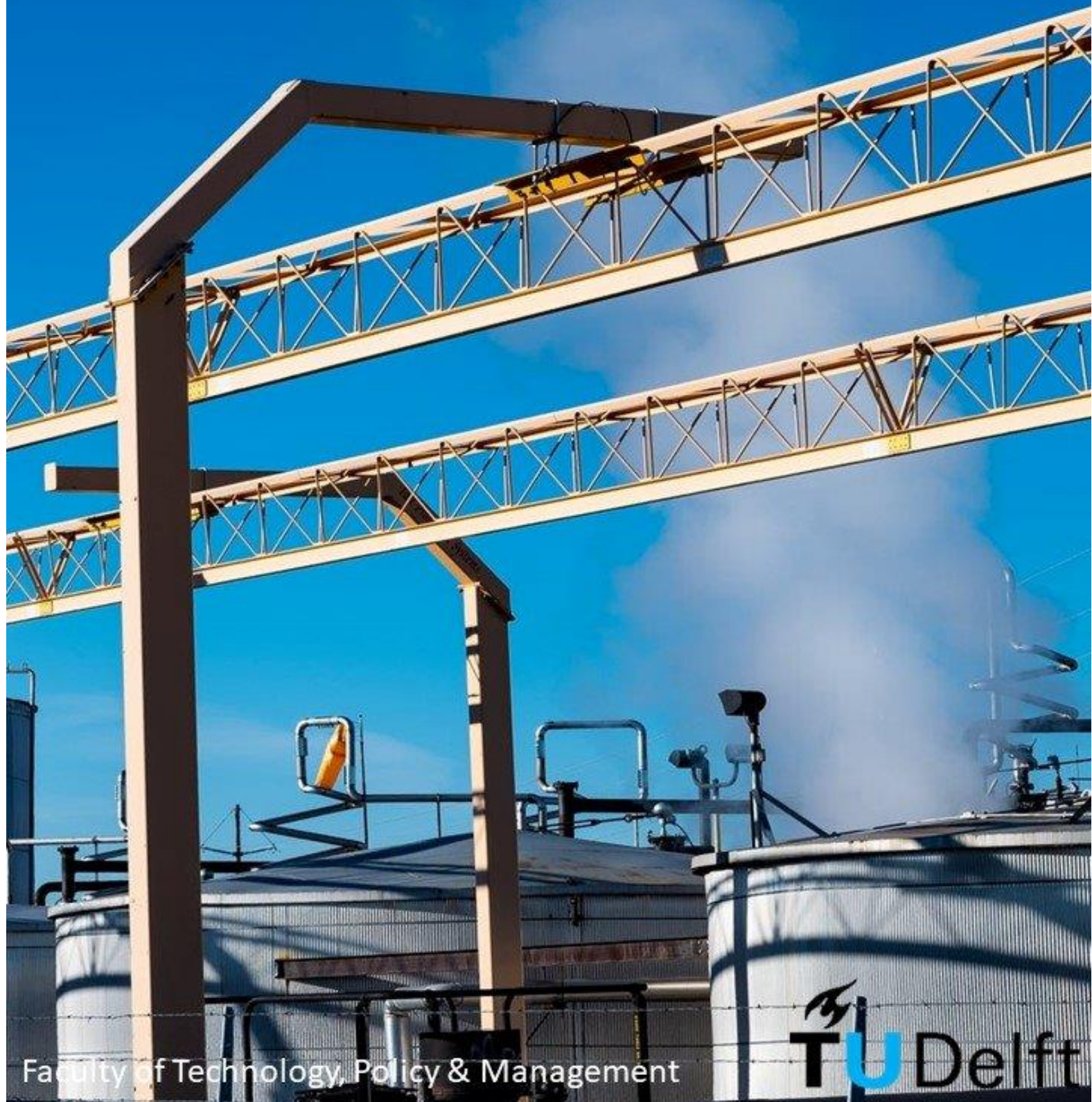


Comparative enviro-economic impact assessment of Dutch chlorine production systems: Investigating different methods for monetizing environmental externalities



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Comparative enviro-economic impact assessment of Dutch chlorine production systems: Investigating different methods for monetizing environmental externalities

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Preface

To my mind, life offers opportunities and it is up to us to decide whether to seize them or not. Two years ago I had the opportunity to change my life in a positive way and start a very challenging but also fruitful academic journey at the Delft University of Technology (TU Delft). After two years of studies, this journey comes to an end. The present report constitutes the conclusion of my graduation project of the Management of Technology master's programme at TU Delft. I feel thankful for all the experiences gained in this two-year programme and especially for the last six months that I had the opportunity to be involved in a master thesis project that was in line with my interests and background. For this, I am grateful for the support, guidance and inspiration of my supervisors whose contribution and aid led me to learn, form and conduct this research.

First of all, I would like to express my sincere appreciation to my thesis supervisor, Dr. ir. G. Korevaar for the insightful, inspiring, and pleasant discussions we had during the last six months and foremost to thank him for giving me the opportunity to work on the particular project. Moreover, I would like to deeply thank my daily supervisor Dr. ir. G.A. Tsalidis for having multiple eye-opening and constructive meetings with me. Thank you for your guidance, valuable time and for challenging me to reach the best out of me, which eventually led me to finalize this research. Furthermore, I would like to express my gratitude to Professor dr. C.P. van Beers and Dr. E. Schröder for their useful comments and feedback throughout the course of this thesis.

This journey would not have been accomplished without the support of my loved ones. I would like to deeply thank my family, my mother Maria, my father Konstantinos and my sister Eleni for their faith in me, motivation and patience throughout this two-year journey. Though you are miles away, your unconditional love and support was the main driver for me to keep pushing forward and achieving my goals. Lastly, I would like to extend my thanks to my close friends in Greece and the Netherlands for believing in me and being supportive during times of difficulty. This thesis is dedicated to all of them.

O.C. Diafonidis

Delft, October 2019

“Look up at the stars and not down at your feet. Try to make sense of what you see, and wonder about what makes the universe exist. Be curious”

Stephen Hawking

Executive Summary

To fend off the probable adverse effects of climate change as well as the subsequent economic and social impacts, the Dutch chemical industry and in particular the chlorine manufacturing sector is required to take courageous decisions and change the way of processing, managing and exploiting natural resources. Given the high energy consumption of chlorine production systems in the Netherlands, it is of paramount importance to thoroughly examine which technical solutions can improve current practices and raw materials' usage. For this reason, we combined the life-cycle assessment and life-cycle costing techniques, in order to identify which chlorine production alternative can lead to the lowest environmental footprint (LCA) and cost-intensity (LCC).

Though the parallel application of LCA and LCC has gained some prominence in academia as the scientific way for diagnosing and assessing environmental and financial discrepancies that occur throughout a production system's life-cycle, their integration still lacks a robust methodological structure. The challenge of integrating LCA and LCC lies in the absence of a standardized technique for converting environmental damages into monetary terms under the prism of LCC. Given that, the present research aims to bring in light valuable insights to the scientific community with respect to the integration issue of the above-addressed techniques by attempting to resolve the following research question,

«How to develop an enviro-economic evaluation method that integrates Life-Cycle Assessment & Life-Cycle Costing techniques and implement it on the Dutch chlor-alkali manufacturing industry?»

To that end, based on a case study that concerns Nouryon's chlor-alkali plant at Rotterdam we attempted to combine these techniques by following the LCA's ISO standard structure and investigating whether the application of five economic weighting sets based on different valuation methods can be used to facilitate LCA's integration with LCC.

To support Nouryon's strategic planning, four different scenarios were developed with a view to assessing potential enviro-economic benefits from the application of zero-gap cell electrolyzers and biomass boilers. In a 'gate-to-gate' analysis, these scenarios were compared in terms of their environmental profile by using SimaPro 8.5.2.0 software and applying the ReCiPe 2016 v1.1 (E) impact assessment method. Private costs were estimated via the ASTM International standard approach, (2002) and summed up with the monetized environmental externalities. Regarding the latter, the economic weighting sets provided by the LCIA methods of ReCiPe, Stepwise, Ecovalue08, Ecotax02 and LIME were used to convert environmental impacts into monetary terms.

From our analysis, a twofold issue was diagnosed. The high dependency of chlorine's production on electricity consumption goes in tandem with a substantial financial burden and negative environmental effects.

In line with the latter, our findings suggest that the most cost-effective and less environmentally-intensive technical solution concerns the modification of the electrolysis cell

from gap to zero-gap one when the heat is supplied by an on-site CHP facility. The implementation of this scenario is anticipated to bring multifaceted benefits to the company and induce a domino of positive effects on society at large.

In particular, the installation of twenty-one zero-gap cell electrolyzers with per unit capacity of 30.5 kton Cl_2 /year is recommended. As such, an initial investment of 77 M€ is required which is anticipated to yield 570 M€ approximately as a consequence of fewer electricity costs when compared to the conventional cell's configuration type.

Moreover, electrolyzers' modification is expected to bring the company closer to its climate change targets, which aim for 25-30% reduction of CO_2 emissions by 2020 and become carbon neutral by 2050. Specifically, our recommendation is accompanied by 39% reduction of CO_2 emissions in the membrane electrolysis stage and 24% reduction in the total CO_2 emissions per ton of chlorine produced. This implies a further reduction in regards to the estimated environmental costs due to on-site generated CO_2 emissions. Furthermore, the suggested alternative can result in 25% reduction in the recorded environmental damage on human health and ecosystems due to off-site power generation. Consequently, chain-related environmental costs decrease by 23% approximately. Lastly, the installation of zero-gap electrolyzers is estimated to yield €1.58 bn in a twenty-year time horizon, thus further investments in researching even more sustainable opportunities can be realized.

As far as the combined LCA and LCC approach followed by this research is concerned, we identified that the environmental cost-related results deviate since the implemented weighting factors are the outcome of different valuation methods. Due to the incompleteness, geographical and cultural bias of the examined weighting factors, we regard that except for one weighting set (Stepwise), which can be representative for certain impact categories, all the others cannot be used consistently in integrated life-cycle studies, and thus lead to generalizable and representative results. As such, we highlight the paramount importance of conducting autonomous valuation research for studies that attempt to combine LCA and LCC with a view to monetizing environmental damages. For this, our suggestion regards the use of the choice experiment method whose multi-attribute valuation scope is perceived to be highly compatible with the rationale of the LCA technique.

Keywords: Life-cycle assessment, Life-cycle costing, Environmental impacts monetization, Dutch chlorine production systems, Membrane cell electrolysis

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List of Abbreviations

BAHY	Biodiversity Adjusted Hectare Year
CBA	Cost and benefit analysis
CBS	Centraal Bureau voor de Statistiek (The Dutch Central Agency of Statistics)
CE	Choice Experiment Method
CHP	Co-generation heat and power
cLCC	conventional Life Cycle Costing
CO ₂	Carbon dioxide
CV	Contingent Valuation Method
EC	Impacts on Ecosystems
eLCC	environmental Life Cycle Costing
EPS	Environmental Priority Strategies
EU	European Union
FU	Functional Unit
GHG	Greenhouse gasses
GWP	Global Warming Potential – Impacts on Climate Change
HH	Impacts on Human Health
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
LCA	Life Cycle Assessment
LCC	Life Cycle Costing
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LCT	Life Cycle Thinking
LCSA	Life Cycle Sustainability Assessment
MAC	Marginal Abatement Cost
NPV	Net Present Value
ODC	Oxygen-depolarized cathode
QALY	Quality-Adjusted Life Year
SETAC	Society of Environmental Toxicology and Chemistry
sLCC	societal Life Cycle Costing
UNEP	United Nations Environment Programme
WTA	Willingness-to-accept
WTP	Willingness-to-pay

Chapter 1: Introduction

1.1 Research background

Nowadays, humanity is facing many challenges through which its future probably will be at stake. The rapid increase of sea levels, atmospheric pollution, the rising temperatures, and the extreme weather conditions comprise major problems for the world society. From the dawn of the 20th century, human and especially industrial activities have intervened in natural ecosystems distilling and deteriorating any available natural resources, thus, leading the planet to an inevitable climate change. Greenhouse gas (GHG) emissions are the most harmful and long-lasting consequence of humans' industrial activities that greatly contribute to climate change (Althor et al., 2016).

To counteract climate change effects, the Europe 2020 Strategy, as well as, the Paris Agreement, are the foundation stones upon which Europe endeavors to collectively restrict energy overconsumption and reduce the associated GHG emissions (Liobikienė & Butkus, 2017; Tol, 2012). However, despite that in the recently ratified Paris Agreement, 196 countries pledged to substantially decrease GHG emissions, the current contribution of each country to tackling the imminent challenges of climate change is still not enough (Canadell et al., 2017; Höhne et al., 2017). To that end, the IPCC (2018) has beaten the drum for more extreme measures, advocating that if by 2050 the world society has not met with success to largely lower GHG emissions, it would be improbable to avoid global warming impacts.

On a global scale, the Netherlands' contribution to climate change is negligible (De Telegraaf, 2019). However, as a consequence of its energy-intensive and fossil-dependent industrial sector, the Netherlands is ranked among the largest GHG emitters in the European Union. That has led the Dutch parliament to repeatedly discuss and enact policies aiming to transition the Dutch economy to its decarbonization. For this, by embracing a long-term, ambitious and demanding climate mitigation plan, the Netherlands wishes to achieve an almost 50% reduction in GHG emissions by 2030 and 85% to 100% respectively by 2050, compared to the reference year of 1990 (van Vuuren et al., 2017).

To accomplish these targets, drastic changes in the sectors that deliberately cause negative environmental impacts are required to effectively limit anthropogenic GHG emissions (Li & Strachan, 2017; York & Bell, 2019). As it is shown in Figure 1, the Dutch chemical industry, which holds a leading position in the global market with 2% share of global sales (Stork et al., 2018), generates the most GHG emissions (40%) in contrast to the other manufacturing sectors (CBS, 2017). In 2016, along with the chemical industry, the petrochemical and basic metals industries have burdened the environment by two billion kg CO₂ more than the previous year. Hence, accounting for 78% of the overall GHG emissions of the manufacturing sector (CBS, 2017). One part of the chemical industry which also contributes to the overall environmental damage is that of the chlorine production sector. The Achilles' heel of this sector is its high energy requirements for the electrolysis of sodium chloride to chlorine and caustic soda (Brinkman et al., 2014). In particular, chlorine production systems demand

between 2,500 and 3,500 kWh per ton of chlorine produced, thus resulting in a substantial environmental burden (Garcia-Herrero, Margallo, Onandía, Aldaco, & Irabien, 2017a).

Greenhouse gas intensity by industry, 2016

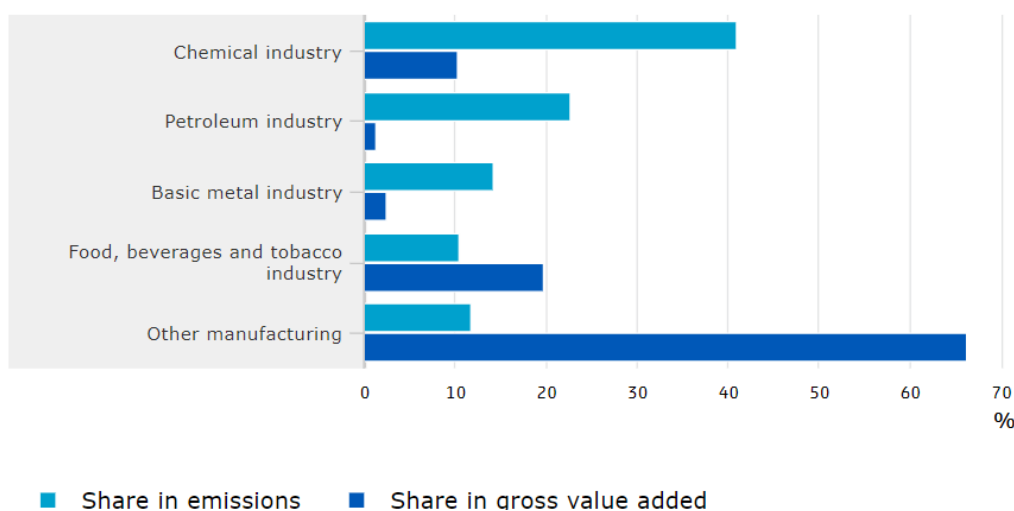


Figure 1: GHG emissions intensity in the Netherlands by industry (CBS, 2017)

Nevertheless, the chemical industry in collaboration with the Dutch government persistently strives to identify alternative solutions through which GHG emissions that are caused due to energy overconsumption can be reduced (Stork et al., 2018). Therefore, the challenge that managers confront, concerns the adoption of energy and resource-efficient technological practices that besides being environmentally and financially sustainable, add value to society.

To that direction, Life Cycle Thinking (LCT) can play a decisive role for the Dutch chemical companies to enhance their competitiveness and social image in terms of economic performance and environmental footprint. LCT is an approach of diagnosing and dealing with systemic problems by getting into the heart of the problem rather than providing short-term solutions to obvious inconsistencies (UNEP-SETAC Life Cycle Initiative, 2017). LCT is stimulated by the life-cycle sustainability assessment (LCSA) which is grounded on the three dimensions of sustainable development – environment, society and economy. The LCSA concept provides the framework through which companies can tackle core problems by assessing the environmental, social and economic impacts of their practices with the view towards the development of more sustainable products (Valdivia et al., 2013). As such, the Dutch chemical firms can be benefited by the use of the LCSA in order to come up with strategies focusing on the abatement of environmental burdens and costs that occur throughout the life-cycle of their production systems.

Within this framework, the Life Cycle Assessment (LCA) and the Life Cycle Costing (LCC) techniques can give precise information to the industry's managers about the environmental performance of the deployed production systems and the directions for their improvement. Both LCA and LCC are designed to serve different purposes. On the one hand, LCA's usefulness lies in its ability to track in a quantitative manner the environmental impacts that occur over a system's life-cycle and compare them with the environmental performance of other systems. On the other hand, LCC is an economic assessment tool for decision-makers to realize the internal and external costs and benefits that arise throughout the life cycle of a production system or a project.

1.2 Research problem

To fend off the probable adverse effects of climate change as well as the subsequent economic and social impacts, the Dutch chemical industry and in particular the chlorine manufacturing sector is required to take courageous decisions and change the way of processing, managing and exploiting natural resources. Given the high energy consumption of chlorine production systems, it is of paramount importance to thoroughly look at which technical solutions can improve current practices and raw materials' usage with a view to achieving a substantial decrease in GHG emissions. However, while the environmental performance of different alternatives is essential, it should not be the only criterion when it comes to deciding what corporate strategies to implement. In principle, every company strives to maximize its profits by adopting strategies that are anticipated to add economic value. Therefore, in order for the companies of this sector to be on an environmentally sustainable track while maintaining their market share and remaining profitable, it is rendered imperative not to confine relevant design decisions on a product's potential environmental impacts without taking into account its economic performance. As such, to be in line with the Dutch government's climate change targets while enhancing the strategic intent of the Dutch chlor-alkali firms, the present study revolves around the following research problem statement,

Problem Statement I: There is a need to identify the less environmentally-intensive and the most cost-effective technical solutions which can improve the overall enviro-economic performance of chlorine production systems.

Thus, to support decision-making under environmental context, it is required to deploy techniques through which the enviro-economic performance of chlorine manufacturing systems can actually be measured. To that end, the LCSA framework and the relevant life-cycle techniques can be used so that to measure the effects that different technical changes in chlorine production can bring on the overall enviro-economic performance of chlor-alkali plants. Both LCA and LCC techniques can be applied to conduct a multi-perspective comparative assessment of different chlorine manufacturing systems in order to identify which alternative can lead to the lowest environmental footprint and cost-intensity.

In principle, the LCSA allows organizations to examine the effects of their decisions and practices over their value chain by providing the conceptual framework to assess the sustainability performance of a system over its complete life-cycle. However, the LCA and LCC techniques differ regarding their level of maturity. Compared to the LCA technique which follows an ISO standard structure, the structure of the economic evaluation concept still lacks robustness and it is under construction and debate with respect to its scope and practicality when it is applied in environmental projects (Neugebauer et al., 2015).

UNEP-SETAC has provided the guidelines and the handbook for the step-by-step execution of an LCA analysis with a view to quantifying potential environmental burdens as a consequence of resources extraction, transportation, manufacturing, consumption and discarding of products. While at the other end of the spectrum, LCC epitomizes the scientific technique to measure the economic performance of a production system on a corporate level. However, until now it has been rigorously focused on providing private costs estimations (Hunkeler et al., 2008; Klöpffer & Ciroth, 2011; Swarr et al., 2011), thus, neglecting other aspects that are difficult to define in monetary terms (e.g. environmental damages) (Neugebauer et al., 2016).

Though there are several methods for the calculation of the financial life-cycle costs of a company's production system, such as the standard approach of the American Society for Testing and Materials (ASTM) (ASTM International, 2002), the scientific community has not yet reached a consensus about the inclusion of non-monetary aspects in the LCC technique. In particular, it still remains debatable which would be the most practical way to incorporate in the LCC structure costs estimates that concern changes in the availability and the quality of environmental goods (e.g. air quality). Hence, an emphasis should be placed on the alignment of the LCC with the LCA technique, which currently constitutes one of the major research themes of life-cycle scientists (Ciroth et al., 2011). To contribute to the scientific debate in regards to the expansion of the LCC scope, the present study attempts to tackle the identified research problem, stated in the following way,

Problem Statement II: There is a lack of consensus over how to convert environmental damages into monetary terms under the prism of the LCC technique.

Despite being debatable whether the LCC should remain restricted to financial costs estimations, a plethora of authors discuss the need for coupling the LCA with the LCC in a structured way (Gluch & Baumann, 2004; Norris, 2001; Zhang, Guo, Gu, & Gu, 2018). In line with the latter, several studies combining LCA and LCC in order to evaluate the ecological and economic performance of a product's or a system's life-cycle have already taken place (Bierer et al., 2015). However, a widely accepted scientific method for their integration with a view to using LCA results for providing environmental costs estimates has not been developed yet. The vast majority of the initiated methods until now are industry-specific, with the chemical industry witnessing the fewer endeavours (Auer, Bey, & Schäfer, 2017). In regards to the chlor-alkali industry, there is not yet a study attempting to merge these two techniques with a view to assessing the ecological footprint of the practices involved in chlorine production, as well as, to estimating the environmental costs of the identified impacts. Notably, the particular industry experiences a variety of published papers (Euro Chlor, 2013; Garcia-Herrero et al., 2017a, 2017b; Hong et al., 2014; Jung et al., 2014; Kätelhön et al., 2015; Lee et al., 2018) focusing on the quantification of the environmental impacts that come from the application of different electrolysis technologies, without providing neither an economic evaluation of the examined technologies nor environmental costs estimates.

To deal with environmental complex decision problems that influence the sustainable development of the Dutch chlor-alkali industry, besides the environmental impact assessment of chlorine production systems, the economic aspects either internal (operational costs) or external (environmental impacts) of the involved practices is imperative to be addressed. Therefore, taking into consideration the scientific debate for the alignment of LCA with the LCC as well as the fact that these two techniques have not been yet implemented on the Dutch chlor-alkali industry in an integrated way, the third research problem can be briefed as:

Problem Statement III: Lack from the academic literature of an enviro-economic assessment, based on LCA and LCC techniques, with the intention to solve complex environmental problems in the Dutch chlor-alkali industry.

1.3 Research objective

The objective of the particular research is to facilitate decision-making pertinent to complex environmental uncertainties that stem from chlorine production systems. Based on a case study that concerns Nouryon's chlor-alkali plant at Rotterdam, we aim to combine the LCA and LCC techniques to assess the enviro-economic performance of the particular chlorine manufacturing system. In line with that, we attempt to examine from a life-cycle perspective the environmental footprint and the associated costs of different technical modifications in the considered production system which can potentially improve its overall performance. To bridge the abovementioned scientific gaps, we further aim to contribute to the scientific debate regarding the expansion of the LCC's scope by aligning the latter with the LCA via the monetization of environmental damages.

As such, our intention lies in the quantification and comparison of the generated environmental impacts of chlorine (Cl_2) production alternatives due to heat and power consumption. The impacts are quantified with respect to two areas of protection and one impact category. The former includes impacts on Human Health (HH) measured in DALY/ ton Cl_2 and impacts on Ecosystems (EC) measured in species.year/ ton Cl_2 . On the other hand, impacts on climate change are calculated through the Global Warming Potential (GWP) impact category, i.e. kg of CO_2 eq. / ton Cl_2 . Moreover, cost estimations in regards to the operation of different alternatives and the subsequent impacts on the environment are provided. Therefore, by comparing the derived results we assess which production alternative can yield the best performance in regards to three dimensions – environmental impacts, environmental costs and the system's economic efficiency.

Hence, in light of the Dutch government's targets set for climate change mitigation until 2050, key technical modifications are pointed out with a view to enhancing the overall enviro-economic performance of the examined production system. The results of the particular analysis are anticipated to be the cornerstone for the industry's managers to take precautionary actions for emissions reduction due to energy overconsumption.

1.4 Research questions

To tackle the abovementioned challenges and trigger the Dutch chlor-alkali sector to counteract climate change effects by transitioning away from carbon-intensive practices, the particular thesis revolves around four major pillars:

- Aligning the LCA with the LCC on the basis of environmental externalities monetization
- Performing an enviro-economic assessment of different technical modifications in chlorine production systems
- Comparing the eco-profile of different technical alternatives for chlorine production in regards to impacts on the environment due to energy and raw materials consumption, the subsequent environmental costs and the economic efficiency of the overall system

- Recommending which technical modifications can potentially improve the enviro-economic performance of the considered chlor-alkali plant

In order to attain the research objective, the following research question is proposed. Consequently, the research question is further divided into five sub-questions to facilitate the research process.

«How to develop an enviro-economic evaluation method that integrates Life-Cycle Assessment & Life-Cycle Costing techniques and implement it on the Dutch chlor-alkali manufacturing industry?»

Sub-questions:

1. How to conduct a comprehensive enviro-economic assessment based on the LCA and LCC techniques?
2. What valuation methods can be used for the monetization of environmental damages and which are the most appropriate ones for life-cycle studies?
3. What are the most environmentally intensive processes in the considered chlorine production system and to what extent technical modifications affect the environmental profile of the system?
4. How do different technical modifications affect the economic performance of the considered chlorine production system?
5. What are the most cost-effective and the least environmentally-intensive technical solutions from a life-cycle perspective in regards to the considered chlorine production system?

1.5 Research methodology

The research methodology that this study follows to answer the above-mentioned questions is an amalgam of two approaches – the inductive and deductive. The inductive approach is suitable for answering the sub-questions 1 and 2. A critical literature review on the fundamental principles and the theoretical background of LCA and LCC as well as on the techniques and methods that can be used for the monetization of environmental damages is conducted. The scope of this process is to explore the linkages between existing theories, highlight their strengths and weaknesses and come up with empirical generalizations that will facilitate us to structure the steps of our analysis.

Thereinafter, a deductive approach is pursued to provide answers to the sub-questions 3 to 5. The aim of that process is the enviro-economic assessment of the considered chlorine production system in the Netherlands. The purpose of the assessment is to identify core inconsistencies of the system as well as which alternative technologies can yield the best enviro-economic performance that can potentially contribute to the energy transition of the particular industry. Figure 2 illustrates the research flow diagram of the present research study.

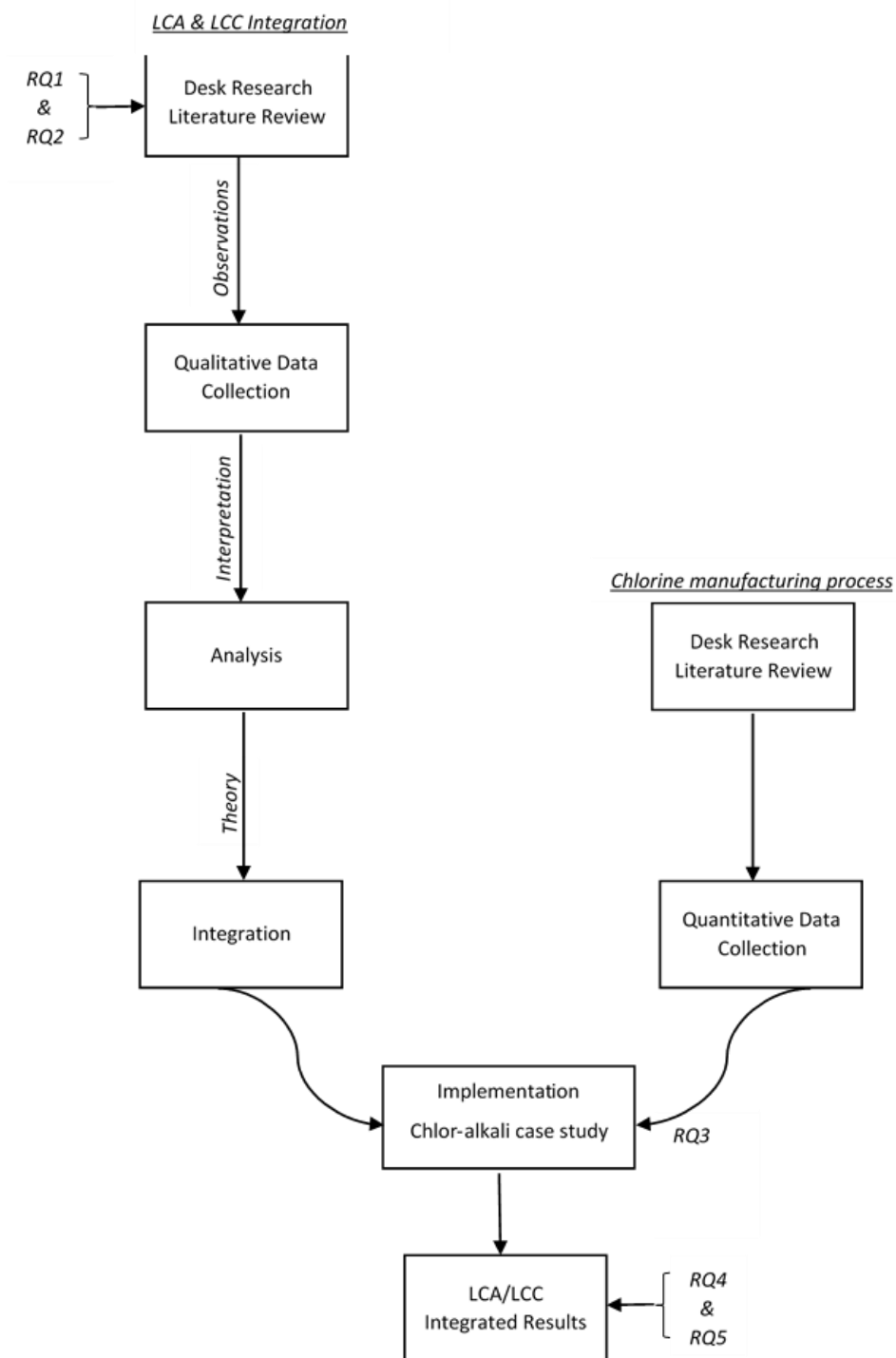


Figure 2: Research flow diagram

The environmental impact assessment concerns the quantification of the environmental damages from the application of different technologies for chlorine manufacturing. In regards to the LCA, the SimaPro software is used to calculate the relevant environmental loads. The environmental impact assessment analysis is executed according to the ISO 14040 and ISO 14044 standards. In order to determine the extent to which certain manufacturing sub-processes burden the environment, the ReCiPe impact assessment method is implemented.

The identification of the chlor-alkali processes that put pressure on the environment requires process-specific data. One part of the gathered data is from the thesis project *“The energy transition in the Dutch chemical industry”*, conducted by Scherpbier (2018), who modelled the material and energy inputs and outputs of the Dutch chlor-alkali industry. Moreover, data that concern alternative technologies and energy resources for the electrolysis process are collected from the literature. The latter requires a thorough literature review on alternative technologies that can be used to serve the same purpose, that of chlorine production.

The LCC analysis is executed in combination with LCA by quantifying internal costs (energy, raw materials) and external costs (environmental). The economic analysis is carried out by calculating the Net Present Value (NPV) of the identified costs within a certain time horizon. The particular economic index can be used to recognize economic inconsistencies in a system by accounting the time value of costs incurred over the life-cycle of a product with the use of appropriate discount rates. The economic analysis requires data about the energy and raw materials consumption as well as the results of the LCA. Moreover, the Euro-Stat Prodcom database and statistical information from the Central Agency of Statistics of the Netherlands (CBS) are exploited to collect economic data necessary for costs estimation.

1.6 Relevance of the study

1.6.1 Scientific and societal relevance

The outcome of this research is expected to add value to academia and society. To start with, the present study becomes relevant to the stakeholders of the Dutch chlor-alkali industry and especially to Nouryon’s technology managers by bringing in light valuable insights about the pivotal paths of transitioning away from fossil-fuel dependency. To be in line with our aim, we seek to contribute to Nouryon’s potential energy transition by highlighting which technologies can play a crucial role in the reduction of GHG emissions while enhancing its financial sustainability. For this, site-specific data are used to assess and compare the environmental and economic profile of different alternatives for chlorine production at Botlek, so that to shed light on where we are now in terms of life-cycle performance and where we can be in the future. To that end, the evaluation of which technology alternative could yield the best environmental-economic performance is anticipated to support strategic planning for the development of carbon-free products and services. Hence, the final results of the study are provided with the wish to make a positive impact on Nouryon’s future considerations towards sustainability.

Moreover, this project is in consonance with society’s interest since it contributes to identify issues of social importance and make recommendations for their improvement. Being aware that fossil fuel-dependent industrial activities lead to the gradual deterioration of the environment and quality of life, we strive for coming up with technical solutions whose implementation will decrease negative impacts on human health and ecosystems. Lastly, this research is anticipated to contribute to attaining the *GOAL 13* of the United Nations Association, which calls for a global collective action to prevent climate change effects and head for a low-carbon economy (United Nations, 2018).

From a scientific perspective, this study intends to contribute to the academic literature by tackling the above-mentioned research problems (section 1.2) and bridging the pertinent knowledge gaps. Though the parallel application of LCA and LCC has gained some prominence

in academia as the scientific way for assessing environmental and financial inconsistencies over a system's life-cycle, their integration still lacks a robust methodological structure. In this regard, it still remains questionable whether the scope of LCC should be expanded so that to be aligned with the LCA technique. A reason for this is that the scientific community has not yet come to a consensus on which is the most scientifically sound and practical way to translate the results of LCA into monetary terms in order to be addressed as an additional component to the LCC assessment. To that end, the present study is engaged in the scientific debate on the application of the LCA and LCC by proposing an approach for their integration on the basis of using the results of the former as inputs to the cost calculation methodology of the latter. The scientific contribution of this research is materialized through the implementation of the findings on Nouryon's chlorine production plant in the Netherlands (Botlek) with a view to assessing the enviro-economic performance of the specific manufacturing system. In particular, the combined application of the LCA and LCC techniques to this specific country and industry is absent from the academic literature, which contributes to this project's scientific relevance.

1.6.2 Relevance to the MoT programme

The Management of Technology (MoT) programme provides deep knowledge on how to manage technology as a corporate resource, develop products that meet customers' needs and increase corporate productivity and profitability in a highly complex and competitive environment. Its main objective is to prepare the future managers, consultants and entrepreneurs to deploy the appropriate strategies and make the right decisions as a response to social, technological and economic changes. To that end, the University of TU Delft has set three axes on which the MoT students should ground their thesis project. Based on the later, the present study corresponds to the MoT requirements in the following ways:

- ✓ "The work reports on a scientific study in a technological context"

The present study uses the case of Nouryon's chlor-alkali plant at Botlek to identify environmental and economic inconsistencies that are associated with the currently employed technologies for chlorine production. Consequently, the nature of this project is inherently based on a technological context since its aim is to assess, report and come up with technological solutions that will strengthen the company's ecological footprint and financial sustainability by tackling the system's energy overconsumption and reducing its negative environmental impacts. To accomplish our goal, initially, a comprehensive literature review on different technological components or concepts linked to chlorine production is conducted. Then, the found technologies are assessed according to three criteria which correspond to the associated environmental impacts, environmental costs and the system's overall economic efficiency. As such, the results of this study are anticipated to support Nouryon's decision-making in environmental context and draw the direction towards energy transition.

