The energy transition in the Dutch chemical industry: Worth its salt?

An analysis of decarbonization pathways in the salt and chlor-alkali industries in the Netherlands

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PBL Netherlands Environmental Assessment Agency

ECN

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by

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Preface

This research is conducted in light of graduation from the master program Engineering and Policy Analysis at the Delft University of Technology. The client, as well as the host of the research project was the Netherlands Environmental Agency (PBL). Together with the Energy Research Center of the Netherlands (ECN), this organization is developing a new knowledge network known as MIDDEN aimed at gaining practical knowledge about CO_2-reducing technologies in specific industries. This research, set up in collaboration with industry stakeholders from AkzoNobel, focusses on the salt and chlor-alkali manufacturing industries and serves as a pilot project for MIDDEN. The research was conducted between March and August in the form of a full-time internship at PBL, as part of the department Climate, Air and Energy.

The research structure can roughly be divided up into two discrete phases; the first involved the understanding of the manufacturing process and the identification of industry-specific alternate technologies that enable the reduction of CO_2 emissions, while the second phase involved an analysis to determine robust strategies for decarbonization. As such, the phases involved in this research are clearly resonated in the name of my intended master degree – Engineering and Policy Analysis. In the first phase of research, while studying the complex and elaborate chemical processes involved in the salt-chlor-alkali chain, I felt that I almost had to become a chemical engineer to properly understand what is truly happening on a process level, and how different technologies can enable the reduction of CO_2 emissions. In the second phase, I noted how from a policy perspective, the importance of specific chemical reactions that occur is obscured by the sheer vastness and complexity of possible futures, most of which are undesirable for all stakeholders involved.

Writing a thesis for university whilst actively collaborating with multiple government agencies and industry stakeholders proved to be both challenging and rewarding to me personally. Although it required a lot of energy to constantly manage and fulfill the expectations of the involved parties (TU Delft, PBL, ECN and AkzoNobel), the extra insights gained by collaborating with so many different experienced individuals were truly worthwhile. Conducting this research has fueled my ambitions to continue working in the field of the future and sustainability of energy usage, and I am grateful that this opportunity has helped me to set out a vision for what I hope to do after graduating.

This research could not have been conducted without the support of certain people around me. Firstly, I would like to thank my two university supervisors Andrea and Jan for their guidance and advice throughout this research. Their complimentary fields of expertise proved to be a perfect match for the way in which this research was set up. Furthermore, I would like to express my sincere gratitude to both of them for their support, understanding and flexibility in the final phase of my research. Secondly, I am indebted to my internship supervisor Hans Eerens, for helping me understand the complex chemical processes at play in the industries under study, and for granting me the opportunity to partake in MIDDEN as the very first intern. Lastly, I would like to thank four people in particular who helped and supported me throughout the whole research process. My parents and my sister Iza, for their encouragements and for reminding me to keep my head up at times when I was struggling; and my girlfriend Jet, for helping me keep focus without losing touch of the joys of life. Thank you all very much.

By finalizing this thesis, I realize that I am also approaching the end of my life as a student. I experience this both as extremely gratifying as well as rather challenging. Although the road ahead is full of uncertainties, I feel privileged and strengthened by the deep friendships and unique experiences I was granted throughout these truly mesmerizing years as a student.

Edzard Scherpbier
Delft, August 2018

Executive summary

Background

Globally, the climate is changing as a result of the emission of greenhouse gases caused by human activity. In 2015, the Netherlands, along with 195 countries pledged to contribute to attaining the long-term collective goal of keeping the increase in global average temperature to well below 2°C above pre-industrial levels and aim for a maximum warming of 1.5°C. In order to achieve this goal, the carbon dioxide emissions should be reduced to approximately 50% by 2030 compared to their level in 1990, followed by a full 100% reduction by 2050.

The Netherlands has pledged to reduce emissions by 49% in 2030, which translates to a national yearly emission reduction of 48.7 megatons, 30% of which must be realized by the Dutch industrial sector. The sheer size of the Dutch industrial sector, combined with the large variety of activities that take place within it, make it a particularly complex field for policymakers to analyze. There is a lack of clarity with regard to the technologies and climate policies that facilitate decarbonization in the industrial sector, as well as a lack in consideration of the effects of uncertainties on this energy transition as a whole.

Research objective

This research focusses on the Dutch salt and chlor-alkali manufacturing industries. The two closely intertwined industries are responsible for roughly 750 kilotons of yearly direct emissions, together with an estimated 1,750 kilotons of yearly indirect emissions. Together, they play a key role in the Dutch chemical chain as their products are used as raw materials across a large range of industries. The central research question is:

What are robust strategies to decarbonize the Dutch salt and chlor-alkali manufacturing industries in light of a deeply uncertain energy transition, analyzed until 2030?

In this research, the specific processes that are at play on multiple levels of aggregation in the salt-chlor-alkali production chain are studied, and emission reduction measures from an industry perspective are analyzed. Thus, this research aims to identify strategies that lower the emission levels of these industries, while characterizing their vulnerabilities and evaluating the tradeoffs among them. Recommendations on how to decarbonize the Dutch salt-chlor-alkali production chain are provided to policymakers and industry stakeholders. The obtained insights feed into a large study of the Dutch industrial sector for the research clients PBL and ECN.

