngas transport	E_7	0.000003	[Mtonne CO_2 - eq / MWh]	(Silva Ortiz 2020)	
CO2 conversion factor for pump/compressors	β_7	0.9839	[MWh/Mton Syngas transported]	(T. Rochelle 2009)	
GWP of Hydrogen gas	GWP_{H2}	5.8	[-]	(Warwick 2022)	
GWP of CO gas	GWP_{CO}	1.9	[-]	(Raman P 2013)	
GWP ofsyngas (2:1) ratio	GWP_{syngas}	4.5	[-]	(ISPT)	

Figure B.3: Symbols overview of objective function

$$\textit{Objective Funtion} = min\{$$

$$\left(\sum m_1 (1-\alpha_{1,j})\right) + \left(\sum m_2 (1-\alpha_2)\right) + \left(\sum m_3 (1-\alpha_3)\right) + \left(\sum m_4 (1-\alpha_4) GWP_{syngas}\right) + \left(\sum E_4\ \beta_4\ m_1\ \alpha_{1,j}\right) + \left(\sum E_5\ \beta_5\ m_2\ \alpha_2\right)$$

$$+\left(\sum E_6\ \beta_6\ m_3\ \alpha_3\right) + \left(\sum E_7\ \beta_7\ m_4 GWP_{syngas}\right) + \left(\sum \varphi_8 + m_9 \varphi_9\right) + \left(\sum \varphi_{12} + m_{13}\varphi_{13}\right) + \left(\sum \delta_{Transport} * m_i\right)\}$$

Inefficiencies in CO₂E SC infrastructure footprint

Energy consumption footprint

Constructional and O&M footprint

Transport footprint

Figure B.4: Simplified overview of objective function regarding direct and indirect CO_2-eq emissions

Description	Symbol	Magnitude	Unit	Reference 1:	Reference 2:
Fixed CO_2 emission due to construction of capture unit	ϕ_8	0.0007	[Mtonne CO_2 -eq/ build unit]	(Koorneef 2008)	
Mass flow of CO_2 captured at site	m_9	Model	[Mtonne CO_2 / yr]		
CO_2 emission due to O&M of capture unit	ϕ_9	0.0001	[Mtonne CO_2 -eq/ Mtonne CO_2-captured]	(Cormos 2014)	(Faruque 2012)
Fixed CO_2 emission due to construction of transport unit	ϕ_{10}	0.0763	[Mtonne CO_2 -eq/ build unit]	(Menin 2022)	
Mass flow of CO_2 transported through pipelines	m_{11}	Model	[Mtonne CO_2 / yr]		
CO_2 emission due to O&M of transport unit	ϕ_{11}	0.0076	[Mtonne CO_2 -eq/km Mtonne CO_2-transported]	(Haaf 2020)	
Fixed CO2 emission due to construction of electrolyser	ϕ_{12}	355.2071	[Mtonne CO_2 / build site]		
Mass flow of CO2 entering the electrolyser	m_{13}	Model	[Mtonne CO_2 / yr]	(A. Alvarez 2011)	(B. Jackson 2014)
CO2 emission due to O&M of electrolyser	ϕ_{13}	35.5207	[Mtonne CO_2 -eq/ Mtonne CO_2-converted]		
Fixed CO_2 emission due to construction of transport unit	ϕ_{14}	0.0763	[Mtonne CO_2 / year]	(ISPT report, 2023)	
Mass flow of syngas transported to demand	m_{15}	Model	[Mtonne syngas / yr]		
CO_2 emission due to O&M of transport unit	ϕ_{15}	0.0076	[Mtonne CO_2 -eq/km Mtonne Syngas-transported]	(A. Alvarez 2011)	(B. Jackson 2014)