- ✓ "The work shows an understanding of technology as a corporate resource or is done from a corporate perspective"

The orientation of this study is company-centered. Precisely, the focal point of the analysis concerns the chlorine production system of Nouryon in the Netherlands. By and large, chlorine manufacturing requires extremely high amounts of energy and raw materials which consequently puts the environment on pressure. Being the market leader in the Dutch chlor-alkali industry, Nouryon has the power to initiate strategies

towards sustainable development and cause a domino of positive effects on the whole industry. From a technology perspective, the present study attempts to identify how different technical modifications in chlorine production can lead to less environmental impacts and costs and increase the economic efficiency of the overall production. To do so, we wish to expand the current knowledge frontiers by assessing the sustainability dimensions of state-of-the-art technologies from a life-cycle perspective. As such, being in line with the aim of TU Delft for knowledge exchange we perceive this study as the breeding ground for Nouryon to exploit the created knowledge body as its primary resource for sustainability and competitive advantage.

- ✓ “Students use scientific methods and techniques to analyze a problem as put forward in the MoT curriculum”

Key theoretical notions and practical knowledge gained from the MoT programme were used to facilitate the research process of this thesis. The following list provides an overview of the MoT courses and their relevance to the present study.

- **MOT2312 Research Methods:** Approaches for conducting scientific research, Interview structure
- **MOT1435 Technology, Strategy & Entrepreneurship:** Technology strategy, Strategic Intent development, Sustainable competitive advantage
- **MOT1461 Financial Management:** Financial Accounting tools (e.g. NPV)
- **SPM9730 Sustainable Innovation & Transitions:** Technology implementation in a socially responsible way
- **SPM9239 Responsible Innovation:** Corporate and social values incorporated in the technological design
- **SPM9716 Cost-Benefit Analysis:** Evaluation of environmental projects from a public and corporate perspective, Calculation of current and potential gains and losses of a project to determine whether its implementation adds value to the engaged actors

1.7 Report structure

In the next chapter, a detailed literature review is conducted to comprehend the core concepts applied in this study. The key aspects, meanings, and applications of the LCA, LCC, and methods for monetizing environmental impacts are provided.

In the third chapter, an overview of the European and the Dutch chlor-alkali industry is given. To start with, the functionality of chlorine production systems along with a description of the electrolysis process is displayed. Then, the focus is concentrated on the membrane electrolysis technologies and the different configuration types that can be implemented. Consequently, European and Dutch chlorine-chains are outlined.

Subsequently, the followed methodology is described in the fourth chapter. Initially, the phases of the enviro-economic assessment are displayed. Secondly, a thorough description of the considered technical modifications (scenarios) compared to the reference case takes place. Then, the inventory lists of the LCA and LCC consisting of the used energy, material and economic data for each scenario are provided.

In the fifth chapter, the results of the enviro-economic assessment distinguished in regards to the identified environmental impacts, the extent of the environmental costs and the operational costs of each scenario are presented. Then, the results are interpreted in the sixth chapter. Firstly, in this chapter, the results of the analysis are compared to other relevant studies. Next, the contribution of each process to the overall impact along with a discussion about the relevance of the used monetization models takes places. Thereinafter, chapter 7 encapsulates the answers to the posed research questions and therefore the conclusions of the study. Finally, our recommendations for the improvement of the considered chlorine production system are presented. In addition to the latter, the last chapter also includes the limitations of the study as well as the directions for future relevant research.

Chapter 2: Theoretical background

2.1 Life-cycle assessment

2.1.1 Structure

Life cycle assessment (LCA) is a well-established standard technique, developed to estimate the environmental burdens of a production system. Its aim is the tracking and quantification of the environmental impacts of a product or service over its complete life cycle, taking into account the additional burdens that emerge from materials or energy flows within certain production processes (de Bruijn, van Duin, & Huijbregts, 2002). According to the standards ISO, LCA is defined as the “compilation and evaluation of the inputs, and potential environmental impacts of a product system throughout its life cycle” (ISO 14040, 1997). That implies the identification of all the environmental implications of a product’s manufacturing process from raw material extraction, its consumption/use to the final disposal. LCA follows ISO 14040 and ISO 14044 standards. In line with that standards, it is structured into four phases: (i) goal and scope definition, (ii) inventory of inputs and outputs, (iii) impact assessment and, (iv) interpretation of results (ISO, 2006b). Figure 3 illustrates the structure of the LCA according to the ISO standards.

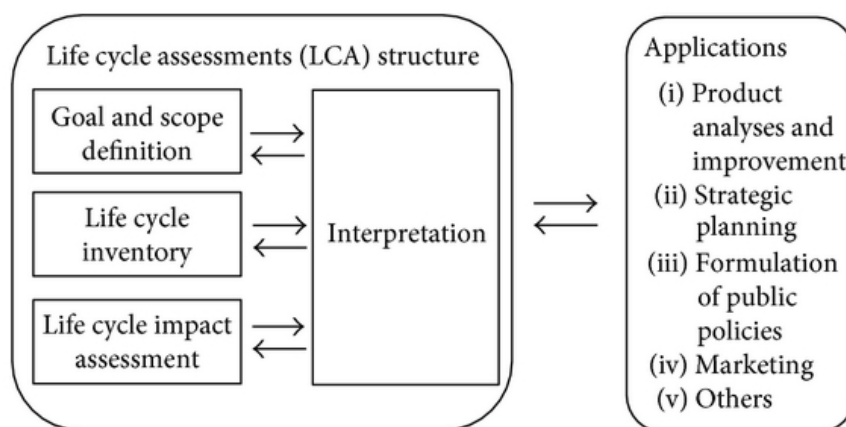


Figure 3: The structure of Life Cycle Assessment (ISO 14040, 1997)

The goal and scope definition is the initial stage of carrying out an LCA analysis. This phase facilitates the simplification of all complex processes that take place within a system and encompasses the purpose, intention and the audience of the study as well as a precise description of the functioning of the system and the involved processes. The latter aims to the restriction of the assessment by clearly defining the functional unit of analysis and establishing the appropriate system boundaries (ISO, 2006b). The functional unit needs to be as precise as possible, especially when the scope of the analysis is to assess and compare the magnitude of the environmental burdens that are associated with the life cycle of a product, process or entire systems. The system boundaries frame all the material and energy flows that can be found in the production system under investigation. The limits of the system may vary, from cradle to grave i.e. from the raw material extraction to the product’s final disposal and even

back to cradle again, to gate-to-gate, which is a partial LCA analysis of specific processes within a system (Horne, Grant, & Verghese, 2009).

The formation of the Life cycle inventory (LCI) constitutes the second phase of the LCA's ISO structure. One could argue that it is the most demanding task when executing an LCA since it requires the development of an environmental model tailored to meet the set goal and scope of the study. This phase includes data collection pertinent to the inputs (material and energy) and the outputs (final products) of the examined system (Horne et al., 2009). Specifically, it concerns a thorough accounting of all flows going in and out of the system boundaries consisting of data regarding energy (by type), raw materials and water consumption as well as relevant emissions to the environment.

All data related to emissions, raw material and energy usage are grouped into categories, known as impact categories, which consist of relevant impact indicators. With respect to the implemented impact assessment method, the impact categories can be divided into midpoint and endpoint ones. The midpoint categories comprise indicators for the quantification of single environmental problems. Their aim is to indicate how fluctuations in the concentration of certain substances affect specific environmental themes such as climate change, water use, acidification etc., (e.g. how rises in CO₂ emissions contribute to Global Warming). On the other hand, endpoint indicators include the major issues of concern, the so-called areas of protection (e.g. human health, biodiversity, etc.), where environmental impacts are aggregated at a higher level (Fokaides & Christoforou, 2016). Hence, all data that delineate a product's life-cycle can be grouped in the LCI and then further processed in the third phase of the LCA structure, i.e. the life-cycle impact assessment (LCIA) (Jolliet et al., 2003).

The LCIA phase is responsible for translating the analysed flows of the LCI into environmental impacts. In line with the ISO standards, the LCIA concerns the quantification of the overall environmental burden of energy and resources consumption as well as process-specific emissions of the system's life-cycle (ISO, 2006a). Thus, the impact assessment facilitates the analyst to comprehend which are the hot-spot processes and the major factors within the studied system that evoke damages to the environment. LCIA can be executed by implementing various methods. The vast majority of these methods operate at midpoint and endpoint level. For instance, the Eco-indicator 99, the Impact 2002⁺ and the ReCiPe LCIA methods consist of three major issues of concern – human health, ecosystem quality and resources – to which the identified environmental impacts are attributed. In addition to the latter, the ReCiPe incorporates eighteen midpoint indicators in its method, which are closely related to those of the CML Baseline impact assessment method (Centre for Environmental Sciences – Leiden University) (Fokaides & Christoforou, 2016). Some examples of that midpoint impact indicators are the global warming potential (GWP), acidification, ozone-layer depletion, eutrophication, photochemical oxidant formation, the impact of land use and human toxicity. Figure 4 gives an example of the midpoint and endpoint indicators that can be included in a life-cycle study. The illustration is based on the structure of the ReCiPe LCIA method (RIVM, 2018).

Consequently, during the last phase, the results are interpreted with respect to the goal and scope of the study, focusing on providing a clear view of the identified discrepancies of the analysed system. Moreover, in the interpretation phase, recommendations that will enhance the sustainability performance of the system are usually given.

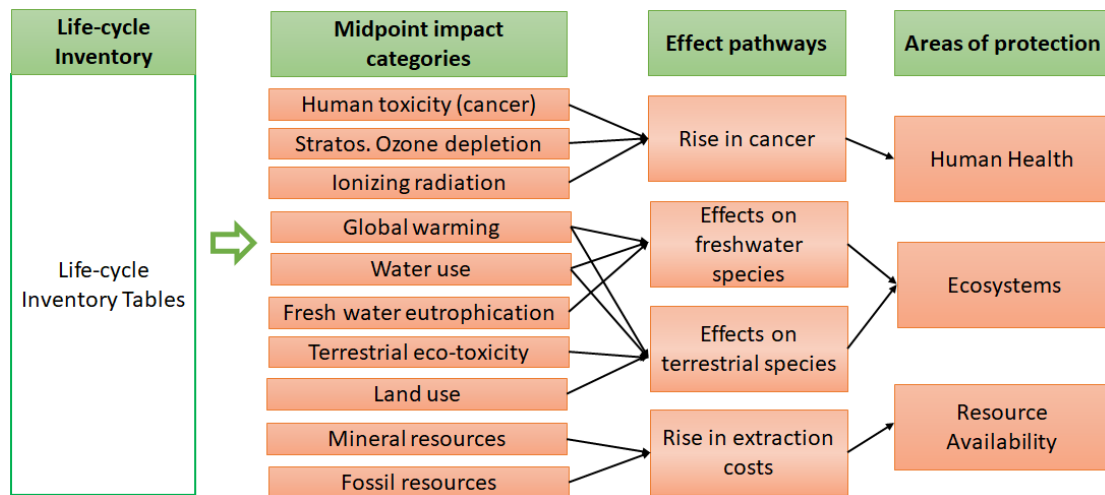


Figure 4: An illustration of midpoint and endpoint indicators based on the ReCiPe model (RIVM, 2018)

To derive sound results during the LCIA phase, two mandatory and two optional consecutive steps are recommended to be pursued – classification, characterization, normalization, and weighting. All steps that correspond to the provided ISO structure of LCA are shown in Figure 5. According to Golsteijn (2014), the features of the four steps within LCIA concern the following:

1. Classification

The sources (chemical substances) of emissions and resource uses are grouped into categories, either at a midpoint or endpoint level, depending on the impact they cause on the environment.

2. Characterization

Characterization factors are used to calculate the relative importance of certain substances. To that end, by multiplying the volume of chemical substances with a relevant factor of characterization, it is feasible to measure the severity of the substance within each impact category. For example, how much 1 kg of CO₂ contributes to the Global Warming impact category?

3. Normalization

The scores of each impact category are analyzed in regards to a certain reference value. That facilitates the comprehension and interpretation of impacts by simplifying the scores of LCAs. A reference value can be the average CO₂ emissions per Dutch citizen per year. Therefore, each impact category is compared to that reference value and the final outcomes are expressed into fractions.

4. Weighting

Its aim is to provide analysts with one aggregated single score of the environmental impacts that certain activities cause. By using value choices as weighting factors, the results from the normalization stage of each impact category are translated into single scores of the same unit, thus, allowing for their integration.

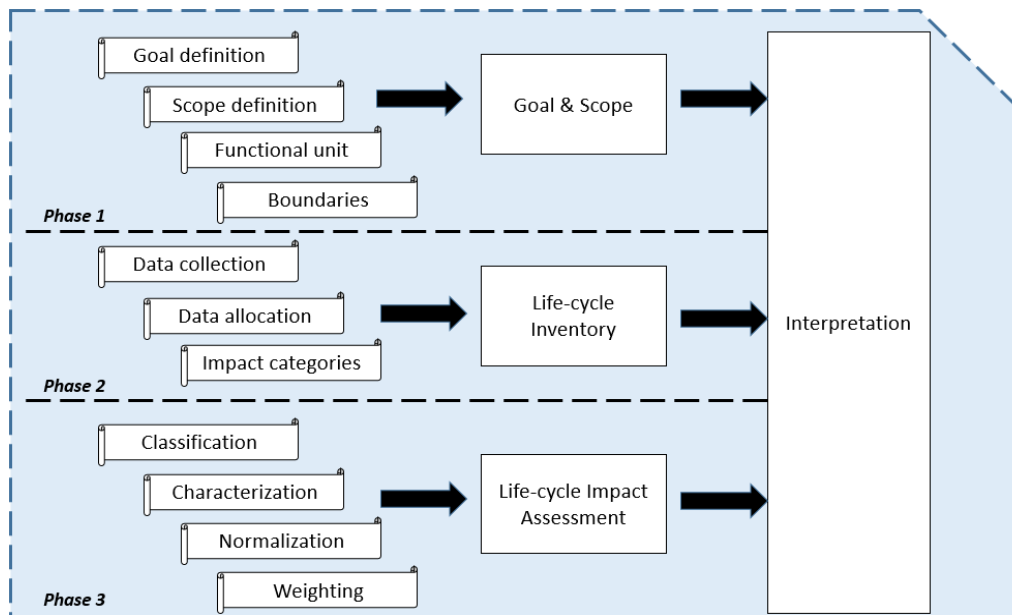


Figure 5: The phases and the subsequent steps of LCA

2.1.2 Limitations of LCA

LCA's scope is limited to the quantification and evaluation of environmental impacts. Decisions for action in a corporate environment such as costs and benefits are not considered by LCA. While the results of an LCA study are used to support decision-making for improving a system's environmental inconsistencies, this approach neglects to regard any economic aspect relevant to the analysed system or the proposed alternatives. Furthermore, internal and external costs, revenue streams and risk of investments are not addressed by LCA. Hence, the shortcoming of the LCA technique to incorporate product performance and economic indicators can be interpreted as "unilateral in nature", prone to a misguided analysis. To that end, an exhaustive analysis that combines LCA with other techniques that focus on the economic aspects of a product/process seems to be necessary for rational decision-making.

2.2 Life-cycle costing

Along with LCA, LCC also belongs in the group of the sustainability assessment techniques of the LCSA framework. LCC is an economic assessment technique appropriate for cost-oriented decision making and the selection of the most cost-efficient alternative. As it is illustrated in Figure 6, LCC has a cost-evaluation scope, concerning the estimation of the overall costs that take place over the complete life cycle of a product, from manufacturing to use, maintenance and disposal (Rebitzer & Hunkeler, 2003). By and large, LCC was developed to address all private costs involved in a production system and impact the financial performance of a company. According to ISO (2017), LCC is "a technique which enables comparative cost assessments to be made over a specified period of time, taking into account all relevant economic factors both in terms of initial costs and future operational costs".

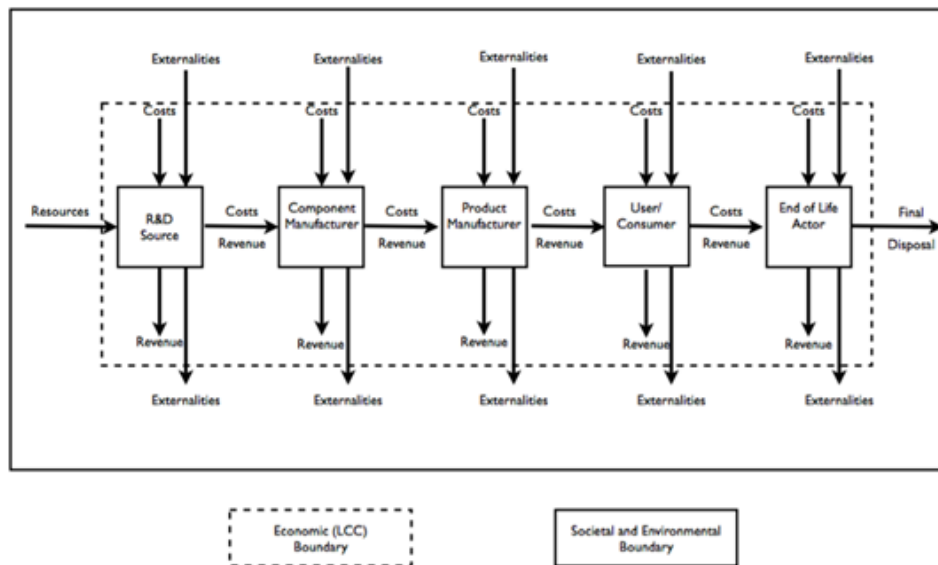


Figure 6: An illustration of LCC's conceptual framework (Rebitzer & Hunkeler, 2003)

2.2.1 Types of life-cycle costing

There are three distinct LCC types – conventional LCC, environmental LCC and societal LCC (Swarr et al., 2011).

- *Conventional LCC (cLCC)*: is an economic assessment approach that concerns the calculation of the internal costs occurred over the life cycle of a product, attributed to the producer or the final user. Usually, use or end-of-life costs are neglected since they are related to other actors' activities. Its linkage to LCA is negligible.
- *Environmental LCC (eLCC)*: the particular approach epitomizes LCA since it encompasses the environmental costs computed through the LCA technique. The environmental LCC takes into account all the internal and anticipated external costs occurred over the complete life cycle of a product, that are attributed to the actors involved in each stage of its life cycle.
- *Societal LCC (sLCC)*: this method evaluates from a society's perspective all the internal and external costs occurred or anticipated to occur within the life cycle of a product.

Each type of LCC includes specific indicators – financial, environmental, or social ones, which are not intertwined with each other. Consequently, the economic performance of a system is analyzed from a certain angle. That restricts the economic analysis since the implementation of a particular LCC-type implies that some other aspects would be left out of the evaluation scope.

Considering that the LCC technique is frequently used to stimulate environmental decision-making by comparing the economic sustainability of products and processes, it is reasonable to be aligned with pure environmental tools such as LCA. In principle, only the eLCC type is highly compatible with the LCA since the results of the latter can be used as inputs to the eLCC approach for the identification of the socially "hot-spot" processes that may affect the performance and image of an organization (Biernacki, 2015; Hunkeler et al., 2008). In a general sense, eLCC allows the internalization of the environmental or social costs that are not directly generated by the main actors involved in a production system (Hunkeler et al., 2008). To that end, its aim is to relate life-cycle costs to environmental impacts and manage costs in a

sustainable manner for future development. As such, the eLCC cannot be seen as an independent technique but to be regarded as a supplement of an LCA analysis. In that sense, they complete one another (Biernacki, 2015). On the one hand, the LCA can produce information about a system's environmental footprint, which is of vital importance when it comes to deciding among different alternatives. While on the other hand, the produced information of an LCA study can be exploited by the eLCC technique to provide environmental costs estimates. For this reason, Biernacki (2015) suggests that both techniques should be implemented together following the ISO structure of LCA.

However, the most debatable issue with respect to the combined application of LCA and LCC regards the methodological approach that life-cycle analysts will follow to calculate costs that correspond to changes in the availability and the quality of non-market goods affected by the LCA-measured environmental impacts. Until now the scientific community has not yet reached a consensus on which is the most practical and robust way to align the results of an LCA analysis with the LCC in order to ease the conversion of the identified environmental damages into externalities costs (Ciroth et al., 2011; Neugebauer et al., 2016). That has led scholars to suggest the use of various decision-supporting tools such as cost-benefit analysis and cost-effectiveness analysis as well as economic valuation methods in order to express LCA results in monetary terms. Relevant examples are accessible in the scientific literature (Y. Dong et al., 2019; Hunkeler et al., 2008; Huysegom et al., 2018; Reich, 2005).

An additional issue with respect to the application of eLCC concerns its scope of analysis. By definition, eLCC's scope does not allow for comprehensive decision-making since it neglects to address the internal costs of a production system such as technical and operational costs (energy demand, raw material expenditures). However, Hunkeler et al., (2008) suggest that the eLCC approach can be used for the monetization of environmental damages in addition to the private costs of a production system, which are typically within cLCC's scope. Figure 7 shows the scope of each LCC type and the costs that it takes into account. The dotted rectangle represents Hunkeler's et al., (2008) recommendations for merging the cLCC and eLCC types.

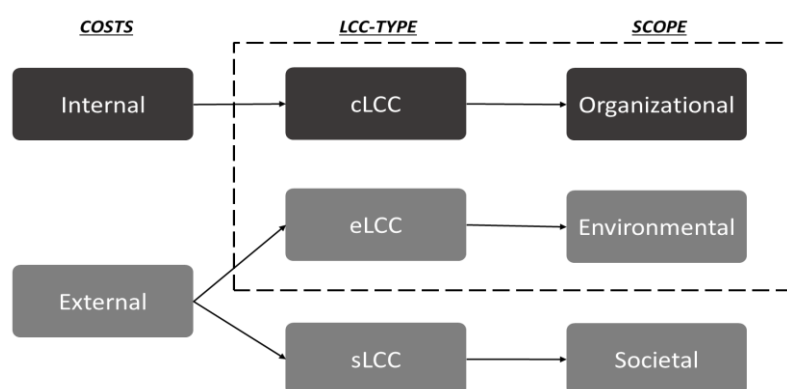


Figure 7: Scope of LCC-types (Hunkeler et al., 2008)

2.3 LCA and LCC integration issue – challenges and trends

In general, LCC's origins stem from the neoclassical economic theory. In consonance with this theory, all firms strive for profit maximization while having perfect information about the market's condition. Moreover, each individual within the market has consistent preferences

and is aware of any other available options (Gluch & Baumann, 2004). To that end, assuming that there is no information asymmetry, it stands to reason that every decision-maker is in a position to know a priori the reverberations and the results of choosing each alternative. Thus, this entails that they adopt rational behaviour when it comes to deciding among alternatives that are expected to bring negative consequences. However, due to the inherent uncertainty and complexity that characterizes decision-making in an environmental context, it is difficult to value all possible consequences in the long-run and estimate the economic impact of their occurrence. Consequently, a decision-maker confronts the following difficulties with respect to the implementation of an LCC analysis (Gluch & Baumann, 2004):

- Make rational decisions due to high uncertainty and information asymmetry
- Translate environmental impacts into monetary terms
- Value goods without an owner (air, water, etc.)
- Attribute environmental costs occurred today to future generations

The abovementioned challenges have led several authors to discuss the importance of establishing a standardized methodology for the integration of LCA and LCC (Gluch & Baumann, 2004; Norris, 2001; Zhang et al., 2018). In line with that, Norris (2001) acknowledges that an integrated life cycle evaluation can enhance the reliability of decision-making process, increase the probability of identifying the most cost-effective ways for environmental improvements and facilitate an organization to remain financially and environmentally sustainable. Nevertheless, due to the absence of a standardized methodology for their coupling, LCA and LCC are usually executed autonomously, and then the distinct evaluation results are combined. According to Meynerts et al. (2017), there is a series of problems that emerge from the separate application of both techniques such as data gathering, discrepancies and loss of significance. Consequently, there is a high chance for providing recommendations that eventually may be rendered either environmentally unfriendly or economically unfeasible.

Besides the very extensive scientific literature regarding LCA and LCC's standalone application, their integration issue has gained some prominence in academia during the last two decades. Recognizing the potential benefits from their combined application, a plethora of studies assessing the life-cycle related environmental and economic performance of industrial production systems do already exist (Bierer et al., 2015). However, the vast majority of the initiated studies that intend to merge LCA and LCC are usually more focused on one part of the assessment.

As it was highlighted by Bierer et al. (2015), the existing integrated life-cycle studies can be clustered in three main categories. The first one concerns the parallel implementation of both techniques and it is divided into two sub-groups. The first sub-group encompasses the studies where LCA and LCC are carried out autonomously, with different goal and scope definition, systems boundaries as well as database. The second group concerns the so-called eco-efficiency studies. In these studies, LCA and LCC share the same system boundaries and time-scales with a view to merging the final results. The second category consists of studies where cost-oriented aspects are defined as additional economic impact categories to those ones of the LCA technique. In this case, the environmental impacts are analyzed and interpreted from

an economic perspective. However, in most of the studies of this category, the procedure followed for cost estimations is not explicitly determined. Lastly, the final category encapsulates studies where LCC's fundamental principles are applied to calculate costs associated with a production system. This cluster of studies is overwhelmingly concentrated on the economic aspects of a system. Usually, they neglect to describe and explain the found environmental impacts, thus, leading to an erroneous interpretation of the results. In most cases, the environmental impacts associated with the analysed production system are not clearly specified. Their goal is primarily cost-oriented.

An additional characteristic of the above-mentioned studies is that the followed procedure to integrate LCC in LCA is tailored to meet the standards of specific industrial applications. The water and building construction industries, as well as the waste treatment sector, possess the largest number of relevant works (Petit-Boix et al., 2017). On the contrary, there is a scarcity of publications integrating ecological and economic assessment in industrial manufacturing systems and especially in the chemical industry (Auer et al., 2017). As far as the chlor-alkali industry is concerned, an integrated analysis that evaluates from both perspectives the chlorine production system is absent. LCA studies assessing and comparing the environmental profile of different technologies engaged in chlorine manufacturing, such as mercury, diaphragm, membrane and ODC (oxygen-depolarized cathode) do already exist (Euro Chlor, 2013; Garcia-Herrero et al., 2017a, 2017b; Hong et al., 2014; Jung et al., 2014; Kätelhön et al., 2015; Lee et al., 2018). However, the combined application of the LCA and LCC techniques in the particular industry is currently missing from the pertinent life-cycle literature.

2.4 Methods for monetizing environmental impacts

An additional decision supporting tool that can be implemented in an environmental context is the “cost and benefit analysis”, aka CBA. In general, CBA appraises the socio-economic value of the overall effects of a policy/project/action to the community at large by calculating a single socio-economic indicator, i.e. net social benefits, which equals the social benefits minus the social costs (Boardman, Greenberg, Vining, & Weimer, 2017). A certain application of CBA is the environmental CBA which concerns the economic evaluation of projects with a view to enhancing environmental services or actions that potentially might exert pressure on the environment as indirect consequences of human activities (Atkinson & Mourato, 2008).

For the monetization of environmental impacts, environmental CBA is based on the fundamental principles of willingness-to-pay (WTP) which aids the analyst to assign economic values to goods and services that are not traded in markets (e.g. air, life and etc.). The WTP principle refers to a “ceiling price” that a consumer is willing to accept and pay for purchasing an additional unit of a product or service so that to increase their utility consumption. Therefore, prices of non-market goods are subjective since they depend on people's preferences and their social values. The WTP principle is suitable for estimating and valuing environmental costs from adverse environmental effects. To that end, two distinct approaches can be found that might ease the monetization of environmental impacts – the equivalent variation and the compensating variation (Venkatachalam, 2004).

The equivalent variation:

Individuals' willingness-to-pay to *prevent* a future welfare loss from taking place as a result of the negative consequences that certain activities may bring on the environment. For instance, the environmental cost of a project that is expected to cause deforestation is people's WTP to avoid impact take place.

The compensating variation:

Individuals' willingness-to-*accept* compensation due to probable welfare loss as a consequence of negative environmental impacts. For instance, the environmental cost of a factory that pollutes and degrades the quality of living in a habitable area is the level of compensation that residents are willing to accept for their relocation.

A wide range of monetary valuation methods that are based on WTP and WTA principles exist and can be used to strengthen decision making. Monetary valuation is a practice of assigning economic values to market and non-market goods, thus facilitating the conversion of social or environmental impacts into monetary terms. It seeks to provide the level of economic price that people are willing to pay or be paid for restoring or accepting changes in the availability and the quality of goods that are free of access (Pizzol, Weidema, Brandão, & Osset, 2015). In line with the latter, in welfare economics relative changes evoked by social and environmental impacts are directly connected to the notion of externalities. Externalities is a market failure that occurs as a consequence of the economic activities of one party that affect the welfare of another either positively (gains) or negatively (loses) (Pearce & Barbier, 2000). When the point of central focus is on determining the non-compensated costs and benefits incurred by environmental impacts, then environmental externalities come into play. To amend market failures, it is required to internalize the externalities and find ways that guarantee the compensation of public or private actors. However, the internalization of environmental externalities within the economic system is not trivial since their quantification process is mainly subjected to people's preferences and behaviour. This is where monetary valuation methods can play a crucial role and stimulate decision making. Pizzol et al., (2015) distinguish five approaches in regards to their core principles for the classification of existing monetary valuation methods for marketed and non-market goods.

<u>Observed preferences:</u>	Consumers' WTP for purchasing a market good whose marginal value is expressed by its market price.
<u>Revealed preferences:</u>	Consumers' WTP for purchasing complement or substitute goods in surrogate markets as a consequence of variations in the availability and quality of a non-market good.
<u>Stated preferences:</u>	Directly asking consumers' WTP for purchasing goods whose market price is inappropriate or WTA compensation due to environmental impacts in hypothetical trade-off situations.
<u>Budget constraint:</u>	Individuals' WTP based on their average annual income as the maximum amount of money that can spend for gaining an additional Quality-Adjusted Life Year (QALY) assuming no externalities.

Abatement cost: Costs for reducing or preventing negative effects from impacts on non-market goods.

Table 1 classifies the existing monetizing methods in accordance with the aforementioned economic valuation approaches. A concise description of each method along with an example is provided. Afterwards, a thorough analysis will take place in the following subsections.

Table 1: Approaches and methods for monetizing non-market goods (Pizzol et al., 2015)

Approach	Method	Description	Example
Observed Preferences	Market Prices	Changes in the market price of an environmental good reflect its value	The market price of soil
Revealed Preferences	Averting Behavior	Individuals' expenditures for market goods as an action to prevent or mitigate environmental deterioration before it takes place	Expenses made for buying bottled water due to the river's contamination
	Travel Cost	Indirectly calculating the value of a non-market good by estimating individuals' full travel expenditures for getting access to it	The travel costs, fees and time spent for visiting the Parthenon (Athens)
	Hedonic Pricing	Fluctuations in the market price of a commercial good as a consequence of changes in the quality features of environmental goods	The difference in the market prices of a house next to the coastline and one's next to a chemical factory
Stated Preferences	Contingent Valuation	Estimating the value of a non-market good by directly asking individuals' WTP or WTA compensation when the quality and availability of the good has changes	Individuals' WTP to clean up the lake
	Choice Experiments	The value of a non-market good is determined by individuals' choices between hypothetical settings of a plethora of alternative attributes for the specific good	Respondents' preferences on the utility of water – e.g. drinking water, water sports, agricultural activities
Budget Constraint	Budget Constraint	The average yearly earnings per capita represent the highest amount of money individuals can spend for sustaining an additional life-year of absolute well-being with no externalities	Income spent on sustaining well-being
Abatement Cost	Marginal Abatement Cost	The costs of the precautionary actions needed for offsetting or mitigating environmental damages reflect the value of environmental goods	Future costs of maintaining buildings and statues due to the effects of acid rain
	Replacement/Mitigation/Prevention Costs		

2.4.1 Market prices

The level of supply and demand of a good determines its value. Changes either from the supply side or the demand side affect the price of a good. A core reason that can influence the supply

and demand of a market good is its exposure to environmental threats, such as air pollution. To that end, by observing changes in the prices of private goods affected by environmental damages, the costs to restore environmental deterioration can be determined.

2.4.2 Averting behaviour method

The averting behaviour or averting expenditures method is a monetary valuation method based on the consumers' revealed preferences approach. When people are exposed to threats of every kind they usually take a preventing course of action to protect themselves from possible hazards. When it comes to threats such as pollution, environmental catastrophes and other relevant hazards, people will adopt a defensive behaviour with the prospect that the benefits from their stance will exceed future costs. In welfare economics, the latter refers to the households and producers' averting behaviour which encompasses their WTP to prevent or mitigate environmental deterioration before it takes place. Individuals' averting behaviour indirectly reveals how much they value a non-market good as a consequence of their expenditures made in surrogate markets. That expenditures reflect on their WTP to prevent or counteract environmental risks (Pizzol et al., 2015).

2.4.3 Travel cost method

Individuals' revealed preference to spend time and money on visiting a site for recreational purposes it is linked to the travel cost valuation method. It is a way to indirectly calculate the implicit price that households place on accessing environmental or cultural services by observing their full travel expenditures incurred per visit (Pizzol et al., 2015). Therefore, the value of non-market goods such as forests, national parks etc., can be estimated through the time and travel expenses of individuals for getting access to them. By and large, the particular method is appropriate for estimating costs and benefits due to variations in the provision of environmental services. However, it is restricted to counting use values of environmental goods, thus neglecting non-users' preferences. Furthermore, additional expenses for purchasing complementary goods required for visiting an environmental site are out of its valuation scope (Bann, 2002).

2.4.4 Hedonic pricing method

Individuals make certain decisions based on their interests and perceptions about what can potentially bring them joy and pleasure. As such, when it comes to their consuming behaviour they reveal their preferences by purchasing goods whose attributes can add value to their way of living. For instance, an individual will probably choose to pay more in order to locate his house in a clean and nice environment instead of a polluted area. Therefore, it stands to argue that the attributes of a good have implicit prices whose aggregation with the actual price of the good compose its total price. The method of monetizing the implicit values that make up the final price of a market good is known as hedonic pricing method. Based on this method, the value of non-tradable goods (e.g. the quality of the natural ecosystem) can be indirectly measured in the overall price of commercial goods. Hedonic pricing finds its common application in environmental services in surrogate markets such as that of the real estate market (Czembrowski, Kronenberg, & Czepkiewicz, 2016). Holding every other factor constant, the implicit values of environmental features can be derived by comparing properties with similar attributes that otherwise would have no difference in their prices (Bann, 2002). Hence, the observed variation in prices demonstrates individuals' WTP for ensuring environmental quality.

2.4.5 Contingent valuation (CV) method

Through the contingent valuation method, the value of non-tradable goods can be estimated by directly asking individuals to express their maximum WTP or WTA compensation when the quality and availability of the good has changed. Frequently, it is applied under the context of environmental CBA or environmental impact assessment in order to draw inferences on individuals' choices for the provision of environmental goods and services (Venkatachalam, 2004). The main technique to elicit individuals' preferences is via surveys. Respondents are directly asked to state the degree to which are willing to pay or being compensated for an environmental attribute such as the reduced risk of water contamination or cleaner air. Commonly, they have to prioritize a series of options in hypothetical situations and money transactions. To that end, non-market goods' value can be directly derived by ranking the gathered responses. However, the creation of a hypothetical market without respondents' actual economic commitment can lead to bias since they might either overvalue or devalue such goods. In addition to the latter, the generalization of the results of a CV analysis is precarious especially when it comes to comparisons of similar burdens between different groups in society (Boyd & Banzhaf, 2007). Snowball (2008) acknowledges that respondents whose answers are based on hypothetical situations may inflate their WTP for a non-market good because of two reasons,

- *Adopting free riders' behaviour:* in hypothetical scenarios where there is no possibility for individuals of paying for a non-market good they can glibly overstate their preference value so that to secure its provision
- *No budget constraints:* In ideal situations, individuals tend to make positive decisions towards a non-market good without taking into account other factors that under real circumstances would have affected their choices. A factor that is deliberately disregarded and affects the validity of the CV method's results is the budget. Therefore, the valuation process is prone to inaccuracy.