Methodology

In this research, an inventory is made of the processes, products and plants involved in the salt and chlor-alkali manufacturing industries. Furthermore, an analysis is conducted of the industries and key driving forces are identified. The inventory is subsequently processed into a database, whereupon a model is conceptualized of each industry. The two models describe how the salt and chlor-alkali industries evolve over time under the driving forces. A series of computational experiments are conducted with these models to explore the way in which the identified uncertainties and decision opportunities influence the way in which the salt and chlor-alkali industries can be decarbonized.

Conceptualization of the salt-chlor-alkali production chain

The Dutch salt industry consists of four production plants in Delfzijl, Hengelo, Harlingen and Veendam, which together produce roughly 6,600 kilotons of salt yearly. The salt industry is especially intensive on its heat consumption; it requires approximately 1.6 PJ of heat energy along with 75 GWh (0.26 PJ) of electricity per megaton of salt produced. As such, the industry, the annual turnover of which is estimated at approximately 230 million euros, spends approximately 35% of its total costs on electricity and gas. The salt manufacturing process can be divided into a series of steps; steam generation, salt extraction, brine purification, brine vaporization, centrifugation and treatment. Across the industry, the steam generation process causes the direct emissions in the salt by the deployment of combined heat and power plants. Most of this steam is generated so that it can be used to vaporize the brine with multiple effect vaporizers. According to the experts consulted for this research, two technologies can enable the emission reduction of the salt manufacturing industry; the replacement of the multiple effect vaporizers by mechanic vapor recompression facilities which reduce the overall steam demand of the industry, as well as the implementation of electric boilers to replace the combined heat and power plants altogether.

The Dutch chlor-alkali industry exists of three production plants located in Delfzijl, Botlek and Bergen-op-Zoom, and together produce roughly 850 kilotons of chlorine, 950 kilotons of caustic soda, as well as 24 kilotons of hydrogen per year. In contrast to the salt industry, the chlor-alkali industry more intensive on its electricity usage; per megaton of chlorine produced, over 3,000 GWh (11 PJ) of electricity are needed in combination with 1.9 PJ of heat energy. The total annual revenue of the Dutch chlor-alkali industry is estimated at 590 million euros per year, with the industry spending almost 40% of its total costs on electricity and roughly 5% on natural gas. The chlor-alkali manufacturing process can be conceptualized in a series of steps; steam generation, caustic soda preparation, brine preparation, electrolysis, caustic soda processing, hydrogen processing and chlorine processing. Across the industry, the electrolysis process is the single largest consumer of electricity causing indirect emissions, whereas the steam generated in combined heat and power plants causes the direct emissions. Based on the empirical research and elicitation with industry experts, the technologies that can benefit the decarbonization of the chlor-alkali industry are the installation of electric and biomass boilers to make the steam generation process more sustainable, the implementation of zero-gap membrane electrolyzers and the flexibilization of the production line to reduce electricity consumption.

A model was developed of each of the industries in which the effect of the implementation of the identified alternative technologies across the two industries, along with gas taxation policies and the reduction of CO_2 intensity of the electricity supply could be investigated. Each conceptual model was run with 500 scenarios over the uncertainty space, and a full factorial design to investigate all policy combinations, resulting in a total of 48,000 and 108,000 experimental runs for the salt and chlor-alkali models respectively.

Experimental results

The computational experiments of the models span an output space that encompasses direct and indirect emissions as well as financial indicators for the selected technological investments (net present value, internal rate of return and the investment cost). Using an open exploration approach, the uncertainty space and decision space of the two models were systematically sampled to identify the way in which these together map to the output space.

A preliminary analysis of the uncertainty space shows that the financial attractiveness of technological investments is largely defined the way in which energy carrier prices develop. Furthermore, the emission levels of the industries are shown to be strongly affected by changes in the production levels, which are affected by market demands. Therefore, an increase in chlorine demand may lead to an increase in salt production upstream, which subsequently causes a further increase in emission levels.

In the output space of the computational experiments, a subspace was identified which contained all cases in which the salt and chlor-alkali industries meet their respective restrictions on direct emissions while showing a decrease in net total emissions, and where the technological investments yield positive business cases. This subspace was identified as the 'desirable' output space within the range of plausible futures according to the experimental runs.

An analysis of this desired output space showed that a significant decrease in CO_2 intensity forms a boundary condition for the decarbonization of the salt-chlor-alkali production chain. Furthermore, it showed that investments in mechanic vapor recompressors, in combination with the small-scale implementation of electric boilers can help to decarbonize the salt manufacturing industry. Lastly, the experiment results showed that investments in zero-gap membrane electrolyzers are the most robust way forward to lowering the emissions of the chlor-alkali manufacturing industry by 2030.

Despite these seemingly concrete findings, certain reservations are in order. The focus of this investigation lies in the reduction of the salt-chlor-alkali production