Figure B.5: Symbols overview of objective function

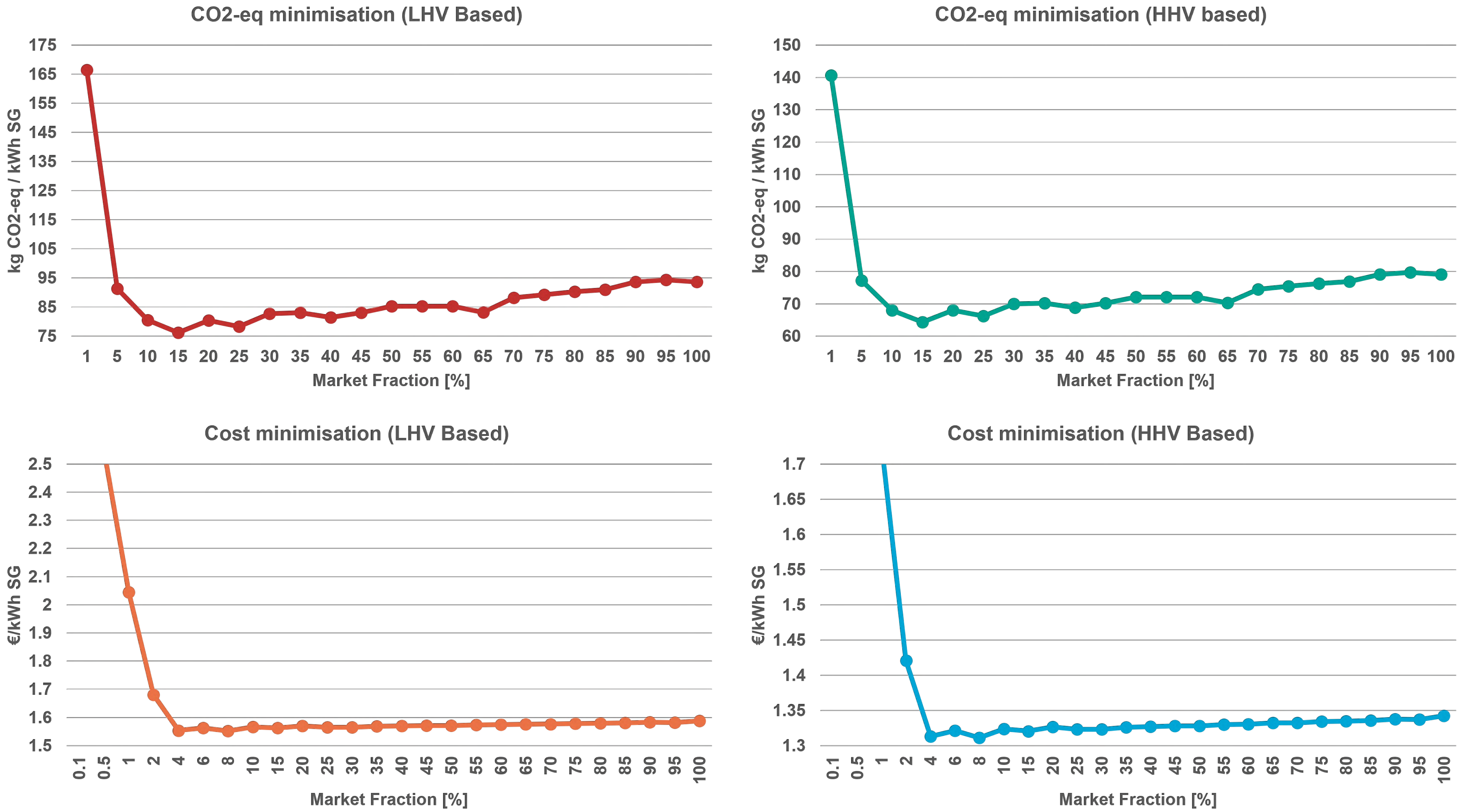

Figure B.6: Objective criteria expressed in energy units

Variables	Description	Type
x_i	Variable containing all possible flows of CO_2 within set i=CCI, CEH, E	Positive Continuous
y_j	Variable containing all possible flows of SG within set j=E, S	Positive Continuous
z	Total CO_2-eq footprint of CO_2E SC infrastructure configured in GAMS	Free
$AllocFlow_{i,j}$	Outcome of the decision variable, to whether or not construct transport use a certain location/pathway within set=i, j	Binary