2.4.6 Choice experiment (CE) method

Choice experiments are part of the stated preference valuation methods. Likewise in the CV, the CE method can be used to determine individuals' WTP or WTA through surveys. In this case, respondents are not directly asked to express their WTP in regards to changes in the provision of an off-market good, but to opt what they would prefer between hypothetical settings of various alternatives of attributes and characteristics of a particular non-market good. The monetary value of a non-market good is usually derived from trade-offs that individuals unconsciously make when they are about to select between a plethora of features at different levels including relevant costs (Alpizar, Carlsson, & Martinsson, 2001).

An essential aspect of the CE method is that it provides a way to assess from a multidimensional perspective the changes that affect the quality of environmental goods and shed light on the associated trade-offs. In contrast to the CV method, choice experiments are more complex and sophisticated because they aim to elicit information by subjecting respondents to make puzzling decisions between multiple tasks. Hence, the latter may lead to cognitive difficulties which probably will result in respondents' contradictory or irrational decisions as well as unsound monetary values (Atkinson & Mourato, 2008).

2.4.7 Budget constraint method

The foundations of the budget constraint method are not based on individuals' revealed or stated preferences but on the accounting perspective of what has been gained must be invested in sustaining their well-being. By this method, it is assumed that the average annual income per capita is the ceiling amount of money that an individual can spend for maximizing their utility (Pizzol et al., 2015). In this case, individuals' utility maximization is expressed in terms of increasing their life expectancy. This is where the Quality-Adjusted Life Year (QALY) perspective becomes relevant. QALY reflects individuals' WTP for gaining an additional life year of absolute well-being assuming with no externality effects. The budget constraint method constitutes an appropriate way for valuing a QALY which inherently encompasses all facets of human well-being. Thus, one may argue that the value of a QALY reflects the highest amount of money that individuals are willing to give up for its preservation (Weidema, 2009).

2.4.8 Marginal Abatement Cost (MAC) method

The particular method addresses the marginal costs resulting from the restoration of environmental degradation as well as the costs of the preventive measures required to avoid environmental damages. Therefore, any present or estimated change in the availability of a non-market good is evaluated as the future expenditures needed for offsetting or mitigating the change. By and large, its common application concerns the deployment of environmental policies and setting targets pertinent to pollution reduction and climate change mitigation. In strict environmental economics, as Mckittrick (1999) denoted, MACs are indispensable costs that private and social actors must bear in order to achieve an additional unit of reduction in GHG emissions. Though it facilitates the development of cost-effective environmental policies, the MAC method cannot estimate costs due to GHG emissions damages but only costs for their mitigation (Watkiss, 2018). To that end, it neglects to value individuals' WTP for reaching such reductions and thus to address the point of maximum social welfare.

2.5 Challenges of monetizing environmental impacts

The aim of this section is to touch upon the crucial challenges that render the monetization of environmental impacts difficult. According to ECON Analysis (2005), there are six major issues that need to be taken into consideration when the goal of a life-cycle study is the economic evaluation of environmental damages. These challenges consist of:

1. Proximity issues – Assessment's Boundaries

Areas in the near proximity of industrial activities that cause damages to the environment are directly affected by them. Hence, the spread of a negative environmental phenomenon directly inflicts the populations of the regions where its source of origin is identified. In environmental impact assessments, it is required to define the boundaries of the life-cycle analysis in order to cover at a high extent the affected areas and populations. However, that is difficult to achieve in practice. Many chemical substances have the ability to travel in long distances, thus causing negative impacts on other regions or even more countries. Consequently, in those situations, the monetary valuation of environmental impacts through the aforementioned methods becomes complicated due to:

- a) Differences in Individuals' preferences and thus WTP from place to place

- b) The degree to which a population/area has been affected by environmental disasters depends on how far its location is from the source of origin
- c) Differences in people's annual income and purchasing power from place to place
- d) Cultural and educational factors

To that end, eliciting individuals' WTP and assigning economic values to environmental impacts that have affected different areas at a different degree requires a lot of effort and time. Moreover, the difficulty to combine data from markets with different characteristics might lead to an incomplete monetary valuation procedure.

2. *Time horizon*

The life span of environmental impacts differs according to their source of origin. A production system has a certain life expectancy, which usually differs from the life span of the environmental impacts that it causes. To that end, when the goal of the analysis is to identify the associated environmental costs, then the chosen time horizon for the monetary valuation of the environmental impacts at least needs to be the same as the life span of the investigated production system. Nevertheless, if the life span of the impacts exceeds that of the production system then the selected time horizon of the life cycle analysis should be adjusted accordingly.

3. *Reference case scenario*

A crucial aspect of a life cycle study that aims at the execution of an economic evaluation is the appropriate delineation of the reference case scenario. The reference case scenario is essential since it refers either to the scenario without the production system or before any technical adjustments to occur. Thus, allowing the life-cycle analyst to identify the environmental impacts before-and-after the establishment or the modification of the production system. Therefore, the economic evaluation of the impacts reflects on the marginal changes in the availability and the quality of environmental goods, as a consequence of the establishment or alteration of a production system.

4. *Lack of data*

One major challenge that life-cycle analysts confront is that some environmental burdens cannot be monetized either due to inadequate or absent data. That means that the analyst has to follow a qualitative approach in order to evaluate the negative and positive socio-economic effects of the identified impacts instead of actually computing environmental costs. At the very least, in the evaluation analysis, an explanation of the most significant impacts that cannot be translated into monetary terms should be included. Additionally, a ranking of the impacts in order of their significance along with who is affected and potentially could be compensated is recommended.

5. *Discount rates*

The money of today has a different value from the money of tomorrow. Typically, the value of one euro gained today is perceived to worth more than one gained in the long term. That creates the problem of making the right decisions, whose benefits and costs cannot directly be realized but only in the future. This is where discount rates come into play. The particular economic notion accounts for the time value of cash flows. It is the rate at which people would be willing to exchange money of today with money of tomorrow and vice versa. Therefore,

the level of the discount rate is a factor that influences the results of economic analyses, especially when tools such as the net present value and internal rate of return are used.

However, it is difficult to select an appropriate discount rate for assessing the enviro-economic performance of a system from a life-cycle perspective. Reason for this is that the effects of environmental impacts (such as CO₂ emissions) occurred today might not be realized until many years to pass from now. Therefore, by selecting a high discount rate for calculating environmental costs, the costs of environmental damages are transferred to subsequent generations. Thus, companies may not be incentivized for future environmentally friendly initiatives. Consequently, a gradually decreasing discount rate (reaching zero) seems to be appropriate for rationally monetizing today's environmental impacts and giving more value to the future.

2.6 Economic weighting of environmental effects

As it was mentioned in subsection 2.1.1, the weighting of environmental effects is an optional step in LCIA. When the aim of the study is to make comparisons between alternative scenarios, then the weighting step can stimulate decision making by providing the results in an easy way to interpret and organize in a hierarchy. To express the severity of certain environmental impacts, weights are assigned to the anticipated effects. In literature, there are three weighting methods (Eldh & Johansson, 2006);

- I. A panel of experts from different social groups are asked to give their weighting factors regarding their perceptions about the effects of environmental impacts
- II. Weighting factors are derived via monetary valuation methods and used for estimating the damage costs or the costs to prevent the environmental effects found in certain impact categories
- III. Distance-to-target methods are used for assigning weights to impacts on the basis of how far the identified environmental effects are from attaining relevant political targets.

Commonly, weights in the form of economic values are applied to convert environmental impacts at midpoint or endpoint level to monetary values (Huysegoms et al., 2018). Moreover, Ahlroth et al. (2011) argue that the weighted monetized results of an LCA study can be used along with LCC to calculate the overall external environmental costs of a production system. The methods that are extensively being used to derive economic values and then put as weights on environmental effects are the described ones in section 2.3. Based on these methods, several LCIA methods have been developed that allow the use of monetary weights. As it follows, six LCIA methods were selected for a detailed discussion through which environmental effects can be aggregated to a single score expressed in monetary terms. Table 2 demonstrates the found LCIA versions and their compatible valuation methods, as well as the relevant midpoint and endpoint indicators of each LCIA method.

Table 2: LCIA methods & compatible valuation methods (Pizzol et al., 2015; Tekie & Lindblad, 2013)

LCIA	Valuation Method	Impact Categories	Areas of Protection	Reference
EPS	Market Prices Contingent Valuation Abatement Costs	No indicators	Biodiversity, Abiotic stock resources, Human health, Cultural & recreational values, Production capacity of ecosystems	(Steen, 1999b)
ReCiPe	Market Prices	Ionizing radiation, Trop. Ozone formation, Human toxicity (none-/ cancer), Stratos. ozone depletion, Water use, Particulate matter, Global warming, Freshwater eutrophication, Freshwater eco-toxicity, Terrestrial acidification, Terrestrial eco-toxicity, Trop. Ozone (eco), Land use, Marine eco-toxicity, Mineral resources, Fossil resource	Human health, Ecosystems, Resource availability	(RIVM, 2018)
Ecovalue08	Market Prices Contingent Valuation	Global warming, Human health, Forming of tropospheric ozone, Acidification, Depletion of abiotic resource, Eutrophication	No indicators	(Ahlroth & Finnveden, 2011)
Stepwise 2006	Budget Constraint	Aquatic eutrophication, Aquatic eco-toxicity, Eutrophication, Acidification Human toxicity, Global warming, Injuries, Mineral extraction, Ionizing radiation, Ozone layer depletion, Nature occupation, Respiratory terrestrial eco-toxicity, Photochemical ozone – Vegetation	Human well-being Ecosystems Resource productivity	(Weidema, 2009)
LIME	Choice Experiment	Eco-toxicity, Air pollution, Land use, Acidification, Global warming Eutrophication, Ozone creation Resource consumption, Ozone layer depletion, Human toxicity	Human health, Biodiversity, Primary productivity & social welfare	(Itsubo et al., 2004)
Ecotax02	Averting Behavior	Ozone layer depletion, Depletion of abiotic resources, Depletion of biotic resources, Terrestrial eco-toxicity, Freshwater aquatic eco-toxicity. Marine water aquatic eco-toxicity, Global warming, Photochemical oxidation, Acidification, Eutrophication, Human toxicity	No indicators	(Eldh & Johansson, 2006)

2.6.1 Stepwise 2006

Stepwise 2006 is an LCIA method which is similar to the LCIA methods EDIP2003 and Impact 2002⁺. The particular method provides impact indicators for three major issues of concern – human health, ecosystems and resource availability. The “Ecoindicator99 method constitutes the baseline for the computation of the pertinent biophysical scores (Weidema, 2009). The primary aim of the Stepwise method is to provide a comprehensive economic weighting set that consists of midpoint and endpoint economic weighting factors to ease the conversion of environmental damages measured in biophysical units into monetary terms (Tekie & Lindblad, 2013). The results in each endpoint impact category are measured in (Weidema, 2009):

- i. **QALYs for impacts on human health;** expressed as a change in the quality of life multiplied by a harshness indicator (which takes values between 0 and 1, i.e. death and prosperity respectively). It expresses a positive state where individuals can gain a life year without externalities. Thus, it is exactly the opposite of one DALY which indicates the extent to which human’s quality of life has declined due to environmental damages (1 QALY = -1 DALY)
- ii. **Biodiversity Adjusted Hectare Years (BAHYs) for impacts on ecosystems;** a loss of BAHYs implies a decrease in the number of indigenous species.
- iii. **Euros₂₀₀₃ for impacts on resource availability;** expressed as a loss of potential economic gains due to environmental impacts that negatively influence resources availability

The particular method allows the integration of the results into one impact category, named as “human productivity and consumption efficiency” (EUROS/QALY). Additionally, the results can be expressed as QALY/BAHY, i.e. the degree to which individuals are willing to give up their well-being (based on their annual income) so that to safeguard the ecosystems or as EUROS/BAHY, i.e. individuals’ WTP to protect the natural environment (Weidema, 2009).

The monetization procedure in the Stepwise 2006 method is grounded on the budget constraint valuation method. However, according to Pizzol et al. (2015), its major limitation of is that the valuation of human well-being can only be expressed as a loss of QALYs, which is debatable whether it actually measures individuals’ WTP or their purchasing power to “buy-out” an additional life-year without the fear of negative externalities.

2.6.2 Eco-value 08

The Eco-value 08 and its updated version Eco-value 12 were developed by Ahlroth & Finnveden (2011). Their aim was the development of an economic weighting set through which environmental impacts would be monetized in a systematic and consistent way. The value of loss of benefits caused by changes in the quality and the availability of environmental goods is built upon individuals’ consuming behaviour in hypothetical or actual markets. This model is based on two monetary valuation approaches – individuals’ stated preferences and observed market prices. The provided weighting factors for the monetization of impacts that affect environmental quality are based on the contingent valuation method. Whereas environmental effects on natural resources are weighted via factors based on observed changes in market prices (Ahlroth & Finnveden, 2011). The particular weighting factors are assigned to the pertinent environmental impacts during the weighting step of the LCIA phase.

For instance, the weighting factor for the GWP indicator takes values between 0.10 SEK/kg CO₂ and 2 SEK/kg CO₂, where 1 EURO = 9 SEK (Ahlroth & Finnveden, 2011). Thus, it can be used for translating biophysical units into monetary terms. It should be noted, that the Ecovalue08 model provides weighting factors only for midpoint indicators and not for endpoint ones due to shortages in relevant market-price data (Pizzol et al., 2015).

2.6.3 Ecotax02

Governments enact policies to protect people against potential threats. To avoid environmental disasters and their impacts on human health, policy-makers are required to act in the interest of society. Based on the assumption that political decisions mirror societal values, Johansson (1999) developed the Ecotax02, i.e. a method to create economic weighting factors for various impact indicators within the LCA context. The particular method makes use of the Swedish taxation system in order to develop a valuation method for LCA by linking environmental taxes and fees to different impact categories.

Based on individuals' revealed preferences and averting behaviour, the weighting factors of the Ecotax02 reflect society's WTP to fix environmental problems through taxes and fees (Ahlroth & Finnveden, 2011; Pizzol et al., 2015). The conversion of the LCA results into monetary terms is realized by connecting a tax or fee on certain substances with impact categories. For instance, taxes related to CO₂ emissions are linked to the global warming impact category. As reported by Eldh & Johansson (2006), the weighting factor for the Global Warming impact category due to taxes for CO₂ emissions reduction is 0.63 SEK/kg CO₂.

The Ecotax02 has a geographical orientation since it is based on taxes and fees that only concern Sweden. An additional disadvantage of the model is that environmental laws and regulations change over time, which means that the weights assigned to certain impact categories will become unsound. Lastly, there are no taxes and fees for all environmental threats, thus some impact categories cannot be monetized (Tekie & Lindblad, 2013).

2.6.4 LIME

LIME is a non-European LCIA method initiated in Japan. It consists of eleven impact categories which are used to assess the damage on four areas of protection – human health, biodiversity, social welfare and plant production (Itsubo et al., 2004). By using the choice experiment method, it provides a set of economic weighting factors for the monetization of environmental impacts. To derive the particular weighting factors, a survey in Japan was conducted, through which respondents were asked to state their WTP to avoid one unit of environmental impact on a specific area of protection. A characteristic example of its logic is how much the Japanese are willing-to-pay to avoid a rise in CO₂ emissions (i.e. the GWP) which will negatively affect human health and biodiversity (areas of protection) (Tekie & Lindblad, 2013).

2.6.5 Environmental Priority Strategies (EPS)

EPS is an LCA-based model developed to facilitate product designers decide between several alternatives which product offers the best environmental performance. To accomplish that, EPS provides a database with environmental damage costs related to a plethora of emissions and resource uses. Therefore, during the design phase engineers can quantify the potential environmental costs over the life-cycle of a product and take appropriate precautionary

measures (Steen, 1999b). The valuation of environmental impacts is based on observed changes in market prices or directly asking individuals' WTP to avoid environmental damages (contingent valuation method) (Pizzol et al., 2015).

The EPS model allows the valuation of environmental impacts on five areas protection – human health, cultural and recreational values, ecosystem production capacity, biodiversity and abiotic stock resources (Steen, 1999b). The valuation procedure consists of three phases; the characterization (impact/kg of chemical compound X), the weighting (euros/impact) and the valuation phase (euros/ kg of chemical compound X) (Tekie & Lindblad, 2013).

2.6.6 ReCiPe

The ReCiPe LCIA method is subdivided into two groups of environmental impact indicators – midpoint and endpoint – that allow the conversion of life-cycle data into performance scores. Endpoint indicators concern three accumulative levels of environmental damage on a) human health, b) natural environment and c) resource availability while the midpoint ones consist of eighteen indicators for the analysis of single environmental issues (Huijbregts et al., 2016).

According to Y. Dong et al. (2019), ReCiPe is the most scientifically comprehensive endpoint method, which allows for the quantification of damage costs (internal or external) from specific activities at three safeguard subjects. Specifically, the valuation of endpoints concerns the translation of the following indicators into monetary terms (Goedkoop et al., 2013):

- *Human health*, measured as the summation of life-years lost because of premature mortality, i.e. DALY – Disability Adjusted Life Year
- *Ecosystem quality*, measured as the Potentially Disappeared Fraction (PDF) of species over space and time
- *Resource availability*, measured as surplus costs

2.7 Economic weighting factors

There are plenty of valuation methods that find application in the weighting phase of LCA studies. In this report, we have investigated six different LCIA methodologies which allow the conversion of environmental impacts into monetary terms by applying relevant weighting factors. As such, an effort to collect the particular weighting factors either at midpoint or endpoint level was made. The identified numerical evidence that facilitates the monetization of LCA results concerns two endpoints and five midpoint weighting factors. For these indicators, scholars have determined an economic weight value to translate environmental impacts into euros per emission unit of substance X. The number of the found indicators was limited since the above-addressed LCIA methods demonstrate significant differences regarding the impact categories and areas of protection which are consisted of.

The economic weighting factors that correspond to the endpoint and midpoint indicators of the identified methods are displayed in Table 3. The vast majority of the factors were derived based on the WTP principle. However, they demonstrate a divergence in their measurement units (currencies) due to their different origin (LIME in Japan, Ecotax02 and Ecovalue08 in Sweden). In order to show the results of our desk research in a consistent way, a conversion

of the units that are used for weighting was conducted either between currencies or between reference substances. Regarding the former, all monetary units were converted into euros by using the appropriate currency exchange ratios. Moreover, the biophysical units that the found LCIA methods use to measure environmental damages on the same impact categories differ from each other. For instance, the characterization factor for the acidification impact category as it was provided by Weidema (2009), was measured in m² UES (un-protected ecosystem) while Ahlroth & Finnveden (2011) gave it in kg SO₂eq. As such, a conversion between characterization factors was conducted according to the values provided by Pizzol et al., (2015).

In the LIME and ReCiPe methods, impacts on human health are expressed in DALY. Disability-adjusted life years (DALY) indicate years of life lost due to premature mortality as well as years spent with disability problems because of environmental damages. Therefore, DALY implies a negative state in human health. On the other hand, in QALY terms, years of well-being gained/lost do not only reflect on health issues but also on other social aspects such as unemployment. Lastly, the EPS model provides estimates for individuals' WTP for one year of life lost (YOLL). Regarding impacts on the ecosystem, all methods' the weighting factors except that of ReCiPe's reflect individuals' WTP to protect species of animals and plants. In ReCiPe, the loss of biodiversity is described as the potential disappearing fraction of species over time and space (e.g. the number of species disappeared on one square meter per year).

Table 3: Midpoint and endpoint monetary weighting factors of six LCIA methods (Ahlroth & Finnveden, 2011; Itsubo et al., 2012; Pizzol et al., 2015; Steen, 1999a; Weidema, 2009)

LCIA method € ref. year	EPS ^[1] € ₁₉₉₉	ReCiPe ^[2] € ₂₀₀₈	Ecovalue08 ^[3] € ₂₀₁₀	Stepwise ^[4] € ₂₀₀₃	LIME ^[5] € ₂₀₁₀	Ecotax02 ^[3] € ₂₀₀₂
Human Health	85000 €/YOLL	60000 €/DALY	-	74000 €/DALY	119805 €/DALY	-
Ecosystems €/Species.yr	110E10 ⁹	* 175E10 ⁹	-	30.8E10 ⁹	115.73E10 ⁹	-
Abiotic resources €/MJ	-	-	0.0037	0.004	-	0.014
Acidification €/kg SO ₂ eq	-	-	2.792	0.146	-	1.675
Global Warming €/kg CO ₂ eq	-	-	0.0093	0.083	-	0.059
Eutrophication €/kg PO ₄ eq	-	-	20.289	1.2	-	2.659
Ozone Depletion €/kg CFC11eq	-	-	-	100	-	111.684

[1] Steen, (1999a); [2] Heijungs, (2008); [3] Ahlroth & Finnveden, (2011); [4] Weidema, (2009); [5] Itsubo et al., (2012) Currency exchange rates used for LIME, Ecovalue08 and Ecotax02: 0.00815 Euro/YEN and 0.09307 Euro/SEK. Units of characterization factors (Pizzol et al., 2015): 19 m²UES/kgSO₂; 12 kgNO₃/kgPO₄;

* Potential loss of biodiversity measured in Potential Disappearing Fraction - PDF m2 years

2.8 Literature findings

In line with the previous sections, we attempted to identify relevant studies where the LCA, LCC and the abovementioned monetization methods have been used to assess the environmental performance of the chlor-alkali industry. According to our findings, there is no study applying the LCC technique to calculate chlorine's production life-cycle costs. On the contrary, a plethora of scientific papers was found in which LCA is extensively implemented to quantify the environmental impacts of the particular industry. However, none of these studies has used economic weighting factors or valuation methods to translate the LCA results into monetary terms. Furthermore, from the published LCA studies, there is none focusing on the Dutch chlor-alkali industry exclusively.

The identified LCA studies were scrutinized to collect quantitative and qualitative data regarding the environmental footprint of the processes engaged in chlorine production systems. Besides gaining a clear understanding of the functionality of the system, our aim was to gather relevant LCA results in order to compare them with the results of our study in chapter 6. To that end, information about those studies' goal and scope, functional unit, system boundaries, LCI and LCIA were gathered. The particular features along with the results found in the GWP impact category are displayed in Table 4.

Eurochlor (2013) constitutes the most comprehensive and up-to-date LCA study of the European chlor-alkali industry. In a cradle-to-gate assessment, i.e. from raw materials extraction and transportation until the final use of the end-products, Eurochlor (2013) calculated the environmental impacts of the chlorine production, taking into account the vast majority of the European chlor-alkali plants of the sector. However, they did not report specific information about the engaged technologies or process-specific contribution to the overall environmental impact.

Interestingly, the vast majority of the studies concern the comparison of the environmental profile of the different technologies that can be used in the electrolysis process. Moreover, in all studies, it is acknowledged that the electrolysis process has the biggest contribution to the identified environmental damage due to its high electricity requirements. Specifically, Garcia-Herrero et al., (2017), Hong et al., (2014) and Jung et al., (2014) concluded that the electrolysis process accounts for over 70% of the overall impact. However, this number varies according to the implemented technology for sodium chloride electrolysis. As it is extensively discussed in chapter 3, the widely applied technologies in the particular process are the membrane cells, diaphragm cells and the mercury cells as well as the ODC technique. Among them, the ODC and the membrane cells technologies record the best environmental performance (Garcia-Herrero et al., 2017a; Jung et al., 2014; Kätelhön et al., 2015).

The main difference between these studies lies in the set functional unit of analysis. Both Garcia-Herrero et al., (2017) and Jung et al., (2014) considered the co-production of chlorine, caustic soda and hydrogen. On the other hand, Kätelhön et al., (2015) computed the impacts excluding hydrogen production, while Hong et al., (2014) focused their study only on the production of caustic soda. Moreover, except for the study conducted by Kätelhön et al., (2015) who excluded from their evaluation scope the processing phase of the end-products, the scope of the others concerns a cradle-to-gate analysis, thus considering in their system boundaries salt mining and all chlorine manufacturing stages.

Table 4: Main features of previous LCA studies in the chlor-alkali industry

Ref #	LCA	LCC	Remarks
[1]	<p><u>Goal & Scope:</u> Comparison analysis of mercury, diaphragm, membrane and ODC technology</p> <p><u>System boundaries:</u> Cradle-to-gate→ salt mining and transportation, brine preparation and purification, electrolysis process, treatment and waste management</p> <p><u>Functional Unit of analysis:</u> 1.13 ton NaOH, 1 ton Cl₂, 0.03 ton H₂</p> <p><u>LCIA method - Classification:</u> CML Guide to LCA (2002) - 12 impact categories</p> <p><u>Allocation:</u> Economic and mass allocation backed up by a systems' expansion - Steam reforming of natural gas (alternative production of H₂)</p> <p><u>Monetary Weighting:</u> No</p>	No	<p>Electrolysis is the most energy-consuming stage, causing more than 70% of the identified environmental impact;</p> <p>Environmental performance rankings of the involved technologies: 1) ODC, 2) Membrane, 3) Diaphragm, 4) Mercury;</p> <p>ODC → 7% less of energy consumption compared to the membrane technology</p> <p><i>*GWP: 2281 kg CO₂/ton FU</i></p>
[2]	<p><u>Goal & Scope:</u> Cost & benefit analysis of the introduction of novel electrolysis technologies</p> <p><u>System boundaries:</u> Cradle-to-gate→ electrolysis; NaOH concentration; inputs supply and concentration process</p> <p><u>Functional Unit of analysis:</u> 1 ton Cl₂ and 1.13 ton NaOH</p> <p><u>LCIA method- Classification:</u> Not Discussed - 1 impact category</p> <p><u>Allocation:</u> System expansion</p> <p><u>Monetary Weighting:</u> No</p>	No	<p>A form of environmental CBA instead of LCC</p> <p>They identified the relationship between electrolysis technologies sales volume and global warming.</p> <p>Global warming effects decrease as the sales volume of the ODC technology increases.</p> <p><u>H₂ used as fuel</u> <i>*GWP: 2700 kg CO₂/ton FU</i></p> <p><u>H₂ used as a commodity</u> <i>*GWP: 2620 kg CO₂/ton FU</i></p> <p><u>H₂ no-use</u> <i>*GWP: 2930 kg CO₂/ton FU</i></p>
[3]	<p><u>Goal & Scope:</u> Comparison of the membrane and ODC technologies</p> <p><u>System boundaries:</u> manufacturing, operation and disposal</p> <p><u>Functional Unit of analysis:</u> H₂-Fuel: 1 ton Cl₂, 1.128 ton NaOH H₂-Commodity: 1 ton Cl₂, 1.128 ton NaOH, 0.028 H₂</p>	No	<p>ODC technology has better environmental performance than membrane cells in six out of seven impact categories</p>

<hr/>		
	<p><u>LCIA method - Classification:</u> ReCiPe - 7 impact categories</p> <p><u>Allocation:</u> H₂-Fuel: avoided burden process – hydrogen used as fuel, substituting natural gas for electricity and heat generation.</p> <p>H₂-Commodity: System expansion - steam reforming process and H₂O electrolysis</p> <p><u>Monetary Weighting:</u> No</p>	<p>Electrolysis power requirements can be reduced by 30% when replacing the standard cathodes of membrane cells with ODC.</p> <p><u>H₂ used as fuel</u> *GWP: 2040 kg CO₂/ton FU</p> <p><u>H₂ used as a commodity</u> *GWP: 2280 kg CO₂/ton FU</p>
[4]	<p><u>Goal & Scope:</u> Environmental impact assessment of NaOH production when using membrane cell technology.</p> <p><u>System boundaries:</u> Cradle-to-gate→ raw material extraction & transportation, electricity generation, infrastructure, caustic soda production & processing, waste disposal</p> <p><u>Functional Unit of analysis:</u> 1 ton of 100% NaOH</p> <p><u>LCIA method - Classification:</u> ReCiPe E (midpoint level) - 18 impact categories</p> <p><u>Allocation:</u> Mass allocation</p> <p><u>Monetary Weighting:</u> No</p>	<p>No</p> <p>Electricity and salt production processes cause more than 90% of the total environmental impact.</p> <p>*GWP: 1590 kg CO₂/ton FU</p>
[5]	<p><u>Goal & Scope:</u> Environmental performance of EU chlor-alkali plants</p> <p><u>System boundaries:</u> Cradle-to-gate→ raw material extraction, grid electricity mix, on-site electricity generation, brine preparation, electrolysis cells, Cl₂ / NaOH / H₂ processing, NaClO production</p> <p><u>Functional Unit of analysis:</u> 1 kg Cl₂ - 1 kg NaOH -1 kg H₂ - 1 kg NaClO and 1 kg NaCl</p> <p><u>LCIA method - Classification:</u> CML 2012 - 10 impact categories</p> <p><u>Allocation:</u> Mass allocation/ Economic allocation and 'Calorific value of hydrogen' (avoided burden)</p> <p><u>Monetary Weighting:</u> No</p>	<p>No</p> <p>On a European level, it is the most complete LCA study focusing on the quantification of the environmental impacts associated with the European chlor-alkali plants</p> <p>LCI data gained from 50 European chlor-alkali plants Plants involved: 21 Mercury, 2 Diaphragm & 27 Membrane</p> <p>The results were presented on an aggregated level (European chlor-alkali industry) and not as technology-specific (membrane, diaphragm or mercury)</p> <p>*GWP: 3890 kg CO₂/ton FU</p>

[1] (Garcia-Herrero et al., 2017a); [2] (Kätelhön et al., 2015); [3] (Jung et al., 2014); [4] (Hong et al., 2014), [5] (Eurochlor, 2013); * GWP results concern CO₂ emissions when membrane cells technology is applied

2.9 Chapter Outcome

In this chapter, the core principles of LCA, LCC, and valuation methods were scrutinized. According to our findings, a common way to apply them in an integrated manner is by using the LCA's structure to encapsulate the environmental impact assessment and the required components for internal and external costs estimations. The latter concerns Hunkeler's et al., (2008) suggestion for a combined eLCC and cLCC analysis. To that end, based on the above-discussed concepts and the four phases that structure the LCA, Figure 8 delineates the approach that this study has used to conduct an enviro-economic impact assessment of Nouryon's chlorine production system at Botlek.

In the first phase, the goal from both perspectives should be defined. Next, the LCI should consist of every flow that goes in and out of the system boundaries, including material, energy and cash inflows and outflows. Then, the quantification of the environmental impacts on the relevant impact categories can be realized. The outcome of this stage in combination with the identified economic weighting factors can be used to translate environmental damages into monetary terms. Within a certain time horizon and by selecting an appropriate discount rate for the involved operational and environmental costs respectively, the anticipated future money flows can be calculated. Lastly, the interpretation of the results can take place considering all the perspectives included in the analysis.

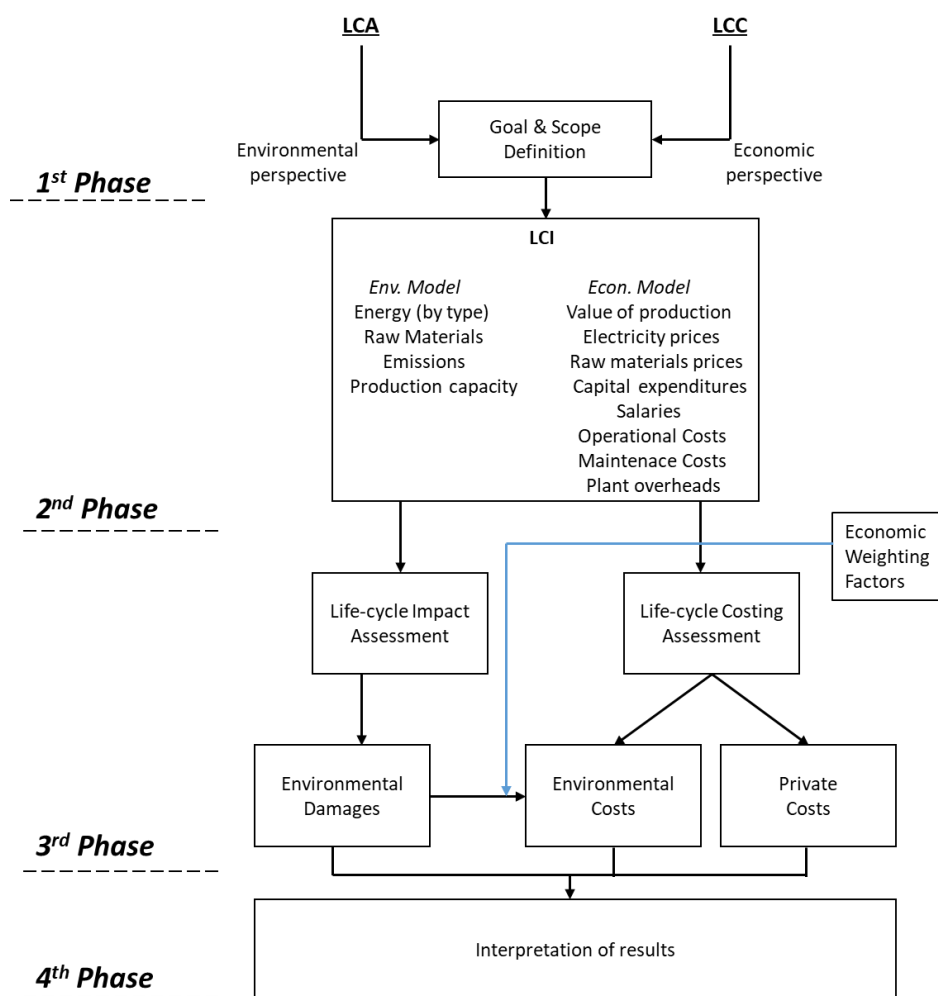


Figure 8: Enviro-economic impact analysis structure

Chapter 3: The European & the Dutch chlorine manufacturing industry

In this chapter, the Dutch and the European chlorine manufacturing industries are outlined. The chapter focuses on the selected case study which concerns Nouryon's chlor-alkali plant at Botlek. Moreover, the fundamental principles of the membrane cells technology along with the available configuration types of the electrolytic cell are discussed in detail.

3.1 Sodium chloride electrolysis

The fundamental process that occurs in chlor-alkali plants is electrolysis. Electrolysis is the process of separating chemical elements, by enforcing a non-spontaneous chemical reaction to take place when a direct electric current (DC) is supplied to an aqueous electrolyte solution. The DC is supplied to the electrolyte through two electrodes – the anode and cathode – that are connected with an external electric circuit. The cathode refers to the negatively charged electrode where the reduction of ions occurs. Cations of the solution move towards the cathode where they absorb electrons and become neutral. On the contrary, the positively charged electrode, anode, is responsible for the oxidation of ions. There, the anions of the solution are discharged by giving up electrons.

Chlorine constitutes the main production line of the chlor-alkali industry, which is obtained from brine electrolysis. As it is illustrated in Figure 9, when an electric current passes through brine, which is the commonly known salt (otherwise sodium chloride - NaCl) in solution, then it breaks down to its constitutive elements. That process causes a chemical change, resulting in the production of chlorine gas. Along with chlorine, (aka sodium hydroxide or NaOH) and hydrogen (H_2) are co-produced via brine electrolysis.

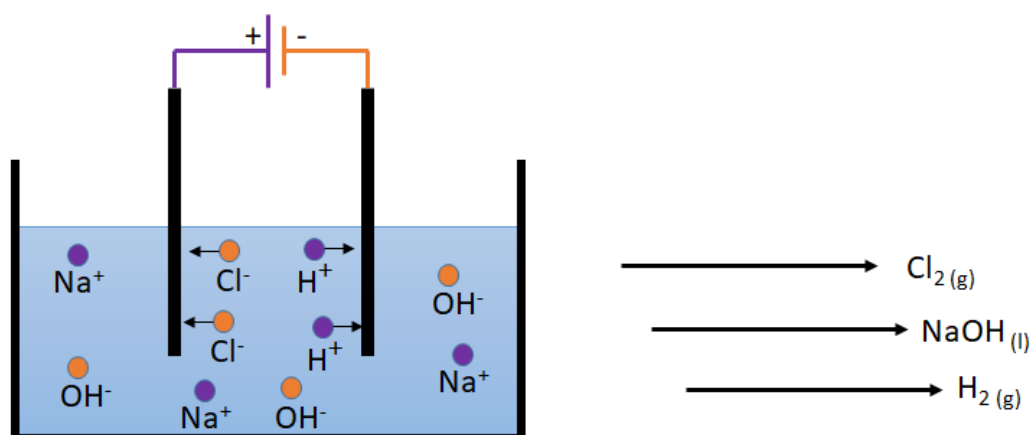
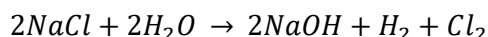


Figure 9: A simplistic depiction of brine electrolysis

By applying the rules of stoichiometry, when one ton of chlorine is produced then around 1.1 tons of caustic soda and 0.028 tons of hydrogen are co-produced (Eurochlor, 2019c). Thus, chlorine and caustic soda industries are inextricably linked to each other.

Currently, there are three technologies that are commonly used for chlorine and caustic soda production on an industrial scale – membrane, diaphragm and mercury. Additionally, the newly introduced ODC technique constitutes a membrane-based alternative for the electrolysis of sodium chloride. Except for the ODC technique, all of the involved technologies co-produce chlorine, caustic soda and hydrogen according to the following reaction,



By and large, membrane electrolysis is a novel technology which is dominantly implemented in the Dutch region. As such, the particular project revolves around the membrane cells technology, which was selected as the focal point of the enviro-economic analysis in chapter 4 and 5. The following section encompasses detailed information about membrane cells and their application in Europe and the Netherlands.

3.2 Membrane cells electrolysis

As the European Commission defines it, the membrane cell technology constitutes the Best Available Technique (BAT) for chlorine production (Brinkmann et al., 2014). Compared to the conventional electrolysis techniques (mercury and diaphragm), it ensures an environmentally friendly and energy-efficient way for brine electrolysis. Ever since the European Commission has compelled the chlor-alkali industry to phase out mercury cells, the diffusion rate of the membrane cell technologies is accelerating. Specifically, the European chlor-alkali industry produces 8,834 kilotons of chlorine (i.e. 78.4% of the total production) by using membrane cells (Eurochlor, 2019a), while in the USA it accounts for 45% of the industry (Lee et al., 2018). Overall, the current world share of membrane technology is 74% (IHS, 2018).

Membrane cells' main feature concerns the separation of the produced chemical elements via a permselective ion-exchange membrane which splits the electrolyzer into two compartments – the anode and cathode respectively. In general, membrane technology is an upgraded version of diaphragm cells (Millet, 2013). The former inhibits the negatively charged chlorine ions to move towards the cathode compartment while the latter allows ion-exchange between the two sides regardless of their electric charge. Figure 10 depicts the configuration of a membrane cell along with its inputs-outputs as well as the flow of the substances.

Firstly, the brine solution is supplied to the anode compartment where elemental chlorine is produced and then collected. Next, water along with sodium ions enter the other side of the electrolyzer and flow towards the cathode. On that side, gaseous hydrogen is produced and then stored. The caustic solution leftover is removed from the cell at 30% concentration approximately (Eurochlor, 2019b). At that point, it is worth mentioning that when gaseous chlorine leaves the cell, it consists of a few molecules of oxygen, thus requiring to be purified and liquefied. Table 5 provides a description of the operating features and requirements of membrane cells.

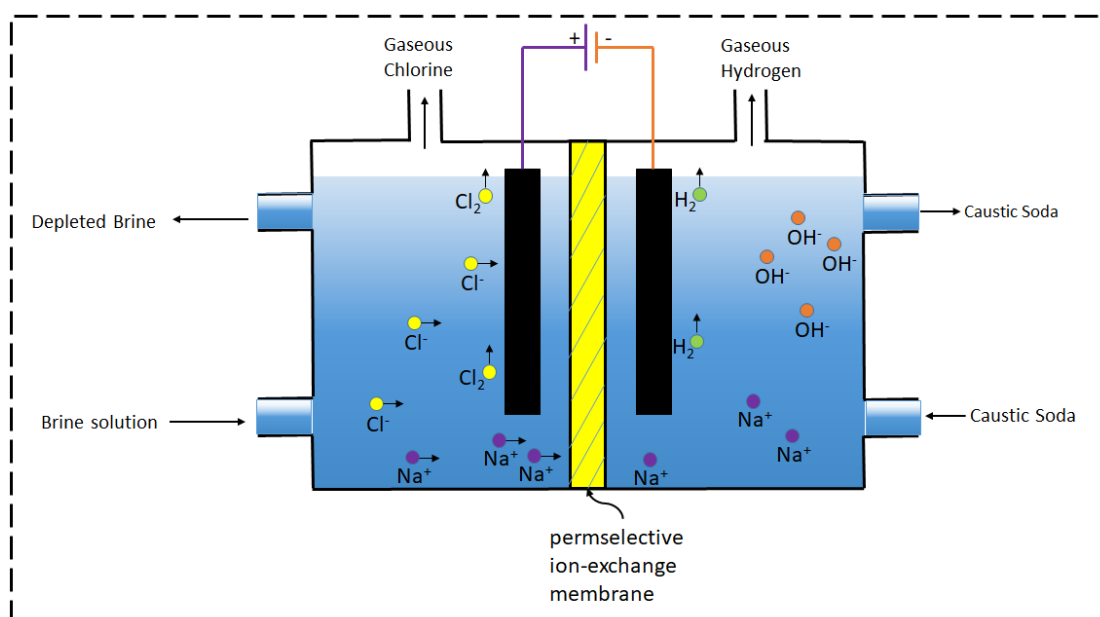


Figure 10: Membrane cells electrolysis

The distance between the two electrodes in the aquatic electrolyte plays a crucial role in the membrane cell's efficiency and energy consumption. According to Ohm's law, the wider the gap between the electrodes, the less the cell's efficiency. There are two possible configurations in regards to the design of a membrane cell; the typical one which is called the gap-cell and the zero-gap configuration (Millet, 2013). The former is the most commonly applied in brine electrolysis systems while the latter constitutes a newly introduced novelty.

Table 5: Operational features of membrane cells for brine electrolysis (Millet, 2013)

Feature	Value
Cell Temperature	85 °C
Pressure	1 atm
Current Density	300 – 500 mA/cm ²
Cell voltage	3.0 – 3.6 V
Energy demand	2600 - 2800 kWh/ton Cl ₂ (at maximum current density)
NaOH Concentration	≈ 35 wt%
Energy demand for NaOH concentration (50%)	≈ 180 kWh/ ton Cl ₂
<i>Raw Materials requirements for producing 1 ton Cl₂</i>	
Sodium chloride	1.7 tons
Water vapour	1 ton

A gap-cell concerns the parallel configuration of two electrodes in the liquid electrolyte while a permselective membrane is placed in between to avoid the compounding of the gaseous products. When the gaseous products of brine electrolysis are generated, the current density capacity of the gap-cell drops and therefore its efficiency. The main reason for this phenomenon is that the electric current cannot flow through the electrolyte because of the presence of gaseous layers (Cl₂ and H₂) over the electrodes (Millet, 2013). Therefore, membrane cells installations that are based on the gap-cell configuration tend to lose their efficiency due to high resistance between the electrodes, thus in high energy consumption.

When the distance between the two electrodes is extremely short then the cell's efficiency increases. This is the idea behind the second type of membrane cells, known as the zero-gap configuration. In this structure, the cell comprises two opposite charged electrodes that are almost attached to the membrane which distinguishes them. More specifically, Brinkmann et al. (2014) indicate that usually in zero-gap cells structures the distance between the electrodes is ≤ 0.1 mm and that the products are bubbled out from their rear side. As a result of the minimum distance between the anode and cathode, the membrane cell shows resistance to ohmic losses (Millet, 2013). Consequently, the cell operates without fluctuations in current density, at its maximum efficiency and with less power consumption rate.

Although the electricity requirements are less, the direct emissions associated with the operation of a chlor-alkali plant do not decline by implementing the zero-gap technology. Nonetheless, the particular approach can lead to a decrease in indirect emissions from electricity generation. Since the structure of the cell is of paramount importance in cutting down electricity demand the zero-gap configuration might constitute a possible solution for the chlor-alkali industry to limit its electricity requirements. Figure 11 shows a schematic illustration of the two configuration options in membrane cells.

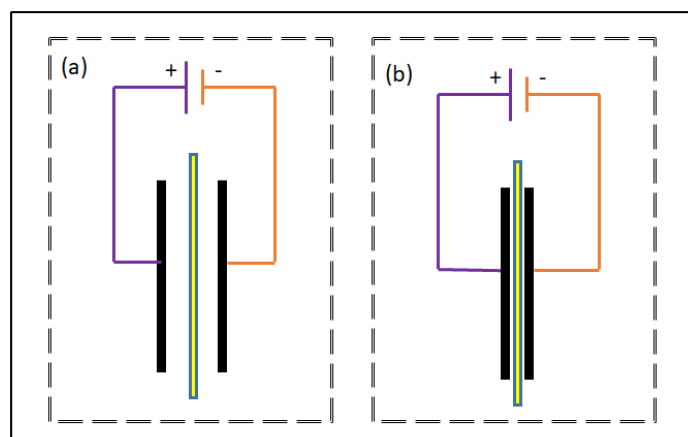


Figure 11: Schematic representation of the two possible configurations in membrane cells; left-side gap-cell and right-side zero-gap cell (Millet, 2013)

Regardless of its configuration type, membrane cell technology causes less environmental impacts and in general, it has greater performance than mercury and diaphragm cells. According to Eurochlor (2019b), the demand for electric power is the minimum of the three techniques and the quantity of steam required to produce one ton of caustic soda is even less than one ton. In contrast with mercury and diaphragm technologies, an additional benefit of implementing the membrane cell technology is the high quality and salt-free caustic soda (<0.02 NaCl) collected at the end of the process. Moreover, it should be underlined that no mercury and asbestos emissions are generated by membrane cells installations (Millet, 2013). On the flip side, high purity sodium chloride is required as raw material. Furthermore, the high investment costs for acquiring and maintaining the membranes along with low chlorine quality are perceived as essential drawbacks of the process (Garcia-Herrero et al., 2017a).

Notwithstanding that the overall electricity demand of electrolysis is substantially decreased by implementing the membrane cell technology, energy consumption yet remains a major sticking point in the environmental performance of the chlor-alkali industry.

To tackle the high electricity requirements of the chlor-alkali industry, an oxygen depolarized cathode (ODC) can be used instead of the hydrogen evolving electrode that is dominantly used in the typical membrane electrolysis cells. The ODC technology is an up and coming way for lessening the electricity usage of the electrolysis process. Actually, the ODC is an alkaline fuel cell cathode which prevents hydrogen formation. The fundamental idea of the technology is the reaction of oxygen with hydrogen ions at the negatively charged compartment of the cell (Millet, 2013). As a result, hydrogen is not co-produced and the cell's voltage declines between 20% and 23% compared to the working voltage of a typical membrane cell. Consequently, the energy consumption of the ODC membrane cell reduces approximately 30% assuming 4 kA/m² current density (Jung et al., 2014).

To sum up, the application of both ODC and the typical membrane cell electrolysis can facilitate the chlor-alkali industry to achieve better environmental performance through fewer energy requirements and rationale utilization of raw materials. Particularly, investments in the ODC technique can drastically scale down the industry's impact on the environment since its main benefit besides less energy demand is the absence of hydrogen production, which otherwise had to be involved in the manufacturing process. This is the reason that gave prominence to the European chlor-alkali industry start implementing the particular technique, which contributes about 4% to the overall chlorine production (Eurochlor, 2019a).

3.3 Chlor-alkali products: Market prices & channels

The production of chlorine via brine solution electrolysis is interdependent with the co-production of caustic soda and hydrogen. These three products have a plethora of applications in multiple industries. Table 6 shows the market value of chlor-alkali products. Despite that the market price of hydrogen is higher than that of chlorine and caustic soda, the profits from caustic soda are greater due to its larger production capacity. The following subsections concern an overview of the utilization pathways of the chlor-alkali products in Europe.

Table 6: The market value of the chlor-alkali products in Europe (EU of 28) (Eurostat, 2018)

Product	Quantity (kg)	€/kg	Margin Profit (€)	Profit Share (%)
Chlorine	1	0.172	0.172	29.1
Sodium Hydroxide (50 wt %)	1.1	0.321	0.353	59.6
Hydrogen	0.028	2.380	0.067	11.3
			0.592	

3.3.1 Elemental Chlorine

Chlorine constitutes an element that can be found in all facets of our everyday life. In some cases, chlorine is part of the end-product but more commonly it is used in the manufacturing process of other industrial products. Chlorine is popularly known as a disinfectant in swimming pools and drinking water systems. Nevertheless, its wide industrial application concerns its use as an intermediate for the production of medicines, chemical products and plastics. Specifically, in Europe, 55% of the total output of the chemical industry is inextricably linked to chlor-alkali products (Eurochlor, 2019a).

Table 7 delineates the applications of chlorine in Europe for 2017 when the overall production capacity had reached 9,915 kilotons. In Europe, over one-third of the total chlorine output is used for the manufacturing of polyvinyl chloride (PVC) and other synthetic plastics based on chloromethane, which then can be used in the construction, agricultural, pharmaceutical and automotive sectors. Additionally, 34% is bound for polyurethane materials production which is extensively used in surface coatings and elastomers.

As far as the pharmaceutical sector is concerned, 88% of breakthrough medications depends on chlor-alkali products for their synthesis. Based on chlorinated solvents, drugs for cholesterol and asthma care can be produced. Furthermore, medicines for diabetes, depression and blood pressure rely on chlorine for their manufacturing (Eurochlor, 2019a).

Table 7: Chlorine applications in Europe, 2017, (Eurochlor, 2019a).

Chlorine applications	kilotons	share
Isocyanates and Oxygenates	3,380	34.1%
PVC	3,200	32.3%
Inorganics	1,234	12.4%
Other Organics	903	9.1%
Solvents and Epichlorohydrin	788	7.9%
Chloromethanes	410	4.1%
Total	9,915	

3.3.2 Sodium Hydroxide – Caustic Soda

Sodium hydroxide constitutes a co-product obtained through chlorine's manufacturing process. Caustic soda's commercial form has two types – a 50 wt% solution (most prevalent) and less often in a solid-state (Brinkmann et al., 2014). By and large, caustic soda is used in a broad variety of industrial applications across multiple domains. Table 8 displays the major applications of caustic soda in 2017. That year the total production capacity in Europe was 9,836 kilotons.

Table 8: Caustic soda applications in Europe, 2017, (Eurochlor, 2019a).

Caustic soda applications	kilotons	share
Organics	3,206	32.6%
Miscellaneous	1,619	16.5%
Phosphates	91	0.9%
Mineral oils	167	1.7%
Rayon	179	1.8%
Bleach	350	3.6%
Alumina and other metals	354	3.6%
Soaps	368	3.7%
Water treatment	466	4.7%
Food industry	591	6.0%
Other inorganics	1,126	11.4%
Pulp, Paper and cellulose	1,319	13.4%
Total	9,836	

As it can be noticed, there are a plethora of industrial applications where caustic soda is involved. Approximately half of its capacity finds use in the production of organic and miscellaneous chemicals. Moreover, 13.4% of the total caustic soda production in Europe was used for recycling and recovering necessary raw materials for pulp and paper industry.

Sodium hydroxide is a constitutive element for the construction sector since it facilitates the separation of alumina from bauxite. Alumina is transformed into aluminium, which is a necessary material in constructions. Furthermore, 6% is used by the food industry and especially for food preservation, 4.7% for water treatment applications and 3.7% by soap and cosmetic industries. Lastly, the rest of caustic soda output is split into multiple other applications, including its use as a bleach, LED light bulbs manufacturing process as well as in the pharmaceutical industry for drugs development such as aspirin.

3.3.3 Hydrogen

Hydrogen is another co-product obtained from salt solution electrolysis. Its production adds value to the whole chlorine manufacturing process since it constitutes an alternative source of energy production which can alleviate the energy demand of sub-processes that otherwise would consume energy from external sources. The end hydrogen-product is highly concentrated (over 99.9 vol %), thus not requiring special treatment (Brinkmann et al., 2014).

In most cases, hydrogen produced via membrane cell electrolysis has two exploitation channels. It can be used either as a fuel for energy generation or as a reagent in chemical reactions. The first channel concerns its on-site combustion for steam and electricity generation while the second one consists of its use for the chemical formation of methanol, hydrochloric acid and ammonia (Brinkmann et al., 2014). Less frequently, hydrogen is sold to hydrogen marketers or released to the atmosphere.

Despite the fact that hydrogen is indicated as an essential contributor to the decarbonization of industrial activities, in Europe, its exploitation either as reagent or as a fuel in chlor-alkali plants is gradually decreasing. Specifically, its utilization rate has fallen since 2010 (90.4%) by 5.6% (2017) (Eurochlor, 2019a). An explanation to the latter can be that its utilization requires further investments in facilities while there are still other alternatives available.

3.4 The European Chlor-alkali industry: figures & facts

The chlor-alkali sector is the foundation for more than half of the European chemical industry. On a European level, the particular industry gives employment to approximately 7,500 individuals, while a plethora of jobs are linked with the various utilization pathways of the chlor-alkali products. As of 2018, the industry produced 11,268 kilotons of chlorine, 7.0% below of the previous year output and 9.3% below the 2016 level of production respectively (Eurochlor, 2019a). Germany dominates the industry by manufacturing almost half of the overall European production capacity. On a country level, the key players are Belgium, France, the Netherlands and the United Kingdom. Figure 12 illustrates the major chlorine producer countries within Europe and their production capacity. Altogether, they manufacture more than 90% of the total European production.

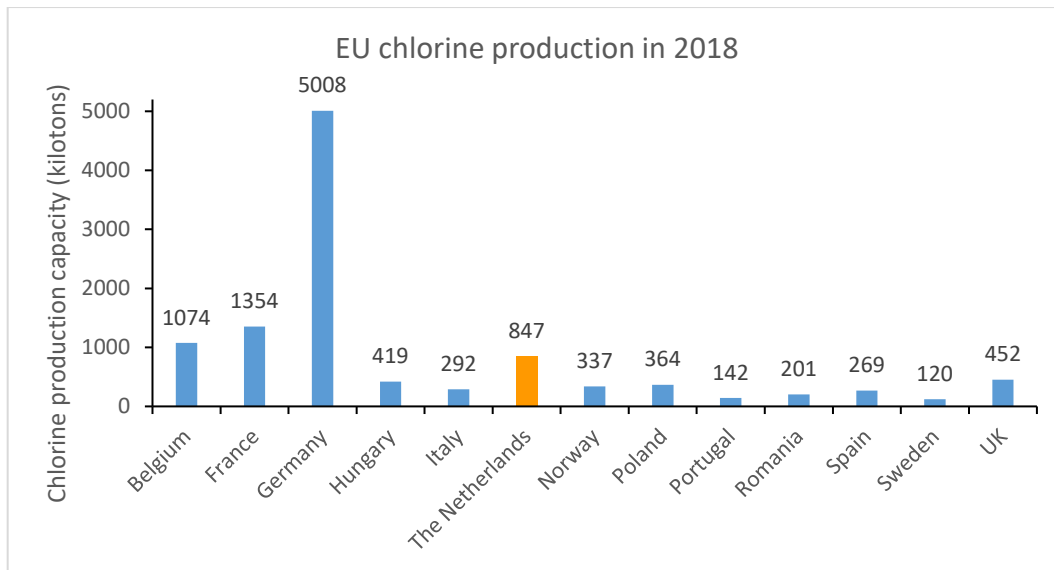


Figure 12: Main chlorine producer countries in Europe for the year 2018

The characteristic feature of the industry is that it consists of multiple energy-intensive processes that require huge amounts of electricity. Electrolysis is the most electricity-demanding process in a chlor-alkali plant. In particular, in 2010, the European chlor-alkali industry consumed 35 TWh (Brinkmann et al., 2014), while in 2017 the level of the energy consumption was decreased by approximately 10% (Eurochlor, 2019a), mainly due to the phase-out of mercury plants or their replacement by membrane cells.

As it is shown in Figure 13, the last two years there is a sharp decrease in chlorine production from mercury cell facilities, which currently account for 6% of the total output. On the contrary, diaphragm cells represent about 17% of the production level in 2018.

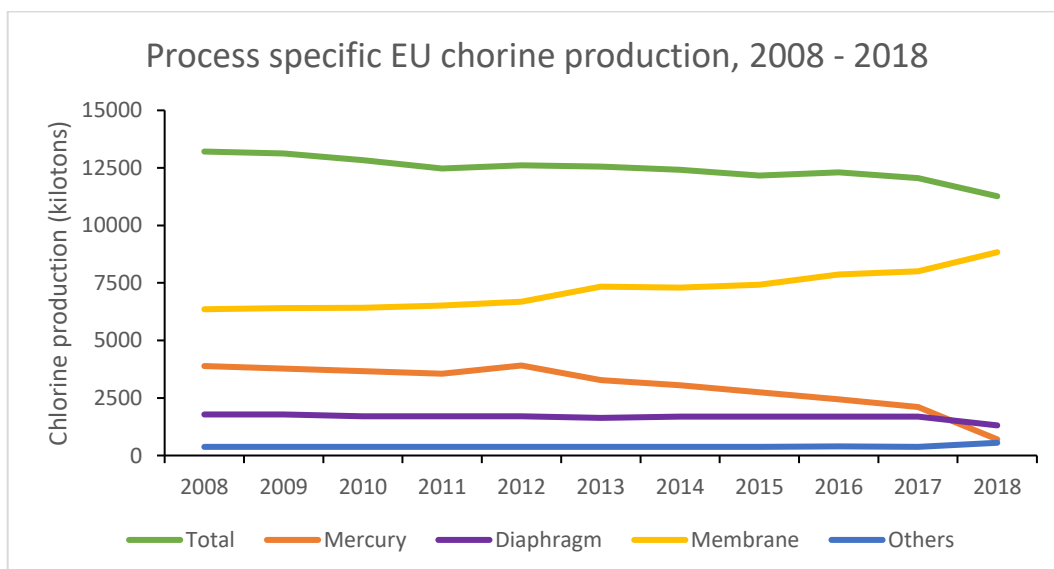


Figure 13: European chlorine production via mercury, membrane and diaphragm cells, 2008 - 2018 (Eurochlor, 2019a)

The technology that dominates the European chlor-alkali industry is the membrane cell electrolysis, accounting for more than three-quarters of the installations. In 2018, 8,834

kilotons of chlorine were produced because of the particular technology (Eurochlor, 2019a). For the same year, Germany, France, Belgium and the Netherlands together produced 72% of the total chlorine output via membrane cell electrolysis. Figure 14 outlines the main European countries that implement membrane cell electrolysis as well as their level of output.

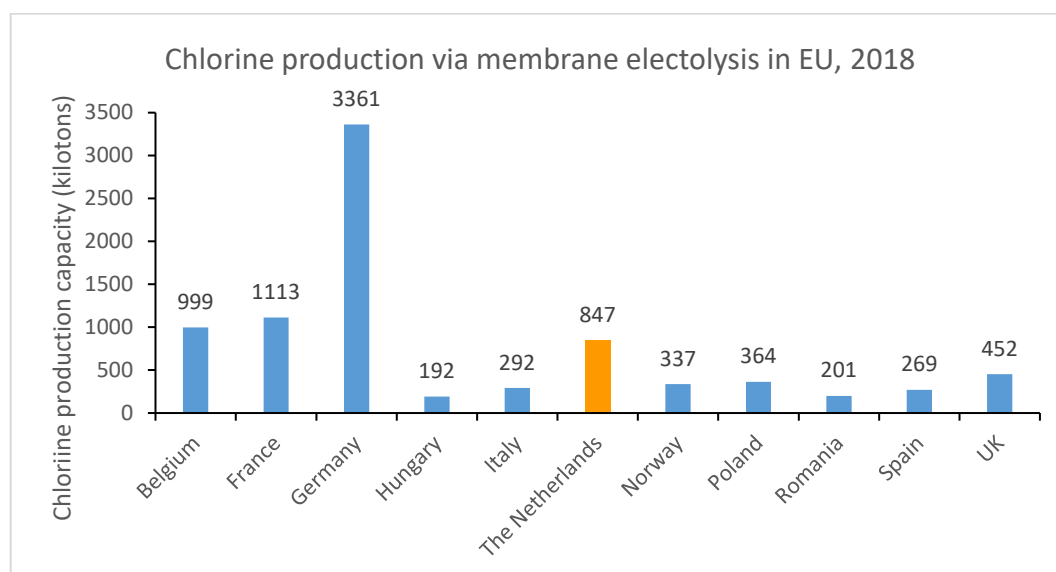


Figure 14: Chlorine production capacity via membrane electrolysis in the EU for the year 2018.

All technologies may result in chlorine and other chemical substances emissions to the environment during the manufacturing, treatment and storage processes. However, the main problem of the industry is concentrated on energy consumption and therefore to the indirect emissions caused by electricity generation. To meet the climate change targets set by the EU, which require 32% better performance in regards to energy efficiency, the European chlor-alkali industry needs to maintain the total energy consumption less than 2,229 Mtoe. To that direction, the industry strives to reach that target and reduce its overall energy consumption (approximately 4.1 Mtoe in 2015) by adopting an energy sharing system among EU countries, developing large-scale energy storage practices and using low-CO₂ electricity techniques (Eurochlor, 2018b).

3.5 Case study: The Dutch Chlor-alkali industry

The Netherlands is among the top-five chlorine producer countries in Europe. Specifically, 7.55% of the total European chlorine production is produced throughout the country. This number is equivalent to 847 kilotons of annual production. With this production capacity, the Netherlands is ranked as the fourth largest country of the European chlor-alkali industry.

In the Netherlands, two companies are mainly engaged in the chlor-alkali market– Nouryon (former AkzoNobel) and Sabic. Nouryon is considered the key player of the chlor-alkali industry, controlling almost 90% of the market. The companies' industrial facilities can be found on three different sides. In all plants, chlorine is produced through membrane electrolysis of undried vacuum evaporated salt solution. Nouryon's major operations in the Netherlands are located at the chemical industry park of Botlek. There, over 640 kilotons of chlorine are produced every year, thus, resulting in being the largest European facility of

membrane electrolysis. In addition to the latter, a membrane electrolysis facility, run by Nouryon, operates at Delfzijl. Delfzijl's membrane electrolysis installation yields 121 kilotons of chlorine annually. The competition in the Dutch chlor-alkali industry is enhanced by the presence of Sabic's (Saudi Basic Industries Corporation) at Bergen op Zoom. Sabic has entered the Dutch market since 2002 when it acquired DSM petrochemical company (Oil & Gas Journal, 2002). Furthermore, in 2007, Sabic has made a breakthrough by purchasing General Electric Plastics for \$11.6 billion and expanding its businesses in the Netherlands at the Chemelot chemical industry park (Bowman, 2007).

Table 9 gives an overview of the engaged actors in the Dutch chlor-alkali manufacturing industry as well as their market share and production capacity. The production capacity of caustic soda and hydrogen was calculated by applying the chemical law for the production of 1 ton of Cl_2 via brine electrolysis. It is worth mentioning that the overall chlorine production in the Netherlands is stable since 2015.

Table 9: Overview of the chlorine production in the Netherlands for 2018 (Eurochlor, 2019b)

Company	Site	Technology	Cl_2 Capacity (kilotons)	NaOH Capacity (kilotons)	H_2 Capacity (kilotons)	Share of Cl_2 production
Nouryon	Botlek	Membrane cell	637	700.7	11.5	75.21%
Nouryon	Delfzijl	Membrane cell	121	133.1	2.2	14.29%
Sabic	Bergen op Zoom	Membrane cell	89	97.9	1.6	10.50%
			847	931.7	15.3	100%

The manufacturing of chlorine is energy and resource-intensive process. As a consequence, huge amounts of GHG emissions are released to the atmosphere. According to Brinkmann et al. (2014), the energy demand in chlor-alkali plants comes from four main stages:

- Raw materials preparation (mainly salt)
- Electrolysis process
- Steam generation for caustic soda concentration (0.4 to 1.5 tons of steam per ton of caustic soda at 100%)
- Supporting equipment (compressors, pumps, heating devices etc.)

Energy can be utilized either as electricity or heat. In the Netherlands, the manufacturing of one kiloton of chlorine requires approximately 3,000 MWh of electric energy. As Scherpbier (2018) discussed in his paper, the particular production level results in 0,21 kilotons of direct CO_2 emissions to be released in the atmosphere. However, the indirect CO_2 emissions account for the greatest part of the environmental damage, due to the fact that the Dutch power system, which is dependent on fossil fuels, mainly covers the electricity demand of the chlor-alkali facilities. Precisely, the Dutch electricity mix is based on 12.1% coal and coal products, 38.5% curdle oil, 41.2% natural gas and 8.2% renewable energy resources (CBS, 2018).

Based on the Energy Agenda of 2016, the Dutch parliament has drawn the direction towards the decarbonization of the national economy by reducing about 50% the direct GHG emissions in 2030. In line with that, the Dutch chemical industry and specifically Nouryon attempts to

adopt sustainable practices and enhance its social and environmental performance (Klein, Ybema, & de Vries, Interview, 2019).

Specifically, Nouryon speciality chemicals, which is a B2B company with a large number of energy-intensive processes, is focused on decreasing CO₂ emissions and energy consumption by adopting the most cost and resource-efficient practices. In 2017, Nouryon reduced its CO₂ equivalent emissions per ton of sold products by 7%, compared to the reference year of 2012. In addition, the company's climate change target concerns a further 25-30% reduction in CO₂ emissions by 2020 and become carbon neutral by 2050 (AkzoNobel, 2017).

For that purpose, Nouryon is willing to reduce the associated environmental burdens by adopting practices to meet the standards of a bio-based and circular economy. Firstly, its collaboration with Phillips, Google and DSM will ensure green energy supply from the Bouwdokken wind park to the chlor-alkali plant at Delfzijl, which is estimated to reduce CO₂ emissions by approximately 100 kilotons per year (AkzoNobel, 2017). Moreover, at the same industrial chemical park, Nouryon aspires through its partnering with Gasunie New Energy to set up a water electrolysis unit with a view to converting electricity generated by renewable energy resources into green hydrogen (Gasunie, 2018). Additionally, the company established a joint venture with Enkchem, Air Liquide, the City of Rotterdam, the Port of Rotterdam, the Province of Zuid Holland and Innovation Quarter, aiming at generating methanol by the gasification of waste from landfills and incineration. The particular endeavour is estimated to bring over 250,000 tons of CO₂ emissions reduction annually (AkzoNobel, 2017).

The abovementioned actions had led the company to obtain in 2017 the first position on the Dow Jones Sustainability Index among other chemical companies. Overall, the sustainability dimension of Nouryon is strengthened by being committed to the national environmental laws and regulations and by taking over environmental clean-up costs and relevant compensations. Lastly, the company's supplier sustainability program facilitates Nouryon to environmentally-wise select its partners and suppliers (AkzoNobel, 2017).

3.6 Nouryon's chlor-alkali plant at Rotterdam

Nouryon's chlor-alkali plant at Botlek was selected as the case study of this project. The environmental profile of the particular plant was structured in terms of its carbon footprint due to the overall power and heat consumption for chlorine production purposes. Along with the environmental profile, an economic assessment consisting of costs from environmental externalities, operational costs and benefits from sold production delineate the overall performance of the plant. In line with the resource and energy requirements of the particular system, the enviro-economic profile of three alternatives was examined.

Several reasons led to the selection of the particular production system. Besides representing Nouryon's largest industrial chemical facility, Botlek's chlor-alkali plant is ranked among the top five plants based on its annual production in Europe. Additionally, in terms of the technology used for the electrolysis process, Nouryon runs the largest membrane electrolysis facility, which is one of the main interests of this study. Furthermore, an underlying reason for this decision is Nouryon's endeavours to modify the electrolyzers from gap-cell technology to zero-gap cells (Klein, Ybema, & de Vries, Interview, 2019).

Specifically, Delfzijl's chlor-alkali plant is exclusively based on zero-gap membrane cells, while chlorine production in Botlek is achieved via gap-cells dominantly. The selected system includes several processes for the treatment and manufacturing of the final products. The main energy and material resources that enter the system are electricity, heat, vacuum salt, demineralized water as well as small amounts of hydrochloric acid (HCl) provided by Nouryon's clients. Cool water at 17 °C, obtained through reverse osmosis, is supplied from a water company operating at the chemical industrial cluster of Rotterdam. Botlek's plant requirements in salt are covered by Delfzijl's salt manufacturing plant (Nouryon's property). Inland ships transport 800 ton on a daily basis (distance: 300km approximately). In order to avoid environmental impacts during salt transportation, the vast majority of the inland vessels use liquefied natural gas fuel (Klein, Ybema, & de Vries, Interview, 2019).

Botlek's plant is distinguished in three major operating phases for chlorine production. The first phase consists of all sub-process involved in the pretreatment of the raw materials that enter in the system. In the second phase, i.e. chlorine manufacturing phase, chlorine is produced via membrane electrolysis. Along with chlorine, caustic soda and hydrogen are coproduced in the manufacturing phase. The last phase concerns the processing of the products obtained in the manufacturing phase. Next, the functionality of the system is concisely described.

23% concentrated brine along with 30% caustic soda, coming from the brine preparation (stage 1) and the caustic soda treatment stages (stage 2), feed the electrolyzer. From the electrolysis process (stage 3), three production lines occur – chlorine, caustic soda and hydrogen. Before reaching its commercial form, chlorine has to be cooled (stage 4), dried (stage 5), compressed (stage 6) and liquefied (stage 7). Like chlorine, hydrogen needs to pass through two stages of treatment before its on-site final use or sale; cooling and compression respectively (stage 8 & 9). Caustic soda at 50% concentration is obtained through multiple-effect evaporation (stage 10), where around 80% of the overall heat demand in the form of steam is consumed. A schematic illustration of the main production stages of the chlor-alkali plant is shown in Figure 15 (chapter 4). All pertinent to the system mass input and output data are displayed in Appendix A, obtained from the Best Available Techniques (BAT) Reference Document for the Production of Chlor-alkali (Brinkmann et al., 2014) and the thesis report of Scherpbier (2018).

Moreover, heat demand is covered by an on-site natural-gas-fired co-generation heat and power (CHP) facility and a waste heat recovery system with 81% maximum efficiency. The CHP plant covers around 10% of the total electricity requirements, while the rest power is supplied by the national electricity grid. Data regarding energy requirements are represented in table 16 (section 4.3).

In the course of the thesis, an interview with Nouryon's experts was conducted in order to grasp further insights about the chlor-alkali plant at Botlek as well as to discuss their considerations regarding future developments of the industry.

Currently, the company examines carbon-neutral technological practices for chlorine production in order to reduce overall electricity and energy requirements. According to Klein, Ybema, & de Vries (Interview, 2019), biomass boilers are considered as a carbon-neutral source for heat generation, which can be used instead of or along with the CHP plant for the vaporization of caustic soda. An alternative option is to cease on-site energy generation, and

instead, develop a network of pipelines that will connect the plant with off-site heat generation facilities. Besides heat requirements, as it was previously mentioned, the Achilles' heel of the system is the huge amount of power needed in the electrolysis process. From the literature research, ODC technique and zero-gap membrane cells electrolyzers are the spotted out alternatives that could lead to a reduction in electricity demand. In line with Klein, Ybema, & de Vries (Interview, 2019), the associated high capital investments as well as the absence of hydrogen production, which can be used either externally (supplying their clients) or internally for heating purposes, constitute the main reasons that the ODC technique fails to meet Nouryon's expectations for a profitable and eco-friendly way for chlorine production. On the other hand, the zero-gap membrane cells electrolysis guarantees the co-production of all chlor-alkali products with fewer power needs. To that end, the company's experts consider zero-gap cells as an unattractive option to invest in, due to the fact that the same level of chlorine production can be achieved with less electricity consumption (Klein, Ybema, & de Vries, Interview, 2019).

Taking all the above-mentioned into account, the zero-gap membrane cells and biomass boilers were chosen to be assessed from a life-cycle perspective. These practices along with the reference case will be examined if can potentially lead Nouryon to better enviro-economic performance and thus, reach the climate change targets set on the Dutch Energy Agenda of 2016.