Table B.16: Description of variables used in the model

C

Appendix C

This appendix contains all LCA data obtained from SimaPro

C.1. LCI data for the capture unit

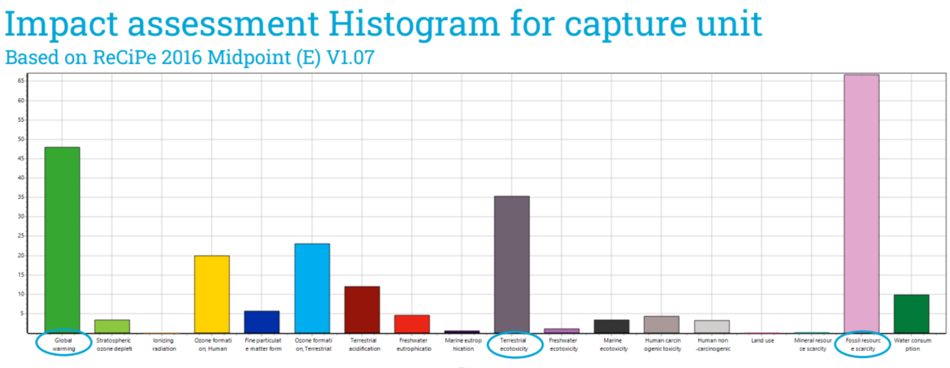

Figure C.1: Histogram for impact assessment of the capture unit

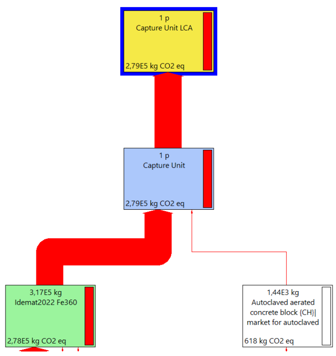

Figure C.2: Characterization network regarding global warming potential of a capture unit

Table C.1: Environmental Impact Assessment for a capture unit (Koorneef 2008) / Idemat 2022

Impact Category	Unit	Total	Capture unit
Global Warming	kg CO_2-eq	2.79E+05	2.79E+05
Stratospheric Ozone depletion	kg CFC11-eq	0.241	0.241
Ionizing radiation	kBq CO-60 eq	28.3	28.3
Ozone formation, Human Health	kg NO_X-eq	410	410
Fine particulate matter formation	kg PM2.5-eq	146	146
Ozone formation, terrestrial ecosystem	kg Nox-eq	410	410
Terrestrial Acidification	kgSO_2-eq	494	494
Freshwater eutrophication	kg P-eq	2.8	2.8
Marine Eutrophication	kg N-eq	2.47	2.47
Terrestrial ecotoxicity	kg 1,4-DCB	5.78E+05	5.78E+05
Freshwater ecotoxicity	kg 1,4-DCB	306	306
Marine ecotoxicity	kg 1,4-DCB	8.21E+06	8.21E+06
Human carcinogenic toxicity	kg 1,4-DCB	1.26E+03	1.26E+03
Human non-carcinogenic toxicity	kg 1,4-DCB	7.16E+06	7.16E+06
Land use	m2a crop-eq	2.55E+01	2.55E+01
Mineral Resource scarcity	kg Cu-eq	1.49E+04	1.49E+04
Fossil resource scarcity	kg oil-eq	6.54E+04	6.54E+04
Water consumption	m3	2.64E+03	2.64E+03

C.2. LCI data for the transport unit

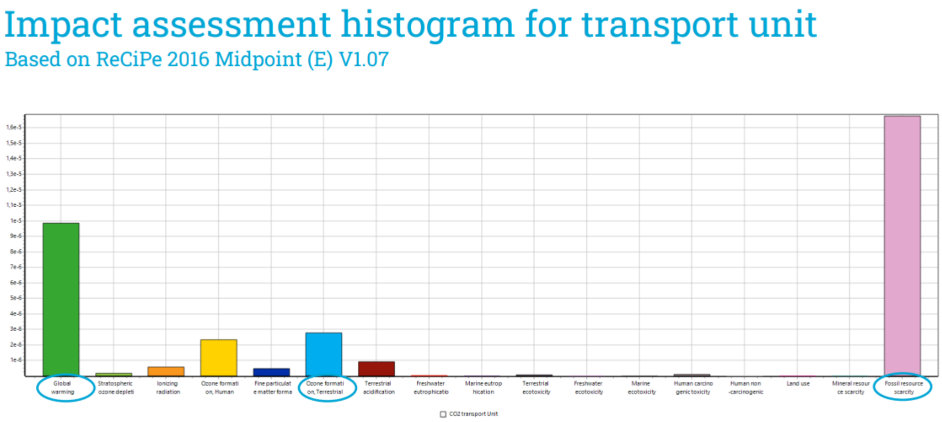

Figure C.3: Histogram for impact assessment of the transport unit

Table C.2: Environmental Impact Assessment of the transport unit (Koorneef 2008) / Idemat 2022