Chapter 4: LCA & LCC Methodology

This chapter discusses the implemented methodology which follows the enviro-economic impact analysis structure developed in chapter 2. In consonance with the ISO 14040 and ISO 14044 standards, the report is structured in four distinct phases: a) the goal and scope of the study, b) the inventory of data, c) impact assessment along with estimations for the operational and environmental costs and lastly, d) the interpretation of the results. The next sub-sections summarize certain research decisions and assumptions that were made. Additionally, an overview of the used energy, material and economic data is provided on the inventory lists of the LCA and LCC analysis. These data can be found throughout chapter 4. Finally, specifications about the characteristics of the analysed technologies become available in sub-section 4.1.5, “Description of the scenarios under evaluation”.

4.1 Goal and Scope definition

4.1.1 Goal of the study

Our primary goal is to carry out an enviro-economic impact assessment analysis of Nouryon’s chlor-alkali plant at Botlek by applying LCA and LCC techniques in an integrated manner. For this, we aim to quantify the environmental burdens from energy and resource consumption at different chlor-alkali production stages and estimate the consequent private and externality costs. To estimate the associated externality costs, we implement different economic weighting factors that are based on a variety of valuation methods through which environmental burdens can be converted into monetary terms. By doing so, we further aim to identify which weighting set and thus valuation method can lead to sound and generalizable results with respect to the present life-cycle study.

Under this project, four scenarios were investigated and compared in regards to three different aspects – environmental profile, energy consumption and economic performance. In that sense, by implementing the NPV rule and analyzing the environmental profile of the considered scenarios, the outcome of the analysis will point out which scenario has better enviro-economic performance. An additional target is to determine the “hot-spots” in terms of process-contribution to the overall environmental impact of the chlor-alkali manufacturing plant for each scenario and discuss opportunities for improvement.

4.1.2 Scope definition & System boundaries

The scope of the project is from “gate-to-gate”, concerning the modelling of the energy, mass, and money flows that take place within the factory (entry-to-exit) and are required to sustain the level of chlorine production stable.

To achieve our goal, we first defined the boundaries of the analyzed system. The system boundaries give an illustration of the time and geographical orientation of the analysis as well as what is included and excluded from the evaluation scope.

The spatial limits of the study concern the production stages of the examined chlor-alkali plant. Moreover, the modelled energy and mass flows are in line with the production year of 2018. Figure 15 portrays the system boundaries of the present study. The production system is divided into three major phases – materials pretreatment, chlorine manufacturing and products processing phases. The first phase consists of the brine and caustic soda preparation stages. The manufacturing phase includes the membrane electrolysis stage as well as the plant's recirculation system. The last phase concerns all sub-processes involved in the processing stages of chlorine, caustic soda and hydrogen until they reach their commercial form. Additionally, in the system boundaries is also included the CHP facility that covers the heat requirements of the production system and covers almost 10% of the total power demand.

Salt mining, products' transportation, waste treatment are excluded from the study since they are out of the selected "gate-to-gate" orientation. Additionally, both the construction work that is required for the installation of new technological systems and equipment maintenance are out of the evaluation scope because previous studies have reported that their share in the overall environmental impact is small due to their long lifespan (Falano, Jeswani, & Azapagic, 2014).

LCC and LCA share the same system boundaries. To that end, money inflows (sold product revenues) and outflows (internal costs along with costs from environmental burdens) arisen from the abovementioned production stages delineate the key features of the LCC analysis. However, as it was highlighted in section 2.2, that LCC can be interpreted as an actor-based economic assessment. Therefore, a decision regarding whose economic-perspective to take into consideration should be explicitly defined. For that purpose, the economic evaluation of this study is conducted from the manufacturer's perspective (Nouryon). As such, since the LCC's scope is manufacturer-cantered we expand our economic analysis in order to investigate which technical modification can yield maximum profits considering two economic aspects – required capital investments (scope's expansion) and total production costs (gate-to-gate). In this report, total production costs refer to the summation of all private costs that are associated with the production and operation of the considered chlor-alkali plant and the environmental costs as a consequence of the identified environmental damages. Regarding the latter five different economic weighting factors were used in the weighting phase of LCA in order to monetize the identified environmental burdens. Lastly, due to the fact that chlorine production takes places in a multi-actor chain, we attempt to come up with an estimation of the overall environmental costs attributed to the chlor-alkali chain by distinguishing environmental impacts in on-site and off-site generated ones.

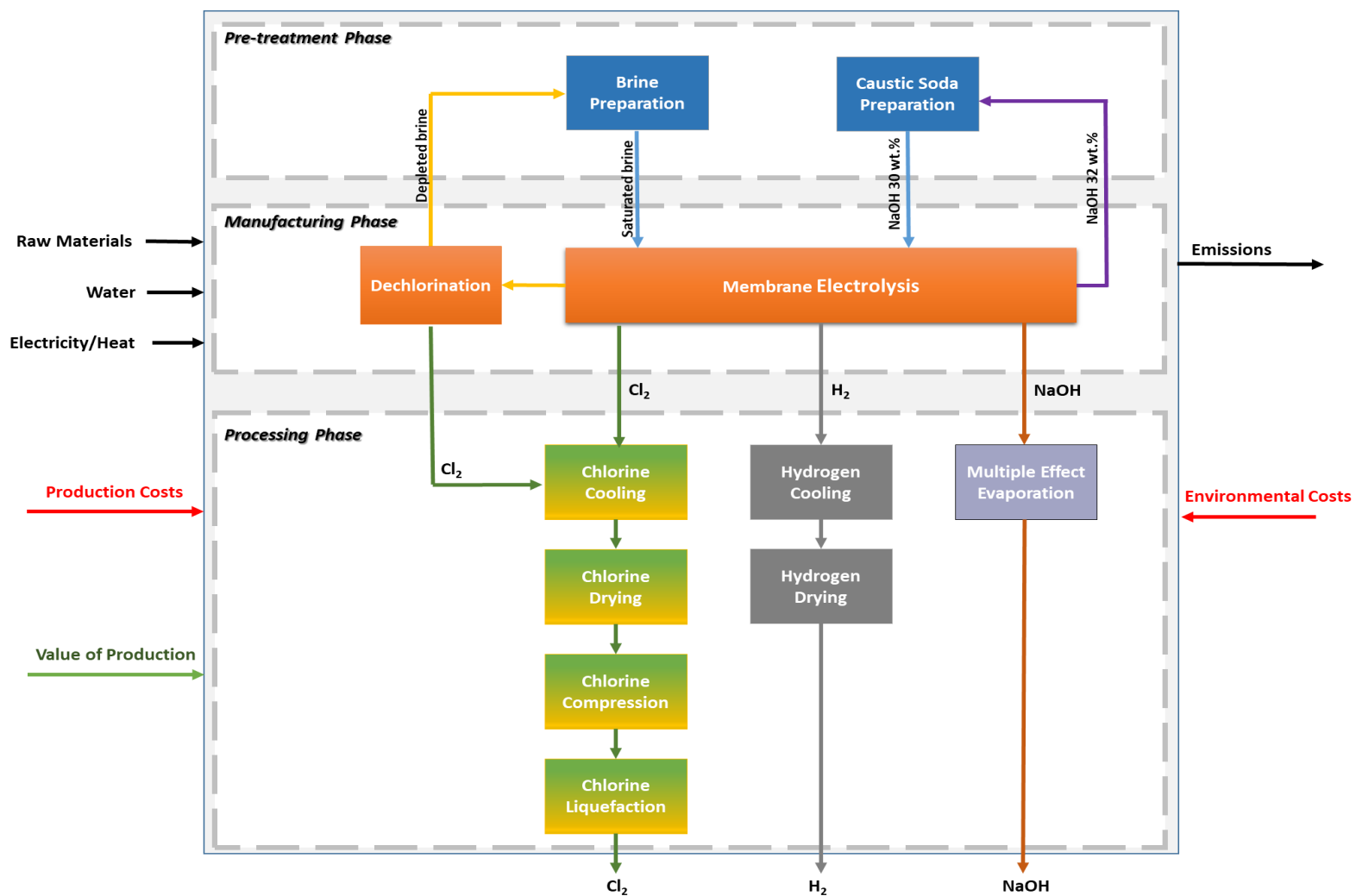


Figure 15: Systems boundaries of the study

4.1.3 Intention and audience of the study

Though the combined application of LCA and LCC has gained some prominence and several integrated studies do already exist, none of them is exclusively focused on the enviro-economic assessment of the Dutch chlor-alkali industry. As such, our primary intention lies in bridging the pertinent knowledge gap by conducting an integrated life-cycle analysis on the basis of environmental externalities monetization through five LCA-related economic weighting sets, which are based on different valuation methods.

Additionally, by carrying out this project, we intend to inform academia, Nouryon and the Dutch chlor-alkali industry about which technical practices and innovations can lead to better enviro-economic performance with respect to the examined chlorine production system. Therefore, the audience of our research's outcome is both academia and the industry's managers, with the ultimate aim to inspire and incentivize them for further actions and research in the particular field.

4.1.4 Functional unit

Determining the functional unit of the analysis is the next step of the implemented structure. The role of the functional unit lies in the development of a common ground upon which the environmental impacts of the four scenarios (see subsection 4.2.5) can be compared. The function of the system under which all scenarios are developed involves the production of chlorine. This results in the co-production of caustic soda and hydrogen. The level of the chosen functional unit is 1 ton of chlorine output, produced via membrane electrolysis. This level of production implies the co-generation of the other two products in the fixed stoichiometric ratio given in subsection 3.1 (1.1 ton of NaOH and 0.028 ton of H₂). Similarly, the function, functional unit and reference flows were defined for the LCC analysis, with the only difference being the unit of measurement – euros per ton of chlorine. Table 10 summarizes the function of the system, the functional unit, and the reference flows for the LCA and LCC analyses.

Table 10: LCA & LCC's systems function, functional unit and reference flows

LCA	
Function	Production of Cl ₂ with co-production of NaOH and H ₂
Functional Unit	1 ton of Cl ₂
Reference flows	Production of 1 ton of Cl ₂ by a gap cell membrane electrolysis Production of 1 ton of Cl ₂ by a zero-gap cell membrane electrolysis
LCC	
Function	Production of Cl ₂ with co-production of NaOH and H ₂
Functional Unit	€ / ton of Cl ₂
Reference flows	Costs from the production of 1 ton Cl ₂ by a gap cell membrane electrolysis Costs from the production of 1 ton Cl ₂ by a zero-gap cell membrane electrolysis

4.1.5 Description of the scenarios under evaluation

The membrane cell technology constitutes the best available technique for chlorine production (Brinkmann et al., 2014). Despite its better environmental performance compared with the mercury and diaphragm cell technologies, it still requires substantial amounts of electricity and heat. As it was mentioned in subsection 3.6, Nouryon investigates what are the best available options for reducing power and heat demand while keeping the level of

production stable. In consonance with Nouryon's considerations, four scenarios were developed in order to assess their enviro-economic performance from a life-cycle perspective in regards to energy and resources consumption. Assuming steady-state production systems, the considered scenarios consist of modifications in the configuration type of the membrane cell. Additionally, two different industrial installations for heat generation purposes are involved. In particular, an on-site natural-gas-fired co-generation heat and power (CHP) facility which co-produces heat and power at a ratio 2:1 and a biomass boiler industrial installation for heat production are examined in this study. For all scenarios, brine, electricity, heat and water are the main inputs in the considered chlorine production system. Overall data used for the development of the following scenarios are displayed in Appendix A. In the following subsections an analysis regarding the specifications of each scenario as well as the sources from which data were gathered takes place.

4.1.5.1 S0: Reference case (base-case scenario)

The particular scenario represents the "do nothing option". Pertinent energy and resource requirements were gathered by the thesis report of Scherpbier (2018), *"The energy transition in the Dutch chemical industry"*, which concerns the modelling of the material and energy inputs and outputs of the Dutch chlor-alkali industry.

For this scenario, the underlying assumption is that sodium chloride is decomposed to chlorine and caustic soda exclusively by gap cell membrane electrolyzers. The electrolyzer is supplied with 20 ton of 23 wt. % saturated brine for the production of 1 ton of chlorine. Caustic soda in 50% solution is concentrated by means of multiple effect evaporation, requiring 0.7 GJ of heat in the form of steam.

An on-site natural-gas-fired CHP facility co-produces heat and power at a ratio 2:1 (1.89 GJ heat and 0.99 GJ electric per ton of Cl₂), covering 56% of the overall heat requirements and almost 10% of the total electricity demand. Approximately 2,850 kWh electricity is supplied by the Dutch power grid for the production of one ton of chlorine. Moreover, an installed waste-heat recovery system (recovering 81% of waste heat thus being capable to recover 1.85 GJ heat per ton of Cl₂ maximum) provides 1.51 GJ heat/ton Cl₂ to the pretreatment stages of caustic soda and brine.

To produce 1 ton of Cl₂ the membrane electrolysis plant consumes around 3,000 kWh (Brinkmann et al., 2014). According to Brinkmann et al. (2014), the maximum current density of the electrolytic room in a membrane cell plant is between 600 and 700 mA/cm². Under these conditions, the cell's room voltage (V) should be:

$$V = \frac{P}{I} \quad (4.1)$$

Where P is the power consumed and I is the current density that the cell operates. Thus, by using the abovementioned equation the cell's voltage is between 4.4 V and 5.1 V respectively. Assuming current density 700 mA/cm² and cell voltage 4.4 V, then, an estimation in regards to the number of electrolyzers and their capacity is presented in table 11. Table 11 also shows the specifications of the electrolyzer in terms of inputs and outputs as they were displayed by Scherpbier, (2018) and Brinkmann et al. (2014). To sustain the chlorine production capacity

stable (637 kton/year), 21 gap-cell configuration electrolyzers with 30.5 kton/year maximum output were estimated.

Table 11: Features of the membrane electrolysis cell in the S0 scenario per ton of chlorine output (Brinkmann et al., 2014; Scherpbier, 2018)

Feature	Value
Current Density	700 mA/cm ²
Cell voltage	4.4 V
Energy demand	3,055 kWh/ton Cl ₂
Brine 23% input	20 ton
NaOH 30% input	38 ton
Brine 17% output	18 ton
NaOH 32% output	3.5 ton
H ₂ output	0.028 ton
Waste heat output	2.2 GJ
Number of cells	210
Number of electrolyzers	21
Single unit capacity	30.5 kton Cl ₂ per year

4.1.5.2 S1: Zero-gap membrane cell electrolysis

Zero-gap membrane cell technology is represented by S1. In this case, gap-cells are replaced with zero-gap cells, keeping all other parameters stable. As it was discussed in sub-section 3.2, the deployment of the particular configuration results in lower raw materials per ton of output, higher operating efficiency and less energy consumption. Specifically, the amount of vacuum salt in solution that is supplied in the brine preparation stage is reduced by 56% with respect to the reference case. Furthermore, around 1,860 kWh are required from the zero-gap electrolytic cell to produce one ton of Cl₂ (Scherpbier, 2018). Assuming 2.8 V cell's voltage (Klein, Ybema, & de Vries, Interview, 2019), table 12 demonstrates the attributes of the zero-gap membrane cell, as well as the number and the capacity of the required electrolyzers. Zero-gap electrolysis cell's specifications in terms of inputs and outputs are available in the pertinent literature (Brinkmann et al., 2014; Scherpbier, 2018; Schmittinger, 2008).

Table 12: Features of the membrane cell electrolysis of S1 per ton of chlorine output (Brinkmann et al., 2014; Scherpbier, 2018; Schmittinger, 2008)

Feature	Value
Current Density	665 mA/cm ²
Cell voltage	2.8 V
Energy demand	1861 kWh/ton Cl ₂
NaOH 30% input	32 ton
Brine 17% output	15.3 ton
NaOH 32% output	2.9 ton
H ₂ output	0.09 ton
Waste heat output	1.6 GJ
Number of cells	170
Number of electrolyzers	20
Single unit capacity	31.6 kton Cl ₂ per year
Capital Investment	120 €/ton Cl ₂

CHP's working conditions and level of output remain the same as they were illustrated in the reference case. More insights about the mass and energy flows of S1 per chlor-alkali production stage are displayed in Appendix A.

4.1.5.3 S2: Biomass boilers for steam generation

As far as the membrane cell's configuration type, energy, and material requirements are concerned, S2 is identical to the reference case. However, the key distinction between them lies in the way on-site heat is generated. While in the reference case a natural-gas-fired CHP facility is used to cover heat demand, in case of S2, the CHP plant is replaced with biomass boilers. Table 13 demonstrates the technical specifications of biomass boilers, their operating conditions as well as the assumptions made to structure the particular scenario.

Table 13: Main features of biomass boilers installation

Feature	Value	Unit
<i>Biomass Boilers- Specifications^[1]</i>		
Power	2	MW
Energy efficiency	85	%
Maximum working pressure	22	bar
Steam temperature	200	°C
Capital Investment ^[2]	246.9	€/kW
<i>Feedstock^[3]</i>	Wood pellets	
Moisture content	8	%
Net calorific value of feedstock	4.8	kWh/kg wood pellet
Load capacity	0.09	ton of wood pellet/ton Cl ₂
Price	235	€/ton of wood pellet
<i>Transportation^[3]</i>	EURO5 truck 16-32 metric ton	
Distance covered	100	km
Freight transportation	9	tkm
<i>Final output</i>		
Number of installed units	19	
Capacity	987.32	TJ/year
Steam	1.55	GJ/ton Cl ₂

[1] Gandras, (2019), [2]including acquisition, installation and pipework costs (University of Strathclyde, 2019); [3]European Pellet Council, (2017)

Using as feedstock organic material such as wood pellets and chips, biomass boilers can be deployed for heat production in the chlor-alkali industry. Biomass combustion is considered to be a green solution for heat generation with a low level of CO₂ emissions in the long-run (Klein, Ybema, & de Vries, Interview, 2019). The critical decision to be made concerns the fuel choice. The key criteria for the selection of the appropriate feedstock were its energy and moisture content as well as its price.

For this scenario, wood pellets with 8% moisture content and 4.8 kWh/kg energy density, transported by EURO5 trucks from a distance of 100 km, was selected as the feedstock to the

boiler (García, Gil, Rubiera, & Pevida, 2019). Based on available industrial applications, a 2 MW biomass boiler system, with 22 bar maximum working pressure and 85% efficiency, capable of producing steam at 200 °C was assumed (Gandras, 2019). Under these working conditions and assuming that the annual chlorine production capacity is stable (637 kton Cl₂/year), nineteen biomass boilers are required for the generation of 987.3 TJ heat/year. Due to the fact that biomass boilers do not generate electricity, it was assumed that total electricity requirements are covered by the national electricity grid exclusively. Specifically, 275 kWh is the additional electric power provided by the Dutch grid with respect to the reference case scenario.

4.1.5.4 S3: Total application of Biomass Boilers and zero-gap cells

S3 concerns the complete application of zero-gap membrane cells along with biomass boilers for heat generation. Same operating conditions for the membrane cell electrolyzers as in S1 are considered, as well as for biomass boilers in S2. However, compared to S2, in S3 two boilers less are required to cover total heat demand.

4.1.6 Allocation

Allocation procedures are required in LCA studies when multifunctional processes exist, i.e. processes that generate more than one products. That's the case with the membrane electrolysis process in chlor-alkali plants, where its multifunctionality lies in the co-production of chlorine, caustic soda and hydrogen. Allocation facilitates the attribution of the identified environmental impacts to the different functions of the system. To deal with the multifunctional issue of the membrane electrolysis process, two allocation procedures were implemented: economic and mass allocation. The former concerns the attribution of the environmental impacts to the functional flows based on the amount of production and its economic value, while the latter is only based on the amount of output. Table 14 and 15 present the mass and economic allocation factors for the four scenarios respectively. Economic allocation was based on Eurostat's 2012 market prices (see table 6, subsection 3.3).

Table 14: Mass allocation factors

Products	S0	S1	S2	S3
Chlorine	0.2208	0.2506	0.2208	0.2506
Hydrogen	0.0062	0.0226	0.0062	0.0226
Caustic Soda	0.7730	0.7268	0.7730	0.7268

Table 15: Economic allocation factors

Products	S0	S1	S2	S3
Chlorine	0.1263	0,1306	0.1263	0,1306
Hydrogen	0.0489	0,1626	0.0489	0,1626
Caustic Soda	0.8248	0,7068	0.8248	0,7068

4.1.7 Selected impact categories

For the LCA analysis, SimaPro 8.5.2.0 software was used for the quantification of the environmental impacts. In this study, the ReCiPe 2016 v1.1 Endpoint method (E) and the ReCiPe 2016 v1.1 Midpoint method (E) are implemented (De Schryver, Brakkee, Goedkoop, & Huijbregts, 2009; Goedkoop et al., 2013). The particular method was selected due to its global

scope and recent introduction in the LCA field. The impact assessment was conducted under the prism of the Egalitarian (E) approach due to its preventive character, which is based on the assumption that environmental damages can evoke adverse effects to nature (Stougie, Tsalidis, van der Kooi, & Korevaar, 2018).

The results are obtained in two endpoint indicators and one midpoint. Specifically, the global warming potential (GWP) category is selected since it reflects climate change effects, one of the most worldwide talked-about topics which currently is at the top of the Dutch political agenda. Furthermore, the Human Health (HH) and Ecosystems (EC) endpoint indicators are included in this study due to the fact that they can provide indications regarding the extent to which the quality of life of every living being is affected by industrial activities. It worth mentioning that the selected endpoint and midpoint indicators are inextricably linked to each other. Specifically, global warming effects negatively influence the quality of human health and biodiversity.

4.2 Life-Cycle Inventory

In this section data used for the LCA are displayed. Table 16 outlines the foreground data used to identify the environmental impacts that stem from power and heat consumption in each scenario. This table is a summary of the energy data displayed in Appendix A and used for assessing the environmental profile of the four above-described scenarios. Data concern the process-specific as well as the overall heat and power requirements for the production of one ton of chlorine. Data regarding the reference case scenario were taken from the thesis report of Scherpbier (2018). S1 was developed following the suggestions and reports of the “Best Available Techniques (BAT) Reference Document for the Production of Chlor-alkali” (Brinkmann et al., 2014), the book “Chlorine: principles and industrial practice” (Schmittinger, 2008) and Scherpbier (2018). Specifically, these reports were used to capture data regarding the functioning and specifications of the electrolysis unit (see table 12) upon which S1 is based.

S1’s electricity requirements of all sub-stages involved in chlorine manufacturing phase remain the same with respect to the reference case since the amount of chlorine produced via the electrolyzer does not change. Taking into account the electrolysis specifications of Table 11 and Table 12, hydrogen production via zero-gap cells increases by approximately two-times more compared to the reference case, thus requiring a proportional increase in electricity requirements with respect to its compression stage. On the contrary, the amount of depleted brine that is sent back to the brine preparation stage and passes through the dechlorination stage is decreased by 15%. Therefore, compared to S0 the electricity requirements of S1 in the dechlorination stage decrease proportionally as required to remove residual chlorine.

Moreover, in the case of S1, it was assumed that the CHP’s working conditions and thus level of heat and electricity output are the same as of S0. As such, 1.89 GJ heat per ton of chlorine can be used to cover on-site demand and the rest requirements can be met via the waste heat recovery system. Since the amount of the recirculated products (NaOH 32% and depleted brine) and caustic soda that leave the electrolyzer and enter the pertinent processing stages decrease by 15% and 16.4% with respect to the reference case, an equivalent decrease in heat requirements of brine preparation, NaOH preparation and caustic soda processing stages it was assumed. As such, total heat requirements in S1 account for 2.858 GJ heat per ton of Cl₂.

CHP's total heat production is supplied to cover the overall demand of the NaOH preparation and processing stages, while the rest is covered by the waste heat recovery system. Furthermore, electricity generated by the CHP facility is supplied to cover the total requirements of the products' processing phase and part of the electrolysis process.

Table 16: Process-specific and overall power and heat requirements of each scenario per ton of Cl₂

Chlor-alkali stage	Source of energy	S0 ^[1]	S1	S2	S3
<i>Heat requirements – GJ consumed</i>					
Brine Preparation	CHP facility	0.00	0.052	0.00	0.00
	Recovered heat	1.20	0.968	1.20	1.02
	<i>Total</i>	<i>1.20</i>	<i>1.02</i>	<i>1.20</i>	<i>1.02</i>
NaOH Preparation	CHP facility	0.39	0.585	0.00	0.000
	Recovered heat	0.31	0.000	0.65	0.396
	Biomass boilers	0.00	0.000	0.05	0.189
	<i>Total</i>	<i>0.70</i>	<i>0.585</i>	<i>0.70</i>	<i>0.585</i>
Multiple Effect Evaporation	CHP facility	1.50	1.253	0.00	0.000
	Biomass boilers	0.00	0.000	1.50	1.253
	<i>Total</i>	<i>1.50</i>	<i>1.253</i>	<i>1.50</i>	<i>1.253</i>
Overall		3.40	2.858	3.40	2.858
<i>Electricity requirements – kWh consumed</i>					
Membrane Electrolysis	National grid	2,844.52	1,669.74	3,055.58	1,861.13
	CHP facility	211.06	191.39	0.00	0.00
	<i>Total</i>	<i>3,055.58</i>	<i>1,861.13^[2]</i>	<i>3,055.58</i>	<i>1,861.13</i>
Dechlorination	CHP facility	0.05	0.04	0.00	0.00
	National grid	0.00	0.00	0.05	0.04
	<i>Total</i>	<i>0.05</i>	<i>0.04</i>	<i>0.05</i>	<i>0.04</i>
Chlorine Compression	CHP facility	33.33	33.33	0.00	0.00
	National grid	0.00	0.00	33.33	33.33
	<i>Total</i>	<i>33.33</i>	<i>33.33</i>	<i>33.33</i>	<i>33.33</i>
Chlorine Liquefaction	CHP facility	21.67	21.67	0.00	0.00
	National grid	0.00	0.00	21.67	21.67
	<i>Total</i>	<i>21.67</i>	<i>21.67</i>	<i>21.67</i>	<i>21.67</i>
Hydrogen Compression	CHP facility	8.89	28.57	0.00	0.00
	National grid	0.00	0.00	8.89	28.57
	<i>Total</i>	<i>8.89</i>	<i>28.57</i>	<i>8.89</i>	<i>28.57</i>
Overall		3,119.52	1,944.74	3,119.52	1,944.74

[1](Scherpbier, 2018); [2](Brinkmann et al., 2014; Scherpbier, 2018; Schmittinger, 2008)

Regarding the membrane cell's configuration type, electricity, heat, and material requirements, S2 has the same specifications with the reference case. However, in this case, heat demand is covered by an on-site biomass boiler installation. Since biomass boilers do not co-produce electricity, it was assumed that total electricity requirements are covered by the national electricity grid. Given the technology specifications displayed in Table 13, 1.50 GJ heat/ton Cl₂ is supplied to the NaOH processing stage while the rest requirements are covered by the waste heat recovery system. With respect to the latter, it was assumed that the system works at its maximum efficiency, meaning it can recover 1.85 GJ heat/ton Cl₂. On the other

hand, in S3, sodium chloride electrolysis is achieved through the same cell's configuration type as in S1. As such, both have the same electricity requirements. However, in the case of S3, electricity demand is totally covered by the national power grid since the CHP facility has been replaced with biomass boilers. Given the number of the required units, biomass boilers, with respect to S3, can contribute to the system's overall heat requirements by supplying 1.44 GJ heat/ton Cl_2 to the processing and preparation of caustic soda stages while the rest demand is covered by the waste heat recovery system.

4.3 Life Cycle Costing Mathematical Formulas

The LCC technique is implemented to investigate the economic performance of the considered chlor-alkali plant with respect to the different developed scenarios. The present study applied a model for environmental and conventional life cycle costing to estimate the financial costs as well as to determine the economic impact of the identified environmental damages per ton of chlorine produced. To quantify the total production costs per functional unit of 1 ton of chlorine, the LCC analysis shares the same system specifications and time horizon with the LCA. The essential aspect of the particular model stems from the fact that besides the financial implications of each production system, the monetized environmental damages of each alternative are incorporated in the particular economic analysis.

The economic and ecological impacts are combined to compare the enviro-economic profile of each scenario. The external costs due to global warming effects (midpoint level) and due to environmental damages on human health and ecosystems (endpoint level) are considered in the environmental component of the economic analysis. Then, the particular costs estimations are summed up with the private costs so that to determine the overall economic impact of each alternative scenario.

4.3.1 Private costs estimations

The conventional LCC concerns the calculation of the internal costs that occur over the life-cycle of the considered chlorine production system due to the implementation of each scenario. In this case, the private costs estimates are attributed to the producer, i.e. Nouryon. The private costs of chlorine production are categorized into investment costs, costs of energy (by type) and raw materials, fixed costs and corporate costs.

To estimate the private costs per functional unit of 1 ton of chlorine, we followed the ASTM standard LCC methodology developed by the American Society for Testing and Materials (ASTM) (ASTM International, 2002). While the particular approach was initially developed to be implemented in the building and construction industry, its application nowadays can be found in various environmental projects where the LCC technique is used (Langdon, 2007).

Within this methodology, the present value approach is applied to determine the financial impact of chlorine production systems. In the present study, it was assumed that all money streams, either internal or external, take place at the end of each year. An exception in regards to the latter constitutes the required capital investments for the implementation of each scenario. For this, it was assumed to occur at day 1 of the first year of their implementation. To that end, all future costs are discounted to the reference date (day 1). The discounted future costs occurring at the end of the year are summed up with the initial investments of

day 1 to quantify the total private costs. It is worth mentioning that costs occurred before the reference date were not considered in the analysis.

The following equations are provided by the ASTM International (2002) for the calculation of the private costs occurring during the life-cycle of a production system. The Present Value of private costs (PV_{PC}) within a certain period of time can be computed by the next equation.

$$PV_{PC}(i, t, C) = \sum_{t=0}^N \frac{C_t}{(1+i)^t} \quad (4.2)$$

Where

C_t	the summation of the internal costs in year t
N	the time horizon
i	the nominal discount rate

The main components of the calculated private costs are shown in the following equation. Data used for the calculation of the internal costs are based on market data relevant to the chlor-alkali industry as well as the Best Available Techniques (BAT) Reference Document for the Production of Chlor-alkali (Brinkmann et al., 2014) which provides pertinent costs estimation for chlor-alkali plants of 500 kton of Cl_2 annual capacity.

$$PV_{PC} = IN + PV(RM + E + FC + CC) \quad (4.3)$$

Where

IN	initial investments
PV	Present value calculated via the nominal discount rate (i)
RM	Raw material costs (natural gas, wood pellets, deionized water, hydrochloric acid, membranes)
E	Costs due to energy consumption (electricity provided by the national electricity grid)
FC	Fixed costs (operating and maintenance costs, plant overheads, payroll, taxes and insurance)
CC	corporate costs

The nominal discount rate (i) can be computed by the following equation in which the inflation rate (I) is taken into account,

$$i = (1 + r) * (1 + I) - 1 \quad (4.4)$$

Where

r	Real discount rate
i	Nominal discount rate
I	Inflation

4.3.2 Internalizing environmental externalities

Externalities costs due to environmental effects are included in the followed environmental LCC model. To estimate the costs resulting from the quantified environmental footprint, this study used the economic weighting factors provided by 5 different LCA models (see section 2.7). As it was described in chapter 2, the identified weighting factors are the outcome of previous scientific studies based on the WTP principle with a view to deriving the value of non-market goods affected by environmental damages. For the selected endpoint and midpoint impact categories, the environmental impacts are monetized through the economic values of table 3 (chapter 2), converted into today's money. In particular, the values found in the ReCiPe, LIME and Stepwise models are used for the endpoint indicators, while for the monetization of the impact on GWP we applied the economic factors provided by the Ecovalue08, Ecotax02 and Stepwise models.

In the weighting phase of the LCA analysis, the economic weighting factors are used to monetize the identified environmental impacts associated with chlorine production. The particular indicators are applied to convert damages on human health – measured in €/DALY, on ecosystems – measured in €/species.yr, and on global warming – measured in €/kg of CO₂ eq. Therefore, the external costs of the production of 1 ton of chlorine are calculated by using the following equations which correspond to the three selected endpoint and midpoint impact indicators.

The externality cost due to impacts on human health can be computed by the following equation,

$$EXC_z^{HH} = \frac{EI_{HH}}{FU} * EWF_z^{HH} \quad z = 1,2,3 \quad (4.5)$$

Where

EXC_z^{HH}	Externality cost of human health derived via model z, expressed in €/ton Cl ₂
EI_{HH}	Environmental impacts on human health, expressed in DALY
FU	Functional unit of analysis – 1 ton of Cl ₂
EWF_z^{HH}	Economic weighting factor of model z for human health, expressed in €/DALY
z	LCA model, z=1 → ReCiPe, z=2 → LIME and z=3 → Stepwise

Secondly, the externality cost due to environmental damages on ecosystems can be computed with the next equation,

$$EXC_z^{EC} = \frac{EI_{EC}}{FU} * EWF_z^{EC} \quad z = 1,2,3 \quad (4.6)$$

Where

EXC_z^{EC}	Externality cost of ecosystems derived via model z, expressed in €/ton Cl ₂
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EI_{EC}	Environmental impact on ecosystems, expressed in species.yr
FU	Functional unit of analysis – 1 ton of Cl_2
$EW F_z^{EC}$	Economic weighting factor of model z for ecosystems, expressed in €/species.yr
z	LCA model, $z=1 \rightarrow$ ReCiPe, $z=2 \rightarrow$ LIME and $z=3 \rightarrow$ Stepwise

Lastly, the externality cost due to global warming effects can be computed according to the following equation,

$$EXC_z^{GWP} = \frac{EI_{GWP}}{FU} * EW F_z^{GWP} \quad z = 1,2,3 \quad (4.7)$$

Where

EXC_z^{GWP}	Externality cost of global warming potential derived via model z , expressed in €/ton Cl_2
EI_{GWP}	Environmental impact on global warming, expressed in kg of CO_2 eq.
FU	Functional unit of analysis – 1 ton of Cl_2
$EW F_z^{GWP}$	Economic weighting factor of model z for global warming potential, expressed in €/kg of CO_2 eq
z	LCA model, $z=1 \rightarrow$ Ecovalue08, $z=2 \rightarrow$ Ecotax02 and $z=3 \rightarrow$ Stepwise

Assuming that the system is on a steady-state, the level of the identified environmental damage will be the same every year for the given production level. Therefore, the PV of the external costs for the endpoint and midpoint indicators can be computed by the following two annuity equations. The annuity formula estimates the total stream of equal cash flows that occur at fixed time intervals. It worth mentioning that the externality costs are distinguished in midpoint and endpoint level in order to avoid double-counting since a fraction of the total environmental damage on human health and ecosystems corresponds to global warming effects.

As such, the present value of the externality cost at endpoint level and for the specific period of study is given by the next equation,

$$PV_{EX_z^{END}} = TP * \frac{[EXC_z^{HH} + EXC_z^{EC}]}{i} * \left(1 - \frac{1}{(1+i)^N}\right) \quad z = 1,2,3 \quad (4.8)$$

Where

TP	Total annual chlorine production, expressed in ton of Cl_2
EXC_z^{HH}	Externality cost of human health derived via model z , expressed in €/ton Cl_2

EXC_z^{EC}	Externality cost of ecosystems derived via model z, expressed in €/ton Cl ₂
z	LCA model, z=1 → ReCiPe, z=2 → LIME and z=3 → Stepwise
N	The length of the study period (same with the LCA analysis)
i	The nominal discount rate

Accordingly, the present value of the externality cost at midpoint level can be computed as follows,

$$PV_{EX_z^{MID}} = TP * \frac{EXC_z^{GWP}}{i} * \left(1 - \frac{1}{(1+i)^N}\right) \quad z = 1,2,3 \quad (4.9)$$

Where

TP	Total annual chlorine production, expressed in ton of Cl ₂
EXC_z^{GWP}	Externality costs of global warming potential derived via model z, expressed in €/ton Cl ₂
z	LCA model, z=1 → Ecovalue08, z=2 → Ecotax02 and z=3 → Stepwise
N	The length of the study period (same with the LCA analysis)
i	The nominal discount rate

4.3.3 Overall economic impact

The monetized environmental impacts at midpoint and endpoint level are summed up with the private costs to derive the overall economic impact of the implementation of each chlorine production scenario. With respect to the applied economic weighting set, the present value of the total costs (PV_{TC}) – at midpoint or endpoint level - of the considered production system occurred over the studied period (N) are given by the next equations,

$$PV_{TC^{END}}(i, N, z) = PV_{EX^{END}}(i, N, z) + PV_{PC}(i, N) \quad (4.10)$$

$$PV_{TC^{MID}}(i, N, z) = PV_{EX^{MID}}(i, N, z) + PV_{PC}(i, N) \quad (4.11)$$

To estimate the economic benefits of each scenario, we implemented the net present value rule. By and large, the NPV calculates the time value of cash flows that emerge at different time periods and it can be used as a decision-making tool in order to opt which alternative demonstrates the best opportunity for investment. To that end, the NPV rule is as it follows (Berk & DeMarzo, 2007), *“When making an investment decision, take the alternative with the highest NPV. Choosing this alternative is equivalent to receiving its NPV in cash today.”*

In the case of the considered chlorine production system, the NPV of each scenario is given by Eq. 4.12. As such, the NPV is defined as the difference between the present value of the total benefits and the present value of the total costs at midpoint or endpoint level for the studied chlorine production systems.

$$NPV_{Sci} = PV_{Sci}(Total\ Benefits) - PV_{Sci}(Total\ Costs) \quad SC_i = 0,1,2,3 \quad (4.12)$$

Therefore, according to the NPV rule and the abovementioned mathematical formulas, the economic assessment of the four described scenarios (SC_i) has taken place.

4.3.4 Discount rate

To a large extent, the final outcome of the cost calculation part is influenced by the decision regarding the time horizon of the study and the level of the discount rate. For both concepts, our choices are in line with the suggested values of the European Commission (2014) which has provided the guidelines for the economic evaluation of environmental projects.

The time horizon of the project was selected to be twenty years for both LCA and LCC analyses. For the purpose of this study, the PV of future costs was computed based on the nominal discount rate (i). The nominal discount rate is adjusted to inflation rates, thus considering changes in the purchasing power of the Netherlands. The nominal discount rate was calculated according to the mathematical formula of Eq. 4.4. The chosen inflation rate was 1.6%, which represents the average rate of the Netherlands for 2018 (Statista, 2019). It was assumed that both the inflation and the interest rate will remain stable for the particular time horizon (20 years).

Two different real discount rates were applied. For the company's private costs, a modest discount rate of 4% was selected. To that decision led the observation that for a long time horizon, as the level of the discount rate increases, the NPV of a project decreases rapidly, thus resulting in unattractive projects. As far as the environmental cost calculation part is concerned, a low discount rate was regarded to be the proper one for this study. The level of the selected rate is near zero (0.01%). By selecting a low discount rate, the costs of environmental damages are avoided to be transferred to future generations. As such, incentives for actions that will lead to environmental costs reduction are given to the involved stakeholders.

Chapter 5:

Enviro-economic assessment results

This chapter summarizes the results of the enviro-economic assessment for the four scenarios. Firstly, the results of the life-cycle impact assessment in the selected endpoint and midpoint categories are displayed. In this case, the ReCiPe method is used to compare the environmental profile of the four scenarios in terms of environmental impacts on *Human Health, Ecosystems & Global Warming Potential* caused due to energy and resource consumption.

Secondly, the costs of the identified environmental externalities of each scenario are estimated. For their calculation, the conversion factors of table 3 are used (section 2.7), converted in today's money. Five economic weighting sets, which are based on different valuation methods, are selected for the monetization of the identified environmental externalities, these are namely ReCiPe, Stepwise, Ecovalue08, Ecotac02 and LIME. Along with the environmental costs, the costs of the deployment and operation of each scenario are presented. Lastly, the costs due to environmental externalities are attributed to the system and summed to the total costs.

5.1 Life Cycle Impact assessment

Table 17 demonstrates the scores of Human Health, Ecosystems and Global Warming Potential categories when economic allocation is applied. By applying economic allocation the environmental impacts are attributed to the functional flows based on the amount of production of Cl₂, NaOH and H₂ via membrane electrolysis and the economic value of the output.

Table 17: Environmental impacts per of chlorine produced

Indicator	Unit	S0	S1	S2	S3
Human Health	DALY/ton Cl ₂	3.02E-02	2.33E-02	3.08E-02	2.39E-02
Ecosystems	species.yr/ton Cl ₂	5.58E-05	4.27E-05	5.90E-05	4.63E-05
Global Warming Potential	kg CO ₂ eq. /ton Cl ₂	2087.96	1593.26	2114.41	1613.23

The environmental impacts of the reference case scenario were quantified in order to be utilized as the reference point against which the results of each alternative scenario are compared. To that end, the relative value assigned to the reference case in all categories is one. In Figure 16, the relative scores of S1, S2, and S3 are compared with regards to the current chlorine production system. Among the four scenarios, the biggest improvement is showed by S1. S3 is the second-best, which besides the zero-gap cell modification it incorporates the installation of biomass boilers.

The modification of the electrolysis cell from gap to zero-gap one results in the lowest environmental and human health damage. Specifically, from the implementation of S1, Nouryon can reduce CO₂ emissions per ton of chlorine by 24% approximately. Additionally, the scores in the human health and ecosystems indicators of S1 with respect to the reference case are decreased by 23% and 24% respectively. At first glance, lower current density and power demand are the main reasons for S1's performance in contrast to the other three. However, taking the uncertainty factor into account, a relative difference is noticed between the results of S1 and S3 in the GWP and HH indicators, thus, rendering these two options to some extent identical in regards to their environmental profile. On the other hand, the deployment of biomass boilers in case of S3's implementation causes an 8.5% increase in the ecosystems indicator when compared to S1. More details about the explanation of this outcome are given in the interpretation phase, chapter 6.

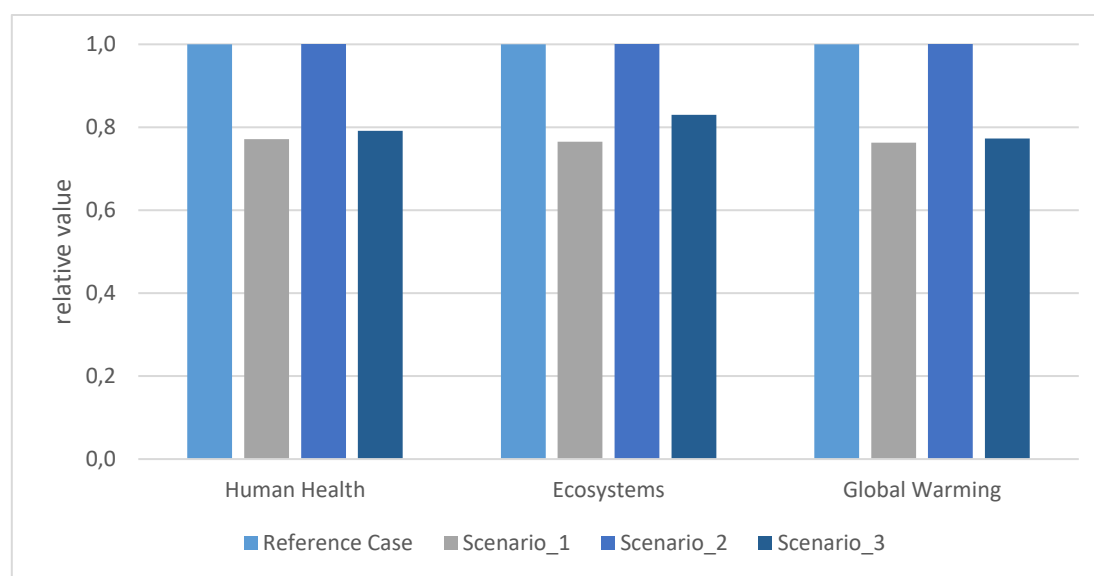


Figure 16: Comparative assessment of the three alternative scenarios with respect to the reference case; Reference Values: HH: 3.02E-02 DALY/ton Cl₂; EC: 5.58E-05 species.yr/ton Cl₂, GW: 2,087.96 kg CO₂ eq. /ton Cl₂

The scenario that exclusively involves biomass boilers shows the poorest environmental performance, scoring slightly higher compared to the reference case. Specifically, when replacing the CHP plant with biomass boilers keeping all other parameters same a 5% increase is recorded in impacts on Ecosystems. Interestingly, S2's scores in the GWP category are greater by almost 2%. However, the results regarding this scenario are dominantly influenced by the assumptions made in the previous chapters. While it seems that the application of biomass boilers does not lead to environmentally friendly results in contrast to the reference chlor-alkali system, when being isolated and exclusively compared to the existing CHP plant in terms of heat output, its performance shows better results. Specifically, to produce one GJ of heat, biomass boilers of S2 burden the environment by 52.7 kg CO₂ eq., while the CHP plant by 72.7 kg CO₂ eq. /GJ of heat.

Overall, the on-site electricity and heat consumption of each scenario is the main reason behind the environmental impacts that can lead to climate change. The results in global warming impact category are the summation of direct emissions produced by on-site power/heat plants and indirect emissions that stem from electricity generation by the national power system. The indirect CO₂ emissions account for the lion's share, as a consequence of the high electricity demands covered by the Dutch electricity mix. Particularly, long before

chlorine's production takes place, half of the identified CO₂ emissions are released to the atmosphere. As Figure 17 illustrates electricity generation based on hard coal and lignite is the largest contributor to the overall impact on global warming, accounting between 27% (S1) and 35.6% (S2) of the identified impacts. On average, energy generated from natural-gas-fired co-generation power and heat plants accounts for 11% of the estimated CO₂ emissions, while the heat generated from the combustion of natural gas and hard coal is responsible for 9.5% of the total impact.

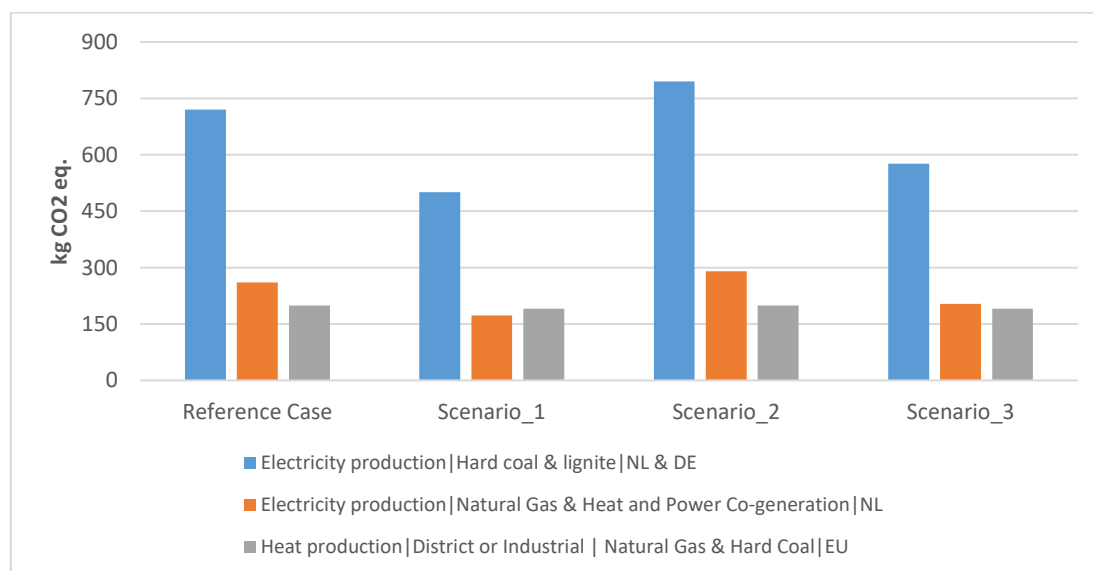


Figure 17: Off-site processes contribution to climate change

5.2 Life-cycle Costing

5.2.1 Monetization of the identified environmental impacts

The purpose of this subsection is to point out the major environmental cost drivers that arise from the deployment of the four scenarios. To do so, the highlighted environmental externalities of the LCA analysis are used as inputs to the economic assessment. The results of the enviro-economic analysis, displayed in Appendix D, are distinguished into environmental costs that concern exclusively Nouryon and those that concern the whole chlorine chain.

As it was mentioned before, almost half of the environmental impacts take place off-site due to energy generation and raw materials extraction. These processes concern the operations of other stakeholders involved in the industry and not the company itself. Therefore, the environmental costs associated with CO₂ emissions due to on-site energy generation are attributed to the company. This means that the environmental costs of the company are directly linked to the impacts generated from the operation of the CHP plants or the biomass boilers facilities. Since human health and ecosystems areas of protection provide indications for damage at an aggregate level, the identified environmental impacts on these categories and hence the associated environmental costs are attributed to the chlorine chain and the involved actors'. Figures 18 and 19 illustrate chain-related costs due to impacts on human health and ecosystems respectively, while the company-related environmental costs are shown in Figure 20.

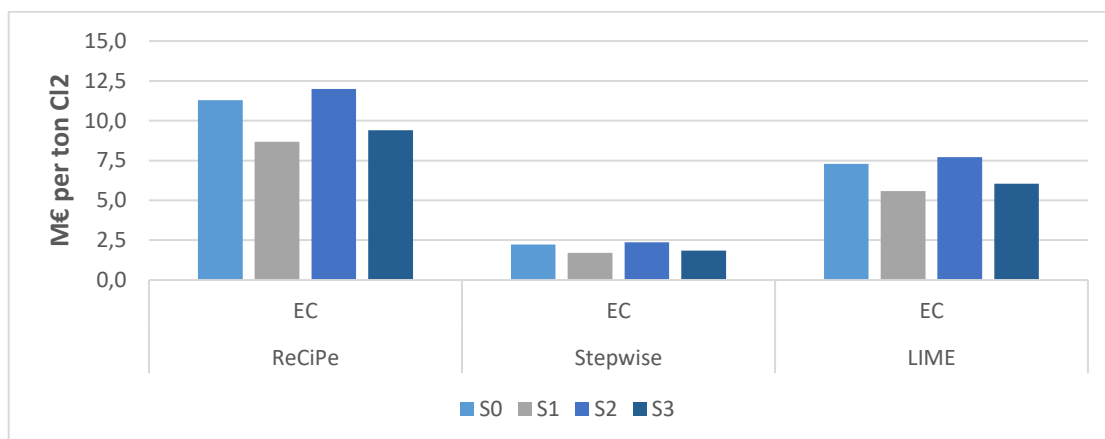


Figure 18: Environmental costs due to impacts on ecosystems per scenario and monetary weighting set

The magnitude of the chain-related environmental costs depends on the calculated accumulative impacts on human health and ecosystems as well as on the applied monetary value. Therefore, the scenario that shows the best performance in the endpoint indicators of the LCA analysis, it also has less environmental costs. As such, the installation of zero-gap cells will bring to the industry the less financial burden per ton of chlorine production, ranging from 1,622 € (ReCiPe) to 3,154 € (LIME) for impacts on human health and 1.71 M€ (Stepwise) to 8.67 M€ (ReCiPe) for impacts on the ecosystems. On the contrary, the execution of S2 will cost the industry between 2.36 M€ (Stepwise) and 12 M€ (ReCiPe) due to impacts on ecosystems. Moreover, the computed costs because of damages on human health from S3's employment are between 2.6% and 3.2% more with respect to the environmental costs of S1. In the case of chlorine production system remains as it is, this can financially burden the involved in the chlorine chain actors by extra 2.2 M€ to 11.3 M€.

Among the values that are applied to convert the environmental impacts on ecosystem into monetary terms, that of ReCiPe result in the highest cost in all scenarios, while impacts on human health are overvalued through the LIME method. At the other end of the spectrum, Stepwise method's values constitute the lower limit of the calculated environmental costs due to impacts on human health, while a more moderate approach for cost estimation is given by the LIME method with respect to impacts on the ecosystem.

The estimated costs for every scenario to avoid environmental damages on human health and ecosystems deviate by 33% from their mean value. As a consequence, it is rendered unfeasible to come up with a reliable estimation. The main reason that the results differ is not actually the values of the used weighting factors but the valuation approach that scholars followed to derive them. Therefore, in the interpretation phase, a thorough analysis of the limitations of each monetary weighting set as well as a discussion about which fits better to this study will take place.

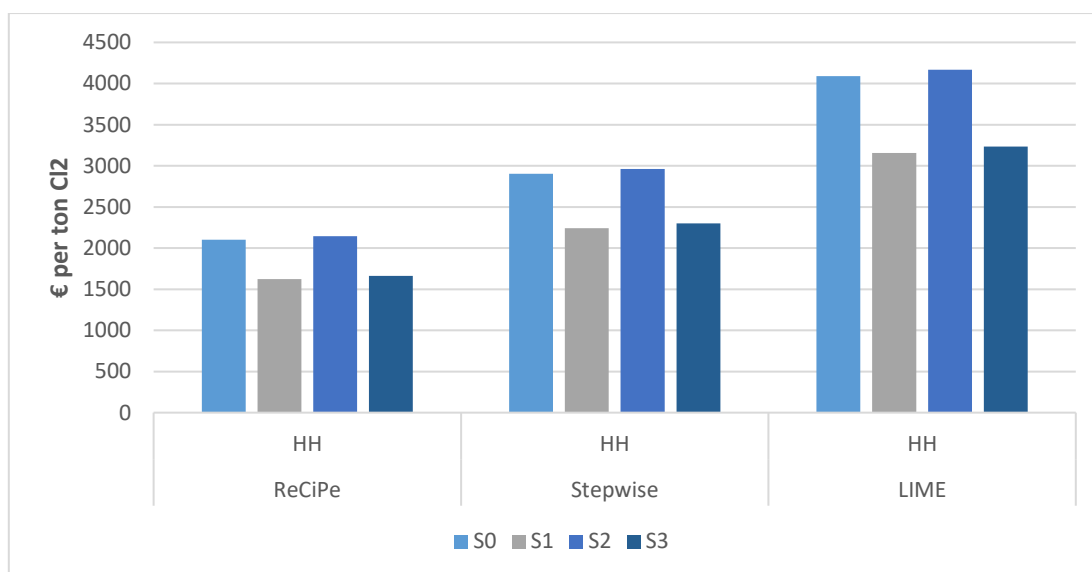


Figure 19: Environmental costs due to impacts on human health per scenario and monetary weighting set

On the flip-side, the environmental costs attributed to the company per ton of chlorine depend on what system is implemented for heat generation. This project examined two ways of covering on-site heat demand – CHP plants and biomass boilers. By and large, the scenarios that involve CHP plants show better environmental performance with respect to those where biomass boilers are engaged. However, as it is illustrated in Figure 20, the contribution of biomass boilers to the overall impact of each scenario is less, compared to the contribution of CHP plants. Specifically, due to CHP's operation 113.72 and 136.36 kg CO₂ eq./ ton Cl₂ are emitted in the reference case and in S1 respectively, while biomass boilers contribute 41.15 and 49.22 kg CO₂ eq./ ton Cl₂ to the overall impact of S2 and S3 respectively.

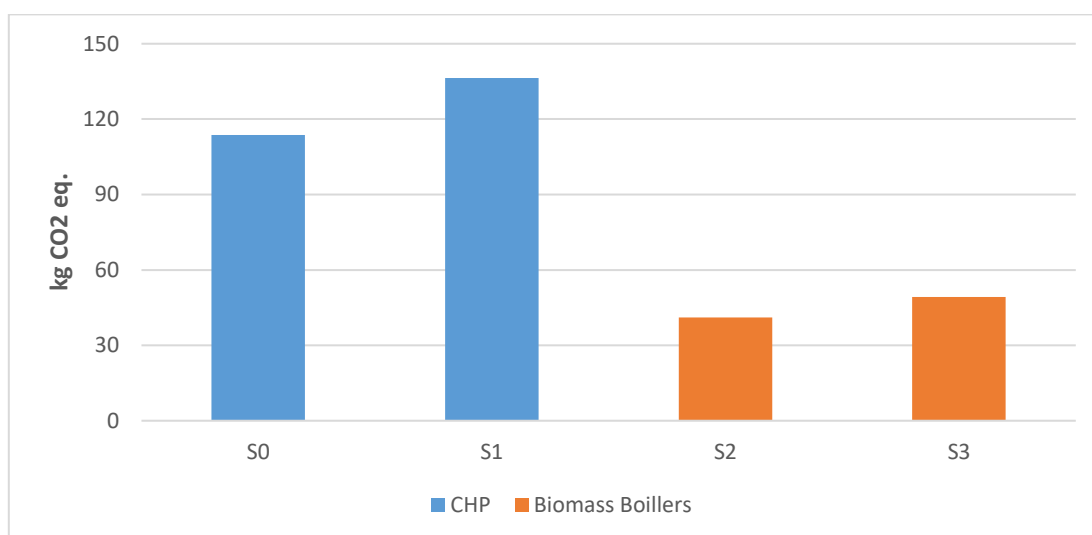


Figure 20: The share of CHP and biomass boilers plant in the total CO₂ emissions

Consequently, the environmental costs for which the company is thought to be responsible are less when biomass boilers are used instead of CHP plants. Figure 21 shows the estimated environmental costs, based on the monetary weighting sets provided by the Ecotax02, Ecovalue08 and Stepwise methods. The upper bound is given by the Stepwise method while the Ecovalue08 sets the threshold of the cost-range. Hence, S2 leads to the lowest financial burden. Particularly, the environmental costs of S2 are almost three times less than those of

the reference case, ranging between 0.43 and 3.23 €/ ton Cl₂. S3 is the second-best, ranging between 0.52 and 3.82 €/ ton Cl₂. On the other hand, the environmental impact from the implementation of S1 will cost to the company between 1.43 and 14.71 €/ ton Cl₂.

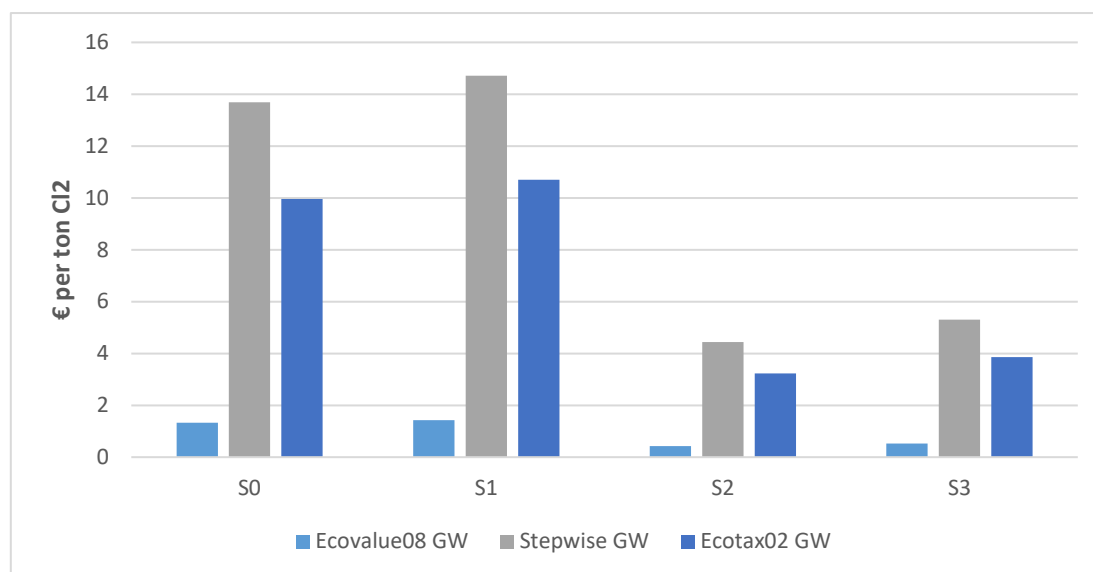


Figure 21: Environmental costs due to the operation of CHP and biomass boilers plants, per scenario and monetary weighting set

5.2.2 Scenarios' implementation – economic performance

To identify which scenario has the best economic performance, we proceeded to an estimation of the relevant benefits and costs that occur within a year after their deployment. As such, the mathematical formulas and data of the LCI in chapter 4 were used. Given that chlorine production is the same regardless of the deployed scenario, table 18 shows the calculated money inflows and outflows according to the company's annual production.

Two main revenue streams that come from the sold production of chlorine and caustic soda along with revenues from hydrogen sales delineate the total economic benefits of each scenario. To that end, the annual revenues from the sold production reach 362 M€ approximately.

Compared to the reference case where no capital investments are required, the deployment of S2 and S3 will cost to the company additional 25.07 M€ and 23.28 M€ respectively during the first year of scenarios' implementation. These costs are mainly due to the required initial investments in changing the configuration of the membrane cell and replacing CHP plant with biomass boilers. In the case of S1's implementation, the initial investment for the installation of zero-gap cells is estimated at 77 M€, while in S2's case, biomass boilers' capital costs reach 23 M€ approximately. On the contrary, the company will substantially increase its savings by investing in S1 as a consequence of its fewer requirements in raw materials and electricity.

Table 18: Internal costs and benefits per scenario (time period: 1 year of implementation)

	Reference Case	Scenario_1	Scenario_2	Scenario_3
Benefits				
Chlorine revenues		109,56		
Caustic soda revenues		224,92		
Hydrogen revenues		27,37		
Total Benefits (M€)		361,86		
Capital Costs				
Initial Investments	0.00	76.44	22.74	97.26
Raw Materials				
Natural Gas	14.93	14.93	0.00	0.00
Wood pellets	0.00	0.00	13.26	12.33
Deionized water	1,27	1,11	1.27	1.07
HCL	1.71	1.49	1.71	1.91
Membranes	12.74	12.74	12.74	12.74
Electricity	190.36	104.08	194.36	121.15
Fixed costs				
Operational	4.78	4.52	4.78	4.52
Maintenance	25.16	23.83	25.16	23.83
Plant overheads	8.92	8.92	8.92	8.92
Payroll	16.76	16.76	16.76	16.76
Taxes and insurance	19.43	19.43	19.43	19.43
Corporate costs				
Corporate costs	11.34	10.74	11.34	10.74
Total Costs (M€)	307.38	294.97	332.45	330.66

In all cases, the main financial burden of the company is due to electricity consumption. The chlor-alkali plant's high dependence on power goes in tandem with high costs. Particularly, 60% of the total costs in the scenarios where chlorine production is achieved via gap-cell membrane electrolysis is due to electricity consumption, while S1 and S2, where the zero-gap configuration is applied, electricity costs account for 36% and 38% of the total costs respectively. Furthermore, the production system is highly dependent on resources consumption. The requirements in natural gas or wood pellets consist of a considerable expense in all scenarios, ranging between 4% and 5% of the overall costs.

An additional essential cost aspect in all scenarios concerns the fixed costs, which comprise of the operating and maintenance expenses, rents, salaries, utilities as well as taxes and insurance. On average, these costs account for 25% of the total costs in each scenario.

From a financial perspective, S1, followed by the do-nothing scenario, constitute the best options for implementation when scenarios are compared with respect to the first year. However, this is the outcome of assessing the calculated costs and benefits of each scenario without taking into account environmental costs. Table 19 gives an overview of the total production costs per ton of chlorine per weighting set implemented for monetizing environmental impacts when initial investments are excluded. For the reference case scenario, total production costs range between 483 €/ton Cl₂ and 496 €/ton Cl₂. In contrast with S2 which shows the worst economic performance, the implementation of S1 is associated

with the least production costs ranging between 344 €/ton Cl₂ and 357 €/ton Cl₂. The provided cost ranges for S0 and S2 are similar to the production costs estimations given by Eurochlor, (2018). In particular, for an electrolysis unit requiring 3 MWh electricity per ton of chlorine, which is also the case in S0 and S2, Eurochlor has estimated that the total production costs can reach 505 €/ton Cl₂ approximately. On the other hand, S1 and S3's total production costs are roughly between 130 €/ton Cl₂ and 150 €/ton Cl₂ less than Eurochlor's costs estimation.

Table 19: Total production costs per ton of chlorine and used economic weighting factor

Model	Reference Case	Scenario_1	Scenario_2	Scenario_3
Ecovalue08	483	344	486	366
Stepwise	496	357	490	371
Ecotax02	492	353	489	370

Considering the time value of money, and the complete time horizon set for the purpose of this study, we implement the NPV rule to identify which scenario can produce maximum economic benefits. Table 20 shows the NPV of each scenario after integrating the estimated environmental costs to the total production expenditures for a 20 years' time period.

According to the NPV rule, all projects are financially viable for implementation. However, they differ in terms of the profits that are anticipated to yield. The option to modify the membrane cell to zero-gap (S1) is the most financially attractive, compensating the company €1.74 bn approximately for the selected time horizon. In that case, taking the environmental costs into account, Nouryon's total costs increase up to 6.33%. The second best option is S3, yielding €1.55 bn approximately, excluding environmental externalities. However, by internalizing to the system the environmental costs, then the NPV of this scenario declines up to 3.8%. From a financial perspective, the worst scenario is represented by S2.

Table 20: Internalizing environmental costs to the total expenditures; time period=20years

LCC - Internal Costs (M€)					
Model		Reference Case	Scenario_1	Scenario_2	Scenario_3
ASTM	Total PV Benefits	4,266	4,266	4,266	4,266
Standards	Total PV Costs	3,499	2,527	3,549	2,723
	NPV	768	1,739	717	1,543
LCC – Internal & External Costs (M€)					
Ecovalue08	Total PV Costs	3,513	2,543	3,553	2,729
	NPV	753	1,723	713	1,537
		[1.95%↓]	[0.86%↓]	[0.56%↓]	[0.39%↓]
Stepwise	Total PV Costs	3,647	2,687	3,597	2,781
	NPV	619	1,579	669	1,485
		[19.40%↓]	[9.20%↓]	[6.69%↓]	[3.76%↓]
Ecotax02	Total PV Costs	3,606	2,643	3,584	2,765
	NPV	660	1,623	682	1,501
		[14.06%↓]	[6.67%↓]	[4.88%↓]	[2.72%↓]

Chapter 6: Results Interpretation

In this chapter, the final phase of the life-cycle study according to the ISO standards is executed. The LCA results of chapter 5 are interpreted by conducting a life-cycle (subsection 6.1.1) and process-specific (subsection 6.1.2) contribution analysis. Thereinafter, the results are compared against that of relevant studies. In line with the scope of our study, we interpret and pinpoint the best of the examined scenarios from an investment and environmental costs perspective. To do so, we first conclude which of the used monetary weighting factors to translate environmental impacts into monetary terms fits better to our study.

6.1 Contribution analysis

The contribution analysis can facilitate the analyst to gain a clear understanding about which are the main sources and causes of the identified impacts. In this section, the results of the LCA analysis are distinguished in contributing processes in order to identify the “hot spots” of the chlorine production system. The system’s life-cycle phases and the per-process environmental impacts make up the structure of the LCA contribution analysis.

6.1.1 Contribution analysis of the life-cycle phases of the chlorine manufacturing system

The examined production system of chlorine is divided into three major life-cycle phases. The pretreatment phase is the amalgam of the stages responsible for the preparation of raw materials, after which chlorine can be produced in the manufacturing phase. Lastly, in order for the products of the membrane electrolysis stage to reach their commercial form, they pass through the processing phase. Table 21 lists the percentage contribution of the life-cycle phases engaged in the production of 1 ton of chlorine.

Table 21: Life-cycle phases contribution per ton of chlorine production of each scenario

Phase	S0	S1	S2	S3
Raw Materials Pretreatment [%]	20.6	26.8	18.5	23.4
Chlorine Manufacturing [%]	71.5	62.0	72.6	63.7
Products’ Processing [%]	7.9	11.2	8.9	12.9

Taking the impact assessment results of the previous chapter into consideration, it can be inferred that the chlorine manufacturing phase for all scenarios has the greatest impact on the environment. The manufacturing phase consists of the membrane electrolysis process and the recirculation system through which a part of the electrolysis products is sent back to the pretreatment phase. For all scenarios, electricity consumption, supplied from the national power system is the most important factor which is directly linked to the identified contribution of the manufacturing phase. Compared to the reference case, an almost 10% decrease in the environmental impact of this phase is noticed when S1 and S3 are implemented.

Besides chlorine’s production line, the production lines of caustic soda and hydrogen are also considered in the products’ processing phase. For each scenario, the environmental impact of

this phase is almost seven times less in contrast to the manufacturing phase, and approximately two times less with respect to the pretreatment phase. The low electricity requirements and the much lower amount of materials that are processed constitute the main reasons behind the level of its contribution. However, the most significant contributor to this phase is the caustic soda evaporation stage due to its high requirements in heat. Compared to the other three scenarios, the processing system of the reference case has the lowest contribution to the overall impact, mainly because the electricity requirements of this phase are not covered by the national power system as in S2 and S3 cases. S1's impact is slightly larger than that of the reference case since the number of products that are processed in this case is marginally increased.

For each scenario, the pretreatment phase has nearly three times less environmental burden than that of the manufacturing phase. In this phase, the pretreatment of caustic soda, brine as well as the supply of the necessary raw materials, such as dry vacuum salt, demineralized water and hydrochloric acid are considered. The biomass boiler scenario (S2) records the lowest impact with respect to the other scenarios. In this case, the heat demand of the pretreatment phase is dominantly covered by the waste heat recovery system with the biomass boilers being negligibly engaged. On the other hand, in the pretreatment phase of S1, where the CHP plant covers around 40% of the total heat requirements, the largest environmental impact in contrast to the other three scenarios is noticed.

6.1.2 Process-specific contribution analysis of the chlorine manufacturing system

Based on the impact assessment results in chapter 5, the process-specific contribution analysis is used to reveal which are the hot-spots in chlorine's production system for the examined scenarios. As such, this analysis will create the breeding ground to first identify and then suggest what parts of the system can be improved.

Figures 22 and 23 show which foreground processes are the major contributors to the overall impact on human health, ecosystems and global warming potential for each scenario. Precise results per examined indicator are displayed in Appendix C.

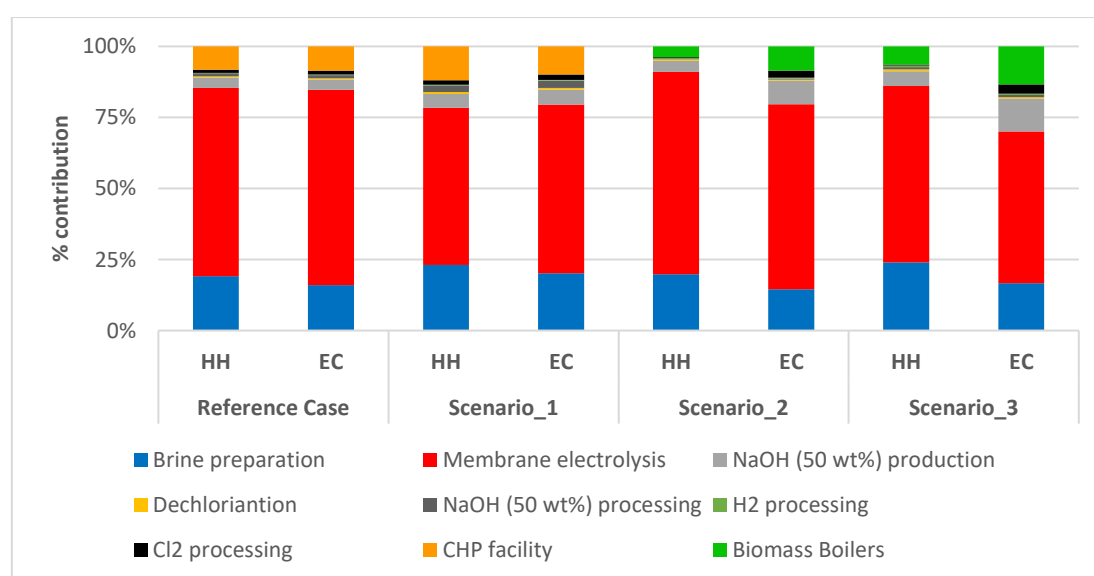


Figure 22: Process contribution analysis for the human health and ecosystems indicators

In all scenarios the ranking of the processes remains the same, however, they differ in regards to their level of contribution to the total impact. Membrane electrolysis has the greatest contribution in all indicators, accounting between 60% and 70% of the overall impact with respect to which scenario is implemented. As far as the reference case is concerned, 985 kg CO₂ eq/ton Cl₂ are released to the atmosphere due to the electrolysis process, while when S1 or S3 are implemented the impact on GWP category is decreased by 39% and 36% respectively. The dominant reason for the electrolysis process being the largest contributor is the power demand of the process which is over 3,000 kWh/ton of Cl₂. The second-largest contributor is the brine preparation stage. As far as the reference case is concerned, the particular stage results in 37.23E-4 DALY/ton Cl₂ damage to human health. The level of the damage due to brine preparation stage in S1 and S2 is roughly 15% less compared to the reference case.