Impact Category	Unit	Total	Capture unit
Global Warming	kg CO_2-eq	2.79E+05	2.79E+05
Stratospheric Ozone depletion	kg CFC11-eq	0.241	0.241
Ionizing radiation	kBq CO-60 eq	28.3	28.3
Ozone formation, Human Health	kg NO_X-eq	410	410
Fine particulate matter formation	kg PM2.5-eq	146	146
Ozone formation, terrestrial ecosystem	kg Nox-eq	410	410
Terrestrial Acidification	kg SO_2-eq	494	494
Freshwater eutrophication	kg P-eq	2.8	2.8
Marine Eutrophication	kg N-eq	2.47	2.47
Terrestrial ecotoxicity	kg 1,4-DCB	5.78E+05	5.78E+05
Freshwater ecotoxicity	kg 1,4-DCB	306	306
Marine ecotoxicity	kg 1,4-DCB	8.21E+06	8.21E+06
Human carcinogenic toxicity	kg 1,4-DCB	1.26E+03	1.26E+03
Human non-carcinogenic toxicity	kg 1,4-DCB	7.16E+06	7.16E+06
Land use	m2a crop-eq	2.55E+01	2.55E+01
Mineral Resource scarcity	kg Cu-eq	1.49E+04	1.49E+04
Fossil resource scarcity	kg oil-eq	6.54E+04	6.54E+04
Water consumption	m3	2.64E+03	2.64E+03

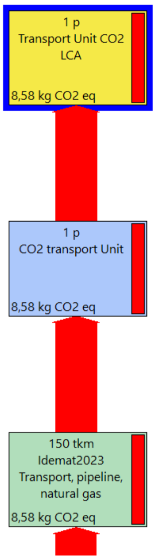

Figure C.4: Characterization network regarding global warming potential of a transport unit

C.3. LCI data for the electrolyser unit

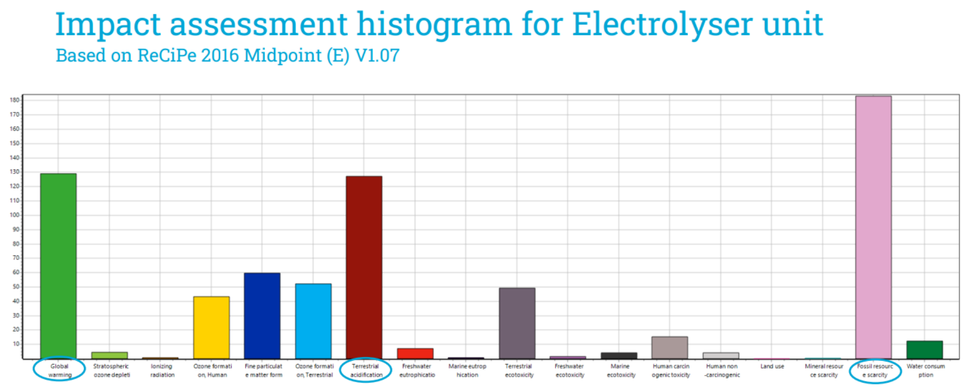

Figure C.5: Histogram for impact assessment of the electrolyser unit

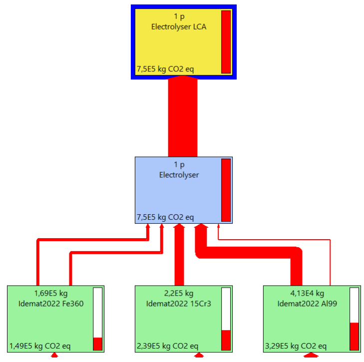

Figure C.6: Characterization network regarding global warming potential of an electrolyser unit

Table C.3: Environmental Impact Assessment for an Electrolyser

Impact Category	Unit	Total	Electrolyser
Global Warming	kg CO_2-eq	7.50E+05	7.50E+05
Stratospheric Ozone depletion	kg CFC11-eq	3.12E-01	3.12E-01
Ionizing radiation	kBq CO-60 eq	615	615
Ozone formation, Human Health	kg NO_X-eq	8.93E+02	8.93E+02
Fine particulate matter formation	kg PM2.5-eq	1.53E+03	1.53E+03
Ozone formation, terrestrial ecosystem	kg NO_X-eq	9.27E+02	9.27E+02
Terrestrial Acidification	kg SO_2-eq	5.22E+03	5.22E+03
Freshwater eutrophication	kg P-eq	4.61E+00	4.61E+00
Marine Eutrophication	kg N-eq	3.23E+00	3.23E+00
Terrestrial ecotoxicity	kg 1,4-DCB	8.07E+05	8.07E+05
Freshwater ecotoxicity	kg 1,4-DCB	4.71E+02	4.71E+02
Marine ecotoxicity	kg 1,4-DCB	1.05E+07	1.05E+07
Human carcinogenic toxicity	kg 1,4-DCB	4.54E+03	4.54E+03
Human non-carcinogenic toxicity	kg 1,4-DCB	9.33E+06	9.33E+06
Land use	m2a crop-eq	1.96E+02	1.96E+02
Mineral Resource scarcity	kg Cu-eq	3.20E+04	3.20E+04
Fossil resource scarcity	kg oil-eq	1.80E+05	1.80E+05
Water consumption	m3	3.33E+03	3.33E+03