Moreover, in the reference case, caustic soda production impacts the environment by 50 kg CO₂ eq/ton Cl₂, while when CHP plant is replaced with biomass boilers the impact is decreased by 24% and 14% in case of S2 and S3 respectively. Furthermore, a small contribution to the overall impact is observed for the caustic soda preparation and the dechlorination stages, due to the fact that a small portion of the former's heat requirements is covered by the CHP plant or biomass boilers and the relatively low power consumption for the latter. For the chlorine processing line, including the cooling, drying, compression and liquefaction stages, as well as, that of hydrogen, consisting of the cooling and compression stages, the contribution to the overall impact is negligible.

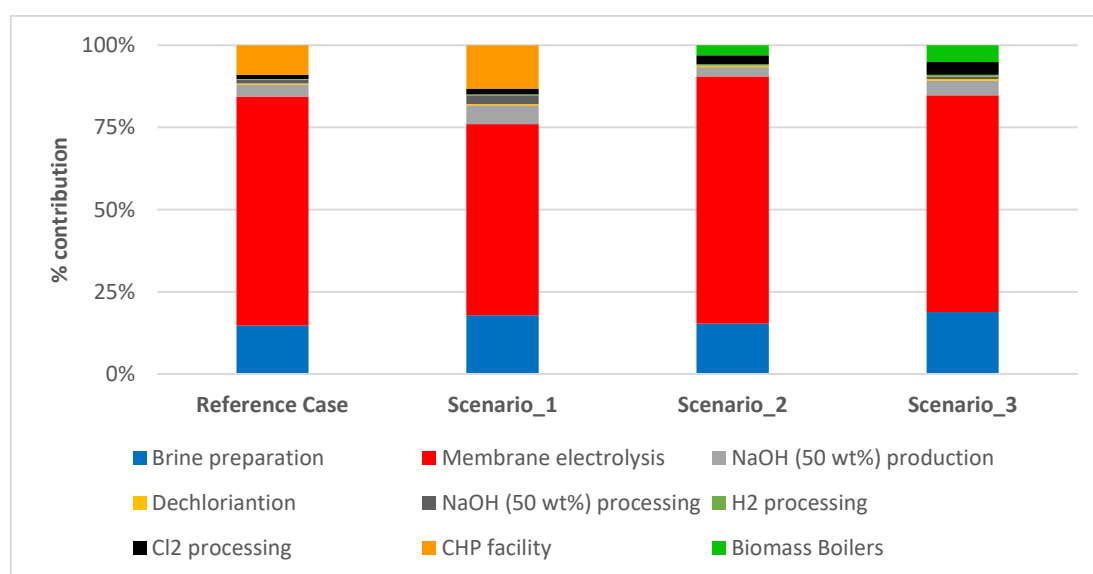


Figure 23: Process contribution analysis for global warming potential

However, this is not the case in regards to what facility is employed for heat generation purposes. Due to the operation of the CHP plant in the reference case scenario 127 kg CO₂ emissions per ton of Cl₂ are released to the environment. Interestingly, despite having the same specifications for the CHP plant, the CO₂ emissions of S0 are relatively lower than S1's. This is due to a difference in the performance level of the caustic soda preparation process which is supplied with heat from the CHP plant in both cases. While in the reference case scenario 1 MJ heat is provided by the CHP plant for the preparation of 97 kg NaOH, in scenario 1 that ratio changes in 1:54, thus burdening a slightly more the environment.

On the other hand, when biomass boilers are employed in S2 and S3, their contribution is decreased by 68% and 61% respectively, compared to the reference case. This big difference in numbers is due to CHP's plant involvement in seven chlor-alkali stages in contrast to biomass boilers which are engaged in only two. By and large, their contribution is not comparable because of one fundamental reason. The CHP plant co-produces power and heat at 1:2 ratio, while biomass boilers generate only heat. Therefore, despite showing in chapter 5 that the environmental impact of CHP is greater than that of biomass boilers with respect to heat generation only, we cannot conclude if the latter is more environmentally friendly since electricity co-generation is absent.

By comparing the results of all scenarios between them, it can be observed that some scenarios record the same level of contribution regarding specific chlor-alkali stages. In particular, the reference case and S2 have the same impact with respect to the brine preparation and the dechlorination stage. In the same way, S1 and S3 show the same results in these stages. This is due to the fact that these scenarios in both cases have the same raw material and energy requirements. Therefore, when being compared in regards to the GWP indicator, S0 and S2's impact is greater than S1 and S3's by 15% for the brine preparation stage and by 22% for the dechlorination stage. For the former, the observed difference is explained because of a decrease in sodium chloride requirements when gap-cells are replaced with zero-gap cells while for the latter due to a small change in power demand.

Because of the same energy and resource requirements in all cases, the scenarios present the same results in all of the sub-processes included in chlorine's production line, with the level of impact ranging between 1% and 4% with respect to GWP indicator. On the other hand, by changing the cell's configuration in zero-gap one, hydrogen production is almost double. Therefore, keeping electricity requirements the same for S0 and S1, as well as, for S2 and S3, but changing cell's configuration, the contribution to the GWP of the hydrogen processing stage after zero-gap membrane electrolysis is greater by 50% than that of gap-cells type.

In regards to the caustic soda processing stage, for the same amount of heat requirements, but supplied in the first case from the CHP plant (S0) and from biomass boilers in the other (S2), a two-times increase in the ecosystems indicator is observed. That's because biomass boilers directly affect the ecosystem due to the fact that they use organic feedstock as fuel.

6.2 Comparison of LCA results with other studies

In Figure 24, the LCA results of our study in the GWP indicator are plotted against the results of relevant studies in the chlor-alkali industry. It worth mentioning that no results in endpoint categories found to compare with. Similarly, there are no studies in the particular field translating the identified impacts in monetary terms.

Our GWP results are in agreement with Garcia-Herrero et al., (2017) who reported a value of 2,281 kg CO₂ eq per ton of chlorine considering a fixed co-production ratio of NaOH and H₂. The authors identified that over 72% of the overall recorded impact comes from the membrane electrolysis process due to high electricity consumption, while in our study the electrolysis stage contributes 60-70% to the total impact with respect to the implemented scenario. Additionally, they reported that 87% of the total energy demand is consumed by the

electrolysis stage, which is close to 91% of our study with respect to the reference case scenario. Despite that the authors have considered multiple chlor-alkali stages, which are also included in our study, the main difference lies in the fact that they have also examined the impact due to salt mining and raw materials transportation, which are out of our system boundaries. Specifically, they argued that 6.5% of the total impact is due to salt mining.

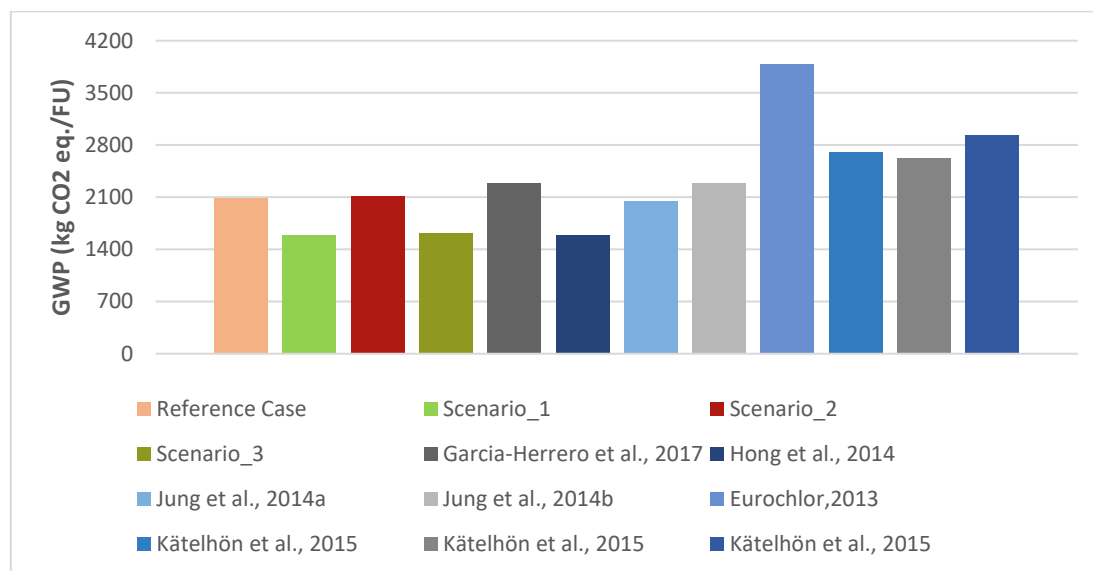


Figure 24: Comparison of the identified results in the GWP indicator with those found in relevant life-cycle studies

Respectively, our results are also in line with Jung et al., (2014), who used the ReCiPe impact assessment method in order to compare the environmental profiles of the membrane electrolysis using standard or ODC cathodes. Under the same system boundaries and functional unit, they considered two scenarios in regards to the utilization of hydrogen obtained from membrane electrolysis with standard cathodes. When hydrogen is used as a commodity they reported 2,280 kg CO₂ eq/FU while when it is used as fuel 2,040 kg CO₂ eq/FU. Additionally, they indicated that electricity consumption is the largest contributor accounting for 70% of the total impact on the GWP category. Furthermore, as we did, they also discussed that heat consumption for caustic soda concentration considerably contributes to the overall impact.

On the other hand, our results are partially in accordance with Kätelhön et al., (2015), who despite not considering raw materials pretreatment and products' processing phase in the set system boundaries, they reported an impact on the GWP category of 2,620 kg CO₂ eq/ton Cl₂ when hydrogen is used as a commodity, 2,700 kg CO₂ eq/ton Cl₂ as fuel and 2,930 kg CO₂ eq/ton Cl₂ when it is flared with of any kind treatment. However, the process-specific contribution is not provided. Additionally, Hong et al., (2014), even though they conducted a comprehensive work with the focal point of their analysis being the chlor-alkali electrolysis process, our results are not comparable due to difference in the used functional unit of the system from both sides. By selecting 1 ton of NaOH as the functional unit, via the ReCiPe impact assessment method they identified a GWP value of 1,590 kg CO₂ eq/ton NaOH. Interestingly, they reported that 72% of the total impact is due to electricity consumption which is in line with our estimate. Moreover, by using the CML baseline impact assessment method, Eurochlor (2013) reported a GWP value of 3,890 kg CO₂ eq/ton of functional unit (1 kg of Cl₂, NaOH, H₂, NaCl and NaClO). However, the results are demonstrated in a different

functional unit and without showing process- and technology-specific contribution results, thus they cannot be compared with the GWP outcome of our study.

6.3 Valuating Environmental Externalities

Monetizing environmental externalities ends to be a challenging task to execute. The present study's intention is placed on merging LCA and LCC by applying five different economic weighting factors to convert environmental damages at midpoint and endpoint level into monetary terms. In addition to the latter, we further aim to provide suggestions regarding which monetizing method might best suit to LCA studies. Since results displayed in biophysical units most of the time are difficult to interpret, our approach is perceived to be a way through which the industry's managers could promptly comprehend the socio-economic consequences of their potential investment decisions. However, that might be questionable regarding our results for the monetization of environmental externalities.

As it is shown from the implementation of the discussed weighting sets in chapter 5, the pertinent results are anything but easy to interpret in the sense that they demonstrate significant differences in their final environmental costs outcome when compared to each other. In particular, the environmental costs for every scenario have a quite high standard deviation, reaching 33%. As such, that raises a question about the extent to which our choice of using five different monetary weighting sets can lead to sound conclusions with respect to our final environmental cost estimations.

One could easily have said that since the used economic weighting factors provided namely by ReCiPe, Ecovalue08, Stepwise, LIME and Ecotax02, differ regarding their value, it would be reasonable the results to deviate from each other (see Table 3 chapter 2). However, our point of view goes way beyond that explanation. To our mind, two issues should be thoroughly addressed in order to examine the compatibility of each weighting set with our study. The first one regards the valuation method upon which scholars were based to derive the particular weighting factors while the second one concerns the methodological steps, intention and scope of their studies. As such, then we can conclude which economic weighting set and thus monetization method is the most representative one for our life-cycle study. Thereby, the final environmental costs associated with the implementation of each scenario would be displayed and interpreted with respect to the outcome of this section's analysis.

By and large, monetary valuation refers to the monetization of environmental and societal consequences by applying relevant conversion factors. The monetization factors implemented in the present study are based on different valuation methods. Specifically, LIME's weighting factors are based on the choice experiment method, Stepwise's on the budget constraint method, while that of Ecotax02, Ecovalue08 and ReCiPe are mainly based on observed and revealed preferences methods.

Observed and revealed preferences methods are inextricably linked to the characteristics of the market in which individuals' consuming behaviour can be interpreted for valuing environmental goods. Changes in the market price of private goods or in individual's consuming behaviour can be perceived as an indicator for explicitly or implicitly deriving the economic value of a non-market good, due to changes in environmental conditions. The primary limitation of that methods is that they fall short to be directly linked to the

environmental burdens identified by the LCA analysis. The main reason for this is that the derived endpoint LCA results indicate environmental and societal damages for which there is no market price. In that sense, there is lack of market data that can be used for assigning economic values in issues of social importance, such as damages on human health and ecosystems, which is the focus of this study. As such, the economic weighting sets (Ecotax02, Recipe and Ecovalue08) used on the basis of the particular methods demonstrate shortage in conversion factors in regards to the LCA endpoint indicators. An additional issue is that the provided factors only mirror use-values, thus neglecting to address the preferences of non-users, who might value the existence of a good to which they do not have access. Consequently, their implementation causes a twofold problem – lack of results' generalizability and representativeness. Which becomes even bigger considering that market prices are usually geographically and time-restricted. That comes into contradiction with the LCA results which account for potential impacts that are aggregated over time and space. Therefore, it is required the used economic weighting factors to be widely applicable, which is not the case in regards to these methods.

The above-addressed issue can be partially overcome in case of applying the economic weighting factors of Ecovalue08, in which non-users values for some midpoint indicators are incorporated (most of the factors are based on market prices). Part of the particular set is grounded on the contingent valuation method in the sense that it provides weighting factors for midpoint indicators whose value to a large extent corresponds to Swedes' perceptions, who were directly asked to state their preferences for non-market goods that reflect on midpoint LCA indicators. However, these factors are limited to few midpoints and none endpoint indicators. Regarding the latter, their absence is directly linked to the followed valuation method. Stated preferences' surveys are insufficient to deal with complex environmental problems such as biodiversity loss, due to the fact that it is difficult to develop hypothetical situations to exchange environmental goods and services for which there is no actual market to be traded. As such, in our point of view, it is rendered unfeasible the particular method, and therefore the pertinent economic weighting factors, to lead to sound results when it is applied in a standalone manner since it is questionable whether or not actual values for environmental costs estimations can be captured.

Moreover, the economic weighting factors of LIME, based on the choice experiment method, were examined. This method also belongs to the family of the stated preferences methods. However, in contrast to the contingent valuation, we perceive the choice experiment method to be highly compatible with LCA for monetizing environmental impacts. Reason for this constitutes the angle from which the monetization of environmental damages can be materialized. To be precise, with this method single damages at midpoint level can be regarded as sub-attributes of the overall impact at endpoint level. By this method, individuals can be asked to place their value and make trade-offs between different kinds of environmental burdens that are linked to a certain safeguard subject (endpoint indicators). As such, the method matches the rationale behind LCA since single environmental problems (midpoint indicators) are aggregated into relevant issues of major concern (endpoint indicators). In other words, a group of midpoint indicators can be regarded as the several attributes that construct a certain endpoint one.

A valuation method that is not related to individuals' preferences but to their purchasing power is the budget constraint method. The budget constraint is a key aspect of the stated preference methods however it is associated with high uncertainty due to the fact the

interviewees may do not state their actual income or even more may not take their actual income as a parameter for answering hypothetical questions. This method has a global scope and can lead to generalizable results since it is based on individuals' average annual income, which can be explored at a country, continent or global level.

The second issue that needs to be examined is whether the used weighting factors can lead to generalizable results. For this, the sets provided by the used methods are scrutinized.

LIME

LIME's purpose was to identify the WTP of the Japanese so that to fend impacts on human health and ecosystems off. It is based on the choice experiment method and provides weighting factors in four endpoint indicators. The derived values are the outcome of personal interviews throughout the country with a random sample. This method cannot lead to generalizable results since its application is spatial-specific and tailored to Japanese conditions. Consequently, we cannot assume that these values are representative on a European level since they are based on Japanese culture, preferences and economy exclusively.

ReCiPe

The monetary weighting factors provided in this method are not based on a certain study for the valuation of non-market goods. Instead, each monetary weighting factor reflects the mean of the values derived from others' studies exploring the value of a human life-year and losses in biodiversity respectively.

Stepwise

Based on the budget constraint method for the valuation of one year of full well-being, the suggested monetary weighting set of the Stepwise valuation technique is grounded on the assumption that an individual's average annual income is the maximum amount of money that they can spend in order to sustain one year without externalities. Therefore, taking into account data regarding the Gross Economic Product (GEP) of USA, Weidema (2009) concluded that one DALY is 74000 EUR₂₀₀₃.

Macroscopically, the assumption and the features of this technique are concrete. Because it makes sense to argue that when human beings are affected by an environmental disaster, they will probably be willing to give up all of their annual income in order to sustain the quality of life that they had before the damage takes place. However, this assumption can only give a good indication for individuals WTP to avoid impacts on human health but not for impacts whose consequences are not directly linked to human health.

Ecotax02

Ecotax02 is a monetary weighting approach in conformity with the Swedish taxation system on emissions and resource depletion. It is based on the hypothesis that the decision-making of governmental authorities mirrors society's values with respect to impacts on the environment. Its scope is geographically restricted as in LIME. Moreover, it has a high level of abstraction since it examines taxes that individuals will have to pay due to CO₂ emissions and

not taxes that concern the source of emissions which is responsible for the environmental burden.

Ecovalue08

For the monetization of impacts on midpoint categories (e.g. GWP), the Ecovalue08 has proposed economic weighting factors based on observed changes in market prices due to resources depletion and on valuation studies in regards to Europeans' WTP to avoid environmental effects. The particular weighting set is suggested to be used in line with the CML Baseline (Centre for Environmental Sciences – Leiden University) impact assessment method (Huysegoms et al., 2018).

While the choice experiment method is regarded as adequate for valuing non-market goods, the implementation of the weighting factors of LIME cannot lead to generalizable conclusions due to their geographical restriction. The same stands for Ecotax02 and Ecovalue08 since they address Swedes preferences. As such, the environmental costs derived by that methods are more likely to represent the WTP of certain social groups rather than that of the Netherlands. Therefore, they are both incompatible with the purpose of this study. We suggest their use when similar studies are geographically oriented in Japan or Sweden respectively because in that case, the results will be more representative.

On the other hand, the weighting set provided to accompany the application of the ReCiPe method might not lead to a consistent outcome since the suggested values do not reflect the actual value placed on human life or biodiversity but the mean of values derived from a plethora of valuation studies. To that end, the use of the particular weighting set is more likely to lead to mean environmental costs, without taking into account the magnitude of the identified impact. Moreover, we are unaware of the criteria on which they were based to choose others' valuation studies and then derive the weighting set as well as the purpose of those studies. Therefore, the particular factors are not appropriate to determine company-specific environmental costs but only mean costs from which it is impossible to conclude what is the company's share.

The application of the weighting factors of the Stepwise method is likely to lead to sound results. The particular method was based on actual economic data to derive its weighting set. The rationale upon which Stepwise is grounded and described above is considered to be compatible with the purpose of the present study, thus it can be used for the monetization of the identified environmental impacts. Therefore, the weighting set of Stepwise is the most representative one for our study because it clearly mirrors an average individual's willingness to sacrifice material things, in order to live a life of full well-being without externalities.

6.4 Economic impact assessment

6.4.1 Investments for improvement

From the economic assessment results in Chapter 5, we can conclude that electricity consumption heavily affects Nouryon's profitability. Its high electricity and heat demand renders the company to a large extent dependent on its suppliers. To that end, we can infer that chlorine's production is influenced by the amount, the price and the source from which

energy is supplied. Moreover, the LCA analysis showed that as the energy demand increases, the environmental impact on the examined indicators increases too. Therefore, in order for the company to reduce the costs and the environmental impact of energy utilization, investments in new technologies and practices are required.

To this direction, we identified that the option to change gap-cells into zero-gap cells can bring to Nouryon several benefits from which not only the company itself is benefited but also the Dutch chlor-alkali industry and the society at large. By investing 77 M€ in zero-gap technology, the company can reduce its electricity costs by 45%, due to fewer energy requirements which subsequently leads to better environmental performance. Excluding the associated environmental costs, in a twenty-year time horizon, this investment can yield two-times more net profits than that of gap-cell configuration.

Furthermore, an additional financially viable option constitutes the replacement of the CHP facility with biomass boilers. From this change, the company can save 1.5 M€/year approximately, due to the fact that natural gas prices are higher than that of wood pellets. However, this is the only economic benefit from the implementation of that scenario. Besides that they require an initial capital investment of 23 M€ approximately, biomass boilers' employment leads to an increase in electricity requirements which will cost to the company around 4 M€ more. Although the particular option yields the lowest economic benefits, it still remains a financially attractive alternative since the gross revenues from the sold production still exceed the associated costs.

6.4.2 Environmental Costs

Given the monetary weighting factors of Stepwise, for the reasons mentioned above, the zero-gap membrane electrolysis scenario has again the lowest environmental costs associated with impacts on human health and ecosystems. Specifically, as it is illustrated in Figure 25, S1's environmental costs are lower compared to the S0, S2 and S3 scenarios by 22.8%, 24.4% and 2.5% respectively in regards to the endpoint indicators. Accordingly, as far as the ecosystem indicator is concerned, the environmental costs of S0, S2 and S3 scenarios are higher with respect to S1 by 30.4%, 38.0% and 8.2% respectively. The second-least expensive scenario from an environmental viewpoint is the S3 scenario which has relatively higher costs than S1 in both endpoint indicators.

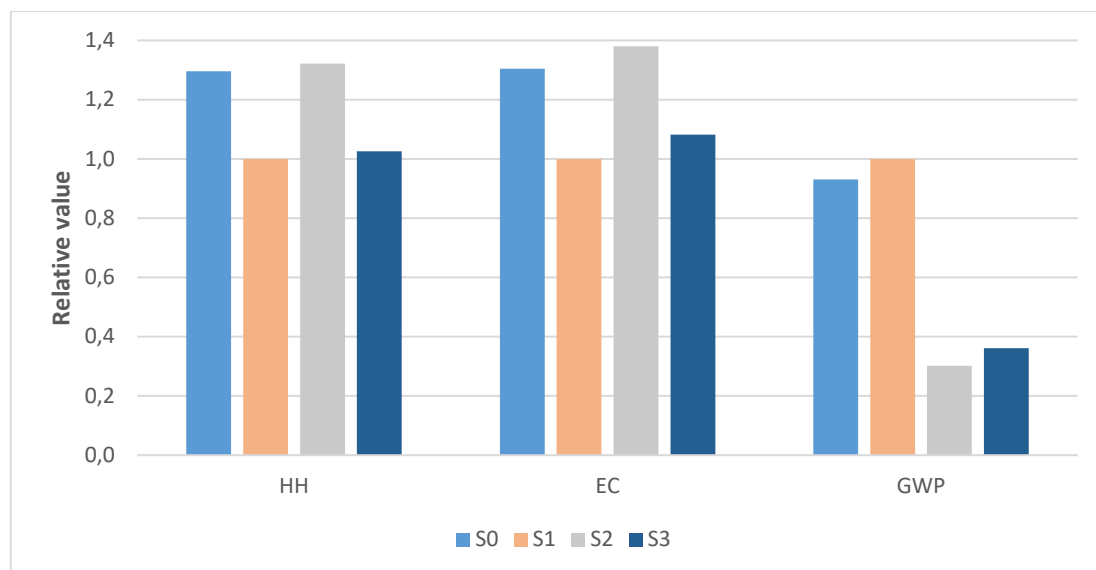


Figure 25: Comparison of S2's environmental costs with the environmental costs of the other three scenarios; Reference values: HH: 2.24E+02 €/ton Cl₂; EC: 1.71E+06 €/ton Cl₂; GWP: 14.71 €/ton Cl₂;

However, the issue that arises is who has to pay for these cost estimations? Taking S1's cost estimation into consideration, the calculated environmental costs for impacts on human health are 2,241 €/ton Cl₂ and 1.71 M€/ton Cl₂ for impacts on ecosystems. The particular cost-estimations result from the environmental footprint of the energy and raw materials consumed on-site but produced from external sources. To that end, it stands to argue that the calculated environmental costs with respect to S1 encapsulate the environmental footprint translated into monetary terms of all energy and raw materials production activities involved in the Dutch chlorine industry. As such, all stakeholders involved in the chlorine production chain are jointly responsible for taking over the identified environmental costs. However, the affiliated stakeholders are not equally responsible. The level of contribution of each stakeholder to the overall environmental impact on human health and ecosystems is linked to the kind of production activities that they implement in order to supply the considered chlor-alkali plant with energy and raw materials. For instance, the environmental footprint of salt transportation via inland vessels has not the same footprint with deionized water production through reverse osmosis. Therefore, to determine the share of each involved stakeholder in the total calculated environmental costs of S1, the environmental footprint of each production system that supplies with inputs the examined chlor-alkali plant has to be assessed. Since the economic analysis is executed from the manufacturer's perspective (Nouryon), determining the share of each stakeholder in the estimated environmental footprint and thus in the environmental costs is rendered beyond the scope and the purpose of this study. Therefore, the costs that can be directly attributed to Nouryon are those that concern CO₂ emissions from on-site energy (either heat and/or power) generation.

By translating via Stepwise's weighting set the environmental impact on the GWP category due to on-site energy generation into environmental costs, the highest increase in the total estimated costs is recorded by S1 while the lowest by S2. Particularly, for a twenty-year time horizon, the calculated environmental costs of S1 are 160 M€ while that of S2 are 48 M€. Incorporating these costs in the overall economic assessment of each scenario's implementation and operation, the NPV of S1 decreases by 9.2%, reaching 1,579 M€. On the other hand, despite that the implementation of S2 is associated with less environmental costs, the particular option yields 670 M€ approximately, thus being the second-worst scenario from

a financial perspective. After S1, the next most attractive scenario to invest in is that of S3, with a calculated NPV at 1,485 M€. The financially-best ranking closes with the reference case scenario, yielding 50 M€ less than S2.

Besides the level of the environmental impact, the next most significant factor that influences the magnitude of the calculated costs is the discount rate used to determine the present value of costs that are anticipated to occur in the future. As it is shown in Figure 26, the higher the level of the discount rate the less the present value of the future environmental costs. By selecting a high discount rate the anticipated future costs are undervalued when a decision about a new investment has to be taken in the present. As such, the costs from the environmental impacts are neglected and not addressed as an equally significant factor for making a design-related choice. As the present study has shown, the impacts on the environment may lead to adverse effects, therefore, the CO₂ emissions and thus the associated environmental costs should be a determinant when making a decision whose effects potentially can affect others. To that end, by selecting a low discount rate we are led to a win-win situation. In that sense, the company is incentivized to invest money today in order to avoid higher costs in the future and as it was revealed by the analysis all investment options are good enough for taking. Consequently, by investing today, operational costs are drastically cut down. But the most important, that justifies the win-win situation, is the rapid decrease of the environmental impact which otherwise would burden the health, quality of life and economy of humanity.

The following graph represents the change in the estimated environmental costs when four different discount rates are applied. For the reasons explained above, the particular study calculated the associated costs with the identified environmental impacts by selecting the lowest possible discount rate, which is 0.01%.

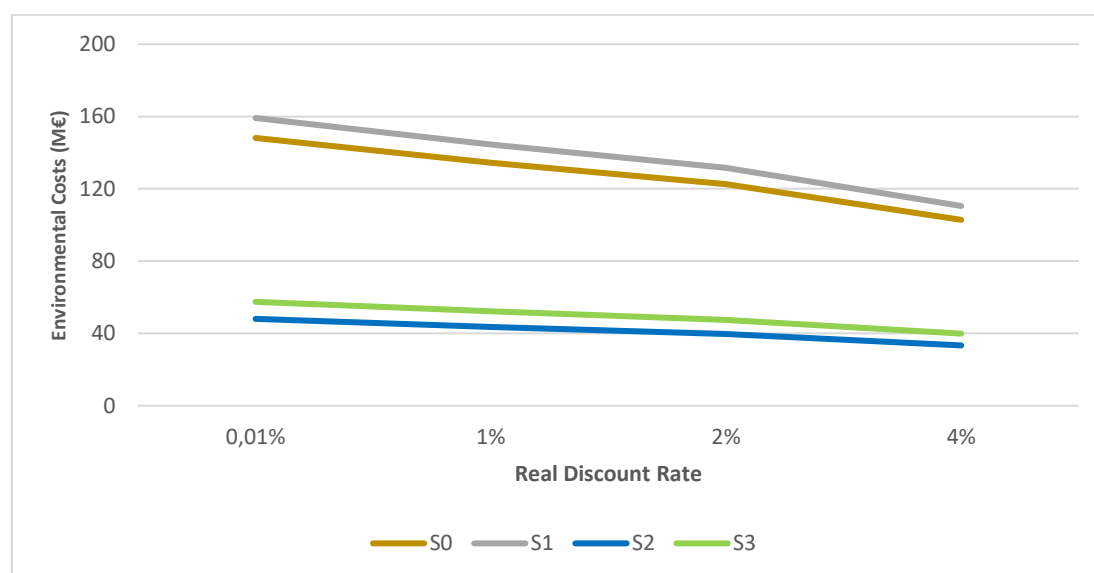


Figure 26 Change in environmental costs as a function of change in the level of the discount rate

Chapter 7: Conclusions

7.1 Answers to RQs

The present project revolved around the identification of the most cost-effective and less energy-intensive technical solutions which can enhance the enviro-economic performance of Nouryon's chlorine production system at Botlek from a life-cycle perspective. For this purpose, the LCA and LCC techniques were implemented in an integrated manner by using five different economic weighting sets to translate the identified environmental damages into monetary terms. To that end, the scope of our project is in line with the recognized knowledge gap in chapter 1 which concerns the absence from the scientific literature of a study merging the LCA and LCC techniques with a view to assessing the enviro-economic profile of chlorine production systems in the Netherlands and suggest ways for their improvement. In order to adequately tackle this issue and bridge the pertinent knowledge gap, our research endeavour was guided by our interest to seek an answer to the following research question,

«How to develop an enviro-economic evaluation method that integrates Life-Cycle Assessment & Life-Cycle Costing techniques and implement it on the Dutch chlor-alkali manufacturing industry?»

The main research question is divided into two parts – the theoretical one, concerning the delineation of the core concepts used in this study and the practical implementation of the findings in the first part on a case study. Therefore, to answer the main research question, five sub-questions were formulated. The first two correspond to the theoretical part while the remaining are focused on providing answers to practical issues regarding Dutch chlorine production systems.

To begin with, we answer the sub-question referring to the following,

«How to conduct a comprehensive enviro-economic assessment based on the LCA and LCC techniques?»

To resolve this question, the key theories and core principles regarding the LCA and LCC techniques were explored. Through our desk research, we identified a suggested in the literature way for the integration of LCA and LCC. This way concerns the parallel implementation of both techniques following the ISO-provided structure of LCA and merging the concepts by converting the environmental impact assessment results into monetary terms with the use of LCA-based economic weighting factors. Given this approach, both eLCC and cLCC are used to conduct the economic analysis of the project consisting of internal and external costs estimations while LCA is applied to quantify the environmental damage associated with the implementation of the project.

As such, the structure of the enviro-economic assessment consists of the four phases of LCA but directed beyond the scope of the environmental impact assessment. Firstly, the goal of the study is defined in such a way so that to be in line with both parts of the assessment. Then,

after establishing the preferred system boundaries the LCI should consist of all flows going in and out of the system including material, energy (by type) and cash flows. Next, by using an appropriate LCA software and selecting an appropriate impact assessment method the environmental damages caused by the operation of the examined production system can be quantified. Then, the obtained results can be expressed in monetary terms after applying economic weighting factors provided by different LCA-based valuation models. To that end, costs estimations regarding the operation of the system and the associated environmental externalities within a specific time horizon can be provided by selecting a proper discount rate for the calculation of the anticipated future money flows. Concluding, the discussion of the results of both parts of the assessment can take place in the interpretation phase.

After structuring the enviro-economic assessment, the methods suitable for the monetization of environmental damages were addressed by answering the following sub-question,

«What valuation methods can be used for the monetization of environmental damages and which are the most appropriate ones for life-cycle studies?»

The monetization of environmental damages can be achieved in two different ways. The first one concerns the implementation of valuations methods to elicit individuals' preferences in regards to the value of non-market goods affected by environmental damages, while the second one refers to the use of LCA-based economic weighting factors that are appropriate to convert environmental damages into monetary terms.

As far as the first way is concerned, based on two fundamental principles, namely Willingness-to-Pay and Willingness-to-Accept, five approaches which are sub-divided in several valuation methods were identified for the monetization of environmental damages (see Table 1, subsection 2.4). Among them, the choice experiment method and the budget constraint method have high compatibility with life-cycle studies whose aim is to provide costs estimations for environmental damages evoked by industrial activities.

Given that LCIA consists of groups of midpoint indicators that are directly linked to endpoint indicators meaning that single impacts such as global warming are connected to impacts on areas of protection such as human health, the choice experiment method is thought to be ideal for monetizing environmental damages due to its multi-attribute valuation perspective. In that sense, single impacts that are linked to midpoint indicators can be seen as the several attributes of an endpoint indicator. As such, following the logic of the stated preferences approach, individuals can be asked to state their preferences by putting economic weights and making trade-offs between midpoint environmental impacts that contribute to the overall identified impact on a certain safeguard subject. To that end, these economic weights would reflect their WTP to avoid or mitigate the consequences of single environmental damages which are aggregated into issues of major concern. Therefore, due to the similar rationale of LCIA and the choice experiment method, life-cycle studies can use the latter to monetize environmental damages. However, an issue that needs to be taken into consideration when the choice experiment method is implemented and might negatively affect the generalizability and validity of results concerns the decision regarding who will be chosen to participate in the pertinent surveys. In case that respondents are not aware or affected by environmental consequences there is always a danger of overvaluing or devaluing environmental impacts. As such, in order to avoid respondents' probable bias, we first believe that the affected area and

the extent to which it is affected should be determined through an LCA study and then conduct surveys to the affected population.

The above-addressed issue can be directly overcome by implementing the budget constraint method which does not make use of surveys but it is based on actual economic data. In particular, it is grounded on the assumption that the average annual income of an individual is the maximum amount of money that they can spend in order to sustain one year of full well-being without externalities. As such, by firstly determining the affected regions and populations and then making an analysis based on data regarding country- or region-specific employment rates, and individuals' average income, the value of one year without externalities effects on human health can be derived. This method can add value to the application of the LCA technique when it is focused on quantifying impacts on safeguard subjects such as human health. The drawback of the method is that the assumption upon it is based might not stand accurate for valuing single impacts that do not directly affect human health. Nevertheless, it can give good economic indicators for monetizing endpoint impacts.

The second way through which the monetization of environmental impacts can be achieved is by multiplying the level of the environmental damage (amount of impact per unit of final output) with relevant economic weighting factors (measured in € per unit of impact). The economic weighting sets applied in this project are provided by the LCA models of ReCiPe, LIME, Stepwise, Ecovalue08 and Ecotax02. The particular factors can be implemented during the weighting step of the LCIA.

After using all of the addressed weighting sets, we identified that the environmental cost-related results differ from each other since the weighting factors applied in this study are based on different valuation methods. Nevertheless, the general conclusion that can be drawn from their application is that all of them indicate a benefit (cost reduction) when environmental performance is improved, whereas costs increase when performance declines. Moreover, the implemented weighting sets are found to be incomplete. Specifically, there is no set through which all LCA midpoint and endpoint indicators can be converted into monetary terms. That means that none of them can be used consistently by LCA studies with a view to monetizing performance scores in all impact categories of both levels. Additionally, cultural, social and economic differences between the studies that conducted to derive the used weighting factors, heavily contribute to the noticed deviation of the results. As such, the generalizability and representativeness of these weighting sets are negatively affected, thus making them incomparable due to their different socio-cultural orientation. In order to overcome the geographical and cultural bias of the used weighting factors, we conclude that only the weighting set of the Stepwise method can be used for our project and can lead to generalizable results. That is because the underlying assumption upon which the pertinent weighting factors are based (budget constraint method) is considered to be an accurate way for valuing impacts on human health since those who are affected by an environmental disaster will probably be willing to give up all of their annual income in order to sustain one year of full wellbeing. But then again, this assumption cannot provide accurate indications for individuals WTP to avoid single impacts that do not affect human health. Moreover, while the weighting factors of LIME were derived through the choice experiment method, which is perceived to be the most compatible valuation method with the LCA technique, they cannot be used to represent the WTP of the Dutch since its application is spatial-specific and tailored to Japanese conditions.

Given the answers to the first two sub-questions, we implemented the literature findings on a case study that concerns Nouryon's chlorine production system at Botlek. Four scenarios were developed in order to assess the enviro-economic performance of the considered chlor-alkali plant in regards to energy and resource consumption. Assuming steady-state production systems, the scenarios consist of modifications in the configuration type of the membrane cell as well as in the industrial installation used for heat generation. In the reference case (S0), chlorine production is achieved through gap cell electrolyzers exclusively, while heat is generated via an on-site CHP facility. The same installation for heat generation is considered in scenario 1 (S1) but chlorine is produced via zero-gap cell electrolyzers. Scenario 2 (S2) and scenario 3 (S3) represent the application of biomass boilers for heat production. In the former chlorine is manufactured via gap-cells while in the latter the configuration type of the cell has changed in zero-gap one. As such, our conclusions with respect to the enviro-economic profile of the four developed scenarios for chlorine production are displayed as the answers to the following three sub-questions.

«What are the most environmentally intensive processes in the considered chlorine production system and to what extent different technical modifications affect the environmental profile of the system?»

For each scenario, the chlorine manufacturing phase results in the greatest impact on the environment. In this phase, the membrane electrolysis stage accounts for the largest contribution to the overall environmental impact, with a value of 985 kg CO₂ eq/ton Cl₂ in regards to S0. The implementation of S1 and S3 can bring 39% and 36% decrease in CO₂ emissions of this phase per ton of Cl₂. Electricity consumption, which is over 3,000 kWh/ton of Cl₂, is the dominant cause behind the identified level of contribution of the membrane electrolysis stage.

Next, the brine preparation is a resource-intensive stage, which due to the pretreatment of raw materials such as dry salt, depleted brine and HCl results in the second-highest process-specific impact of the considered chlorine production system. The deployment of zero-gap cells which is associated with less amount of raw materials processed per ton of chlorine can lead to less environmental damage.

Furthermore, due to the high heat requirements of the caustic soda production stage, 50 kg CO₂ eq/ton Cl₂ were recorded when the heat demand was covered by the on-site CHP facility (S0). In the case of biomass boilers' employment (S2), the impact of the particular stage can be decreased by 24% approximately.

Additionally, the industrial installation for on-site heat production plays a crucial role in regards to the overall environmental impact. The operation of biomass boilers is associated with less environmental damage compared to the CHP facility. However, the environmental impact of both installations might not be comparable since it was considered that the CHP facility co-produces power and heat at 1:2 ratio while biomass boilers generate only heat. When comparing their environmental profile in regards to heat output exclusively, then biomass boilers (S2) impact the environment by 52.7 kg CO₂ eq. /GJ of heat, while the CHP plant (S0) by 72.7 kg CO₂ eq. /GJ of heat.

Lastly, the indirect emissions account approximately half of the identified environmental impact in regards to the global warming indicator because of the overall high electricity

demand and the Dutch electricity mix which is supplied on-site. Electricity generation based on hard coal and lignite is the largest contributor to the overall impact on global warming, followed by the natural-gas-fired co-generation power and heat plants.

Overall, the modification of the electrolysis cell from gap to zero-gap one results in the lowest environmental and human health damage. Due to lower current density and electricity consumption, the particular production system demonstrates the lowest scores in all of the examined indicators. Similar results to the latter are obtained from S3 which concerns the parallel deployment of zero-gap cells and biomass boilers. However, in this case, an increase in the score of the ecosystems indicator is recorded. Additionally, from an environmental impact perspective, the reference case, as well as the scenario that exclusively involves biomass boilers, show the poorest environmental performance, since both constitute the most energy and resource-intensive scenarios.

«How do different technical modifications affect the economic performance of the considered chlorine production system?»

From an operational cost perspective, electricity consumption constitutes the major financial burden in all cases. When chlorine is produced via gap cell electrolyzers, electricity costs account for 60% of the total costs. 45% reduction in the electricity costs can be achieved when zero-gap cells are implemented. Overall, zero-gap cell electrolyzers are associated with the least operational costs, requiring an initial investment of 77 M€. Moreover, by changing the cell's configuration in zero-gap one, the company will substantially increase its savings, as a consequence of its fewer requirements in raw materials and electricity. On the other hand, though the deployment of biomass boilers (S2) requires the lowest capital investment (22.75 M€), it has the highest operational costs due to an increase in electricity demand. Besides the plant's dependency on electricity, the production system consumes considerable amounts of natural resources. Expenses for natural gas or wood pellets requirements account between 4% and 5% of the total identified costs.

The chlorine-chain related environmental costs depend on the overall identified impact of each scenario. Therefore, the installation of zero-gap cells results in the least environmental costs reaching 2,241 €/ ton Cl₂ for damages on human health and € 1.71 bn/ton Cl₂ due to damages on ecosystems. Compared to the latter, the deployment of biomass boilers (S2) will bring 32% and 38% increase in the environmental costs of both indicators due to higher electricity consumption.

Company-related environmental costs are inextricably linked to what system is implemented for heat generation. Under this project, two ways for on-site heat generation were explored – CHP plants and biomass boilers. The total identified impact of the scenarios in which heat demand is covered by an on-site CHP plant is less than those where biomass boilers are engaged in. However, the contribution of biomass boilers to the overall impact of each scenario is less, compared to the contribution of CHP plants. Specifically, due to CHP's operation 113.72 and 136.36 kg CO₂ eq./ ton Cl₂ are emitted in the reference case and in S1 respectively, while biomass boilers contribute 41.15 and 49.22 kg CO₂ eq./ ton Cl₂ to the overall impact of S2 and S3 respectively. To that end, the company's environmental costs due to on-site energy generation are less when CHP plants have been replaced by biomass boilers. In particular, when S2 is implemented, i.e. the CHP facility is replaced with biomass boilers, the level of the environmental cost reaches 4.44 €/ ton Cl₂. On the contrary, the operation of

the CHP facility is anticipated to financially burden the company by 14.73 €/ ton Cl₂, if S1 is followed.

Taking into account the total production costs including environmental costs and according to the NPV rule, all projects are financially viable for implementation. The most attractive option for investment concerns the modification of the membrane into zero-gap one (S1), yielding €1.58 bn for a twenty-year time horizon. The second best option is S3 with €1.48 bn for the same time period. On the other hand, the financially worst scenario concerns the installation of biomass boilers when gap-cell electrolyzers are employed.

«What are the most cost-effective and with the least environmental damages technical solutions regarding the considered chlorine production system from a life-cycle perspective?»

Firstly, we identified that the deployment of zero-gap cell electrolyzers with or without biomass boilers is associated with the least environmental burden. Notably, the scores of these two scenarios in the examined indicators have a small difference. However, the most environmentally friendly solution concerns the installation of zero-gap cell electrolyzers when the heat is generated by an on-site CHP facility, followed by the scenario that consists of the same configuration type but the CHP plant is replaced with biomass boilers.

Again in the same ranking, these two options are the most financially attractive for implementation, yielding in a twenty-year time horizon € 1.58 bn and € 1.48 bn approximately. Both technical solutions go in tandem with the least operational expenses since power and raw materials requirements are drastically decreased. Moreover, their results regarding the chlorine-chain environmental costs are the least, as a consequence of fewer damages on human health and ecosystems with respect to other examined scenarios. On the other hand, the company's share in the computed environmental costs is higher when the CHP facility is employed due to higher CO₂ emissions. On the contrary, by replacing the CHP plant with biomass boilers in case of S3's implementation, the environmental costs attributed to the company are less due to the installation's better environmental performance. However, in both cases, the financial burden that the company has to bear due to CO₂ emissions is negligible when considering all other expenses associated with chlorine production. Specifically, for the selected time horizon, the environmental costs of the first option account for 6% of the total costs while for the second one 2% approximately. Therefore, both technical solutions represent our suggestions to Nouryon in order to enhance the enviro-economic performance of Botlek's chlor-alkali plant. The particular recommendations are displayed in Chapter 8.

7.2 Research contribution

Though academia extensively addresses the combined implementation of LCA and LCC as the appropriate scientific way for assessing the environmental and financial life-cycle performance of a production system, their integration still lacks a robust methodological structure. For this is responsible the scientific debate with respect to the expansion of LCC's scope (from financial to environmental orientation) so that to be aligned with LCA in the sense to provide costs estimates for environmental damages. Given that, we engage in the pertinent scientific debate and contribute to academia by proposing an approach for their integration

on the basis of investigating whether different valuation methods can be used for environmental externalities monetization. As such, we implemented LCA-related economic weighting sets that are based on different valuation methods in order to convert the identified environmental damages into monetary terms and then added them as a cost-component in the LCC structure. However, due to the incompleteness, geographical and cultural bias of the examined weighting factors, we conclude that except for one weighting set, which can be representative for certain impact categories, all the others cannot be used consistently in LCA studies. Therefore, we end up suggesting the importance of autonomous valuation research for monetizing environmental damages under the combined context of LCA and LCC.

Moreover, this research contributes to academia by integrating and implementing the LCA and LCC techniques with a view to assessing the enviro-economic performance of Nouryon's chlorine production system in the Netherlands (Botlek). Specifically, the combined application of the LCA and LCC techniques to this country and industry is absent from the academic literature, which adds to the scientific contribution of this project. Lastly, we also contribute to Nouryon's efforts to achieve its climate change targets by pointing out which technical modifications can lead to GHG emissions reduction and enhance the company's financial sustainability. As such, we wish to have through our suggestion a positive impact on Nouryon's future considerations towards sustainability.

Chapter 8: Recommendations & Reflection

8.1 Recommendations to Nouryon

In this project, the environmental footprint, as well as the environmental, and operational costs of four different scenarios in regards to Nouryon's chlor-alkali plant at Botlek were examined. From our analysis, a twofold problem was identified. Firstly, chlorine's production high dependency on power and heat consumption constitutes a substantial financial burden for Nouryon, which is even higher when considering the associated environmental costs from impacts on the environment. Secondly, the production system's energy-intensity is inextricably linked to a significant environmental footprint which goes in tandem with multifaceted negative effects on the society but also to the overall social image of the industry. Hence, after the identification of the hot-spots of the chlorine production system two recommendations can be made. These recommendations can potentially lead to lower energy consumption, less environmental impact and thus higher economic output. Therefore, their employment is not only expected to bring benefits to the company and enhance its social image but also to create a domino of positive effects on the chlor-alkali industry and society at large. The following suggestions are the outcome of the comparison between the results of each examined scenario and the reference case where chlorine's production exclusively takes place by gap-cell electrolyzers.

1st suggestion

The electrolysis process has between 60% and 70% contribution to the total environmental impact due to the high electricity requirements. To tackle the high power demand and the caused environmental impact, the modification of the membrane's cell configuration is suggested. Specifically, twenty-one zero-gap cell electrolyzers with per unit capacity of 30.5 kton Cl_2 /year are recommended for transitioning from gap cell to zero-gap cell membrane electrolysis. In line with that, an initial investment of 77 M€ for the installation of zero-gap cells is required which in five years will yield 570 M€ approximately.

By changing the cell's configuration from gap-cells to zero-gaps cells the total electricity requirements are decreased by 38% while keeping the level of production capacity constant. Consequently, almost two-time fewer electricity costs are estimated than that of the conventional configuration, resulting in 85 M€ savings per year approximately.

Moreover, this change is accompanied by environmental benefits which will bring the company more close to its sustainability target that concerns a 25-30% reduction of CO_2 emissions by 2020 and become carbon neutral by 2050. In particular, with our suggestion, it is estimated 39% reduction of CO_2 emissions in the membrane electrolysis stage, or in other words 24% reduction in the total CO_2 emissions per ton of chlorine produced. To that end, the

company's environmental costs due to on-site generated CO₂ emissions will account just for 6% of the total estimated costs.

As a consequence of this change, positive side effects are anticipated in the long-run. Firstly, environmental impacts on human health and ecosystems due to off-site power generation will decrease by one-quarter of the initial impact. To that end, the quality of life is improved drastically and the industry's social image is enhanced. In addition to the latter, chain-related environmental costs will decline by 23% which otherwise would have to be paid by a plethora of industry's stakeholders in the form of compensation to society. Finally, in a twenty-year time-horizon, the expected profits for the company are estimated to reach €1.58 bn which can be further invested in improving the identified hot-spots.

2nd suggestion

Along with the change in the membrane cell's configuration, the replacement of the current CHP plant with biomass boilers for on-site heat generation is recommended. By selecting this alternative, besides the results of the zero-gap cell electrolysis, Nouryon can achieve a further reduction in environmental costs due to lower on-site generated CO₂ emissions. However, the overall enviro-economic performance of this option is slightly lower than that of the first suggestion.

The installation of sixteen 2 MW biomass boilers is recommended for the production of 918.5 TJ/year steam at 200 °C which will mainly cover the demand of the caustic soda concertation stage. As such, an investment of 97 M€ is required which in turn will yield 490 M€ in five years. Electricity costs are estimated to decrease by 36%.

Moreover, the employment of this option is anticipated to bring a 60% reduction in the on-site generated CO₂ emissions and 23% in regards to the whole production system respectively. Additionally, impacts on human health and ecosystems will drop by 21% and 17% respectively. As such, the company-related environmental costs are estimated to be 2% of the total costs. Therefore, in a twenty-year time-horizon, this project is expected to yield € 1.48 bn.

Overall, an organization's inherent intent is to create value. This implies more than just optimizing production or finding the most cost-efficient solutions, but it means to create value for customers, society and enhance the economic benefits for the shareholders. As it is shown, Nouryon is currently on a sustainability track by including in its mission the reduction of CO₂ emissions while remaining profitable. In consonance with that, we have suggested two possible solutions with similar environmental benefits but differing from a financial perspective. Nevertheless, both can add value to the company and society. Moreover, our recommendations are in line with the company's eco-footprint targets which are based on the Dutch government's goals for mitigating climate change.

8.2 Limitations of the study

Environmental model – LCA

This project, like any scientific research, undoubtedly has its constraints. First of all, the decision of structuring the reference case scenario on the basis that chlorine is exclusively produced via gap-cells electrolyzers does not reflect on Nouryon's actual production system.

Currently, at Botlek's chlor-alkali plant, a portion of the total electrolysis cells is of zero-gap configuration type. Therefore, we cannot claim that our results regarding the environmental and financial performance of Nouryon's chlorine production system are representative. Nevertheless, the outcome of this study shows that the particular technical adjustment is associated with several enviro-economic benefits.

Furthermore, despite that we recognized that the overall environmental performance of the production system is affected by the power consumption of the membrane electrolysis stage, the developed scenarios include just technical adjustments and not technological alternatives for chlorine production, such as the diaphragm and ODC technologies. Therefore, an analysis in regards to these technologies might have led to the identification of different 'hot-spots', and thus to a totally different outcome.

Thirdly, the assumption regarding a steady-state production system might fit with the purpose of this project but restrains us from deriving reliable conclusions about the actual performance of the system. On an industrial scale, companies operate in a dynamic environment in which they try to meet customers' needs by adjusting to the constantly changing market conditions. As such, taking into account contingent fluctuations in the market prices and the availability of the products required for chlorine production, the hypothesis that the total production capacity, the operational expenses and the environmental costs of the considered chlor-alkali will remain stable over the examined period is not in line with the actual market conditions.

Moreover, the limitations of the decisions regarding the scope of the analysis should be addressed. The extent to which the outcome of the study is reliable depends on the selected scope and system boundaries. Our decision to exclude from the system boundaries the construction of the suggested installations as well as the waste management does not allow us to draw comprehensive conclusions in regards to the overall performance of the system. Therefore, the particular project is limited in the quantification of the environmental impacts that exclusively come from energy and raw materials consumption. To that end, our study cannot be considered as a full life-cycle analysis, but instead as an energy and resources consumption assessment from a life-cycle perspective. Lastly, while we applied an impact assessment method with a global scope, we did not try other methods in order to ascertain any differences in the final results, thus affecting the reliability of the outcome.

Economic model – LCC

The first issue regarding the economic analysis is that it was based on the LCA's standards. That has limited its broadness since in order to be in line with the ISO structure and consistent with the LCA analysis both perspectives shared the same system boundaries and scope. Therefore, costs associated with raw materials transportation, marketing, end-products delivery, logistics and every other money flows outside of the selected boundaries were not incorporated in the analysis. As such, while we identified that every scenario constitutes a financially viable solution for the company to pursue, this might not be the case if all costs related to the company's supply chain would have been considered.

Moreover, the decision to focus the scope of the economic analysis only on the manufacturer's perspective has inhibited us from inferring conclusions in regards to the probable positive or negative effects that the implementation of each scenario might bring to the stakeholders involved in the chlorine chain. Therefore, being unaware of the side-effects

that they might cause, we cannot claim that our suggestions would be in everyone's interest. To that end, a stakeholder analysis is imperative in order to ascertain if the proposed changes in the considered chlorine production system are indeed positive for the industry and society at large.

Lastly, our choice to base the monetization of the environmental impacts on economic weighting factors derived from different valuation studies, and not to conduct independent valuation research, constitutes one of the project's limitations. To some extent, this decision has influenced the reliability of our results since the used economic weighting sets are based on economic and demographic data of the regions where the valuation studies have taken place. That means that they represent the preferences of certain social groups, and not in particular that of the Netherlands. Consequently, we should state that we have only provided estimations for environmental costs due to the fact that there is a high chance for people's preferences to differ from place to place.

8.3 Directions for future research

Considering the limitations of our study, we can provide some directions for future research in this field. Firstly, since we identified that the "hot-spot" in a chlor-alkali plant is that of electrolysis stage, several life-cycle studies can be conducted in order to diagnose which electrolysis technology can yield the best results. Therefore, it would be very interesting for future researchers to explore if novel practices, such as the ODC technique, can result in less energy consumption and better environmental performance by replacing the currently adopted technologies. Moreover, since the chlor-alkali industry is inextricably linked with the salt manufacturing industry, a broader LCA scope, in which the production activities of both industries will be included, might give insights on how changes in one industry affect the other. Additionally, our suggestion is that every LCA study which aims to provide policy suggestions should be accommodated by stakeholders and political analyses. That would facilitate the researchers to identify what are the interests of the society and the political views so that to be able to propose well-founded solutions.

As far as the monetization of the environmental impacts is concerned, we suggest the following steps through which future researchers would be able to derive reliable economic results. Initially, the environmental impacts of the examined system should be quantified. Then, we suggest that stakeholder analysis is imperative in order to first identify all actors involved in the considered production chain and then determine their share in the found environmental impact. Consequently, an investigation regarding which regions and populations are affected by the environmental damage should take place. To that end, we recommend future researchers to conduct a valuation study based on the choice experiment method to elicit from the affected population the value that they would place on several environmental impacts that affect human life and ecosystem. Therefore, after analysing the results of the valuation study the environmental costs as a consequence of the damage can be determined and attributed to those being responsible for it.

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Appendix A

Energy & Material flows for 1 ton of chlorine production per examined scenario

Reference Case (S0)

	Input	Quantity	Units		Output	Quantity	Units
CHP plant	Natural Gas	63,33	m3		Electricity (internal use)	275	kWh
					Heat (internal use)	1,89	GJ
					CO2 emissions	210	kg
NaOH preparation	Total Heat	0,7	GJ		NaOH (30%)	38	ton
	Heat (CHP plant)	0,39	GJ				
	Heat (Recovered Heat)	0,31	GJ				
	Dimineralized water	2,4	ton				
	NaOH (32%)	36	ton				
Brine preparation	Heat (Recovered Heat)	1,2	GJ		Saturated brine (23%)	20	ton
	Dry Salt	1,6	ton				
	Dimineralized water	510	kg				
	HCL (32%)	0,18	kg				
	Depleted brine (17%)	18	ton				
Dechlorination stage	Electricity (CHP plant)	0,05	kWh		Chlorine gas	5,4	kg
	Depleted brine (17%)	18	ton		Depleted brine (17%)	18	ton
	HCL (32%)	16	kg				
	NaOH (32%)	21	kg				
Membrane electrolysis	Electricity (CHP plant)	211,06	kWh		NaOH (32%)	3,5	ton
	Electricity (National grid)	2844,52	kWh		Cl2 (90°C)	1	ton
	Mebr. Electr. total electricy	3055,58	kWh		H2 (90°C)	28	kg
	NaOH (30%)	38	ton		Waste heat	2,2	GJ
	Saturated brine (23%)	20	ton		Depleted brine (17%)	18	ton
					Recirculated NaOH (32%)	36	ton
Multiple effect	Heat (CHP plant)	1,5	GJ		NaOH (50%)	2,2	ton
	NaOH (32%)	3,5	ton		Mother liquor	1,3	ton
Hydrogen cooling	H2 (90°C)	28	kg		H2 (20°C)	27	kg
					Waste heat	0,029	GJ
Hydrogen compression	Electricity (CHP plant)	8,89	kWh		H2 (300 bar)	2,7	kg
	H2 (20°C)	27	kg		H2 (100 bar)	24	kg
Chlorine cooling	Cl2 (90°C)	1000	kg		Cl2 (20°C)	800	kg
	Chlorine gas	5,4	kg		Waste heat	0,055	GJ
	Total	1005,4	kg				
Chlorine drying	Cl2 (20°C)	800	kg		Cl2 (20°C)	800	kg
Chlorine compression	Electricity (CHP plant)	33,33	kWh		Compressed Cl2	800	kg
	Cl2 (20°C)	800	kg				
Chlorine liquefaction	Electricity (CHP plant)	21,67	kWh		Cl2 final use	800	kg
	Compressed Cl2	800	kg				
Total Electricity rq.	Electricity (CHP plant)	275	kWh				
	Electricity (National grid)	2844,52	kWh				
	Total Electricity Demand	3119,52	kWh				
Total Heat rq.	Heat covered by CHP	1,89	GJ				
	Total Waste Heat	2,28	GJ				
	% max. waste heat reuse	81%					
	Max. recovered waste heat	1,85	GJ				
	Actual Recovered Heat	1,51	GJ				
	Total Heat Demand	3,4	GJ				

Scenario 1 (S1)

	Input	Quantity	Units		Output	Quantity	Units
CHP plant	Natural Gas	63,33	m3		Electricity (internal use)	275	kWh
					Heat (internal use)	1,89	GJ
					CO2 emissions	210	kg
NaOH preparation	Heat (CHP plant)	0,585	GJ		NaOH (30%)	32	ton
	Dimineralized water	2,01	ton				
	NaOH (32%)	30,1	ton				
Brine preparation	Total Heat	1,02	GJ		Saturated brine (23%)	17	ton
	Heat (Recovered Heat)	0,968	GJ				
	Heat (CHP plant)	0,052	GJ				
	Dry Salt	1,36	ton				
	Dimineralized water	434	kg				
	HCL (32%)	0,15	kg				
	Depleted brine (17%)	15,3	ton				
Dechlorination stage	Electricity (CHP plant)	0,04	kWh		Chlorine gas	4,6	kg
	Depleted brine (17%)	15,3	ton		Depleted brine (17%)	15,3	ton
	HCL (32%)	14	kg				
	NaOH (32%)	18	ton				
Membrane electrolysis	Electricity (CHP plant)	191,39	kWh		NaOH (32%)	2,9	ton
	Electricity (National grid)	1669,74	kWh		Cl2 (90°C)	1	ton
	Mebr. Electr. total electricy	1861,13	kWh		H2 (90°C)	90	kg
	NaOH (30%)	32	ton		Waste heat	1,6	GJ
	Saturated brine (23%)	17	ton		Depleted brine (17%)	15,3	ton
					Recirculated NaOH (32%)	30,1	ton
Multiple effect	Heat (CHP plant)	1,253	GJ		NaOH (50%)	1,84	ton
	NaOH (32%)	2,9	ton		Mother liquor	1,1	ton
Hydrogen cooling	H2 (90°C)	90	kg		H2 (20°C)	86	kg
					Waste heat	0,092	GJ
Hydrogen compression	Electricity (CHP plant)	28,57	kWh		H2 (300 bar)	8,7	kg
	H2 (20°C)	87	kg		H2 (100 bar)	77	kg
Chlorine cooling	Cl2 (90°C)	1000	kg		Cl2 (20°C)	800	kg
	Chlorine gas	4,6	kg		Waste heat	0,055	GJ
	Total	1004,6	kg				
Chlorine drying	Cl2 (20°C)	800	kg		Cl2 (20°C)	800	kg
Chlorine compression	Electricity (CHP plant)	33,33	kWh		Compressed Cl2	800	kg
	Cl2 (20°C)	800	kg				
Chlorine liquefaction	Electricity (CHP plant)	21,67	kWh		Cl2 final use	800	kg
	Compressed Cl2	800	kg				
Total Electricity rq.	Electricity (CHP plant)	275	kWh				
	Electricity (National grid)	1669,74	kWh				
	Total Electricity Demand	1944,74	kWh				
Total Heat rq.	Heat covered by CHP	1,89	GJ				
	Total Waste Heat	1,747	GJ				
	% max. waste heat reuse	0,81					
	Max recovered waste heat	1,415	GJ				
	Actual Recovered Heat	0,968	GJ				
	Total Heat Demand	2,86	GJ				

Scenario 2 (S2)

	Input	Quantity	Units		Output	Quantity	Units
Biomass boilers	Wood pellet	89,70	kg		Heat (internal use)	1,55	GJ
NaOH preparation	Total Heat	0,7	GJ		NaOH (30%)	38	ton
	Heat (Recovered Heat)	0,65	GJ				
	Heat (Biomass Boilers)	0,05	GJ				
	Dimineralized water	2,4	ton				
	NaOH (32%)	36	ton				
Brine preparation	Heat (Recovered Heat)	1,2	GJ		Saturated brine (23%)	20	ton
	Dry Salt	1,6	ton				
	Dimineralized water	510	kg				
	HCL (32%)	0,18	kg				
	Depleted brine (17%)	18	ton				
Dechlorination stage	Electricity (National grid)	0,05	kWh		Chlorine gas	5,4	kg
	Depleted brine (17%)	18	ton		Depleted brine (17%)	18	ton
	HCL (32%)	16	kg				
	NaOH (32%)	21	kg				
Membrane electrolysis	Electricity (National grid)	3055,58	kWh		NaOH (32%)	3,5	ton
	NaOH (30%)	38	ton		Cl2 (90°C)	1	ton
	Saturated brine (23%)	20	ton		H2 (90°C)	28	kg
					Waste heat	2,2	GJ
					Depleted brine (17%)	18	ton
					Recirculated NaOH (32%)	36	ton
Multiple effect evaporation	Heat (Biomass Boilers)	1,5	GJ		NaOH (50%)	2,2	ton
	NaOH (32%)	3,5	ton		Mother liquor	1,3	ton
Hydrogen cooling	H2 (90°C)	28	kg		H2 (20°C)	27	kg
					Waste heat	0,029	GJ
Hydrogen compression	Electricity (National grid)	8,89	kWh		H2 (300 bar)	2,7	kg
	H2 (20°C)	27	kg		H2 (100 bar)	24	kg
Chlorine cooling	Cl2 (90°C)	1000	kg		Cl2 (20°C)	800	kg
	Chlorine gas	5,4	kg		Waste heat	0,055	GJ
	Total	1005,4	kg				
Chlorine drying	Cl2 (20°C)	800	kg		Cl2 (20°C)	800	kg
Chlorine compression	Electricity (National grid)	33,33	kWh		Compressed Cl2	800	kg
	Cl2 (20°C)	800	kg				
Chlorine liquefaction	Electricity (National grid)	21,67	kWh		Cl2 final use	800	kg
	Compressed Cl2	800	kg				
Total Electricity rq.	Total Electricity Demand	3119,52	kWh				
	Electricity (National grid)	3119,52	kWh				
Total Heat rq.	Heat covered by biomass boilers	1,55	GJ				
	Total Waste Heat	2,28	GJ				
	% max. waste heat reuse	81%					
	Max. recovered waste heat	1,85	GJ				
	Actual recovered heat	1,85	GJ				
	Total Heat Demand	3,4	GJ				

Scenario 3 (S3)

	Input	Quantity	Units		Output	Quantity	Units
Biomass Boilers	Wood pellet	83,40	kg		Heat (internal use)	1,44	GJ
NaOH preparation	Total Heat	0,585	GJ		NaOH (30%)	32	ton
	Heat (Recovered Heat)	0,396	GJ				
	Heat (Biomass Boilers)	0,189	GJ				
	Dimineralized water	2,01	ton				
	NaOH (32%)	30,1	ton				
Brine preparation	Heat (Recovered Heat)	1,02	GJ		Saturated brine (23%)	17	ton
	Dry Salt	1,36	ton				
	Dimineralized water	434	kg				
	HCL (32%)	0,15	lg				
	Depleted brine (17%)	15,3	ton				
Dechlorination stage	Electricity (National grid)	0,04	kWh		Chlorine gas	4,6	kg
	Depleted brine (17%)	15,3	ton		Depleted brine (17%)	15,3	ton
	HCL (32%)	13,6	kg				
	NaOH (32%)	17,85	kg				
Membrane electrolysis	Electricity (National grid)	1861,13	kWh		NaOH (32%)	2,9	ton
	NaOH (30%)	32	ton		Cl2 (90°C)	1	ton
	Saturated brine (23%)	17	ton		H2 (90°C)	90	kg
					Waste heat	1,6	GJ
					Depleted brine (17%)	15,3	ton
					Recirculated NaOH (32%)	30,1	ton
Multiple effect evaporation	Heat (Biomass Boilers)	1,253	GJ		NaOH (50%)	1,84	ton
	NaOH (32%)	2,9	ton		Mother liquor	1,09	ton
Hydrogen cooling	H2 (90°C)	90	kg		H2 (20°C)	86,7	kg
					Waste heat	0,093	GJ
Hydrogen compression	Electricity (National grid)	28,57	kWh		H2 (300 bar)	8,7	kg
	H2 (20°C)	86,7	kg		H2 (100 bar)	77	kg
Chlorine cooling	Cl2 (90°C)	1000	kg		Cl2 (20°C)	800	kg
	Chlorine gas	4,6	kg		Waste heat	0,055	GJ
	Total	1004,6	kg				
Chlorine drying	Cl2 (20°C)	800	kg		Cl2 (20°C)	800	kg
Chlorine compression	Electricity (National grid)	33,33	kWh		Compressed Cl2	800	kg
	Cl2 (20°C)	800	kg				
Chlorine liquefaction	Electricity (National grid)	21,67	kWh		Cl2 final use	800	kg
	Compressed Cl2	800	kg				
Total Electricity rq.	Total Electricity Demand	1944,74	kWh				
	Electricity (National grid)	1944,74	kWh				
Total Heat rq.	Heat covered by biomass	1,442	GJ				
	Total Waste Heat	1,748	GJ				
	% max. waste heat reuse	81%					
	Actual recovered heat	1,416	GJ				
	Total Heat Demand	2,858	GJ				

Appendix B

Data used for the calculation of the internal costs relevant to the chlor-alkali are displayed in the following table. Costs associated with the production, operation and installation of chlor-alkali equipment are in line with the Best Available Techniques (BAT) Reference Document for the Production of Chlor-alkali (Brinkmann et al., 2014).

Commodity	Unit	Price (€/unit)	Reference
Natural Gas	kWh	0.036	Eurostat, (2019)
Deionized water	ton	0.69	(Evides, 2017)
Hydrochloric acid	ton	165.5	(KEMCORE, 2019)
Electricity	kWh	0.0978	(Eurostat, 2019a)
Wood Pellets	ton	235	(European Pellet Council, 2017)
Employees' salaries ^[1]	Annual income	35467	(OECD, 2018)

[1] OECD TOTAL – 2016, Assumption: number of workers 3786 workers (checked on LinkedIn) from which 60% is paid by 35467 €/year and the rest are paid by 15% more.

Appendix C

Process contribution to the overall impact in each category per ton of Cl₂ (economic allocation)

Chlor-alkali Stage	Reference Case			Scenario_1			Scenario_2			Scenario_3		
	HH	EC	GW	HH	EC	GW	HH	EC	GW	HH	EC	GW
Brine Preparation	37.23	5.90	208.20	32.46	5.16	182.20	37.23	5.90	208.20	32.46	5.16	182.20
NaOH Preparation	2.20	0.43	17.66	3.39	0.68	27.15	0.28	0.13	1.64	1.19	0.26	6.87
Dechlorination	0.80	0.16	5.50	0.90	0.14	4.30	0.80	0.16	5.50	0.90	0.14	4.30
Membr. Electrolysis	128.59	25.44	985.48	78.92	15.55	599.34	133.41	26.40	1018.50	84.11	16.52	635.82
NaOH Evaporation	7.12	1.35	50.14	7.04	1.39	58.86	7.26	3.35	38.35	7.05	3.59	43.81
Cl ₂ Compression	1.30	0.30	11.00	1.30	0.30	11.00	0.30	0.60	23.00	0.30	0.60	23.00
Cl ₂ Liquefaction	0.90	0.20	7.00	0.90	0.20	7.00	0.19	0.40	14.00	0.19	0.40	15.00
H ₂ Compression	0.30	0.06	2.50	0.30	0.06	2.50	0.70	0.13	5.00	0.70	0.13	5.00
CHP Facility	15.87	3.18	126.90	17.04	2.58	136.36	0.00	0.00	0.00	0.00	0.00	0.00
Biomass Boilers	0.00	0.00	0.00	0.00	0.00	0.00	7.23	3.47	41.15	8.63	4.15	49.22
Foreground Pr. Impact	194.31	37.02	1414.38	142.65	26.17	1030.91	187.40	40.54	1355.34	135.53	30.95	965.22
Rest	107.92	18.78	673.58	90.8	16.56	562.35	120.94	18.47	759.07	103.59	15.31	648.01
TOTAL	302.23	55.80	2087.96	233.45	42.73	1593.26	308.34	59.01	2114.41	239.12	46.26	1613.23

HH: Human Health (10⁻⁴ DALY); EC: Ecosystems (10⁻⁶ species.yr); GW: Global Warming Potential (kg CO₂ eq.)

Appendix D

Chlorine chain & company related environmental costs per weighting set

Chlorine-chain Environmental costs (€/ton Cl₂)					
<i>Model</i>	<i>Impact Category</i>	<i>Reference Case</i>	<i>Scenario_1</i>	<i>Scenario_2</i>	<i>Scenario_3</i>
ReCiPe	Human Health	2,101.92	1621.68	2143.68	1663.44
	Ecosystems	1.13E+07	8.67E+06	1.20E+07	9.40E+06
Stepwise	Human Health	2905.24	2241.46	2962.96	2299.18
	Ecosystems	2.23E+06	1.71E+06	2.36E+06	1.85E+06
LIME	Human Health	4088.47	3154.35	4169.69	3235.57
	Ecosystems	7.30E+06	5.58E+06	7.72E+06	6.05E+06
Company's Environmental costs (€/ton Cl₂)					
Ecovalue08	Global Warming	1.33	1.43	0.43	0.52
Stepwise	Global Warming	13.69	14.71	4.44	5.31
Ecotax02	Global Warming	9.96	10.70	3.23	3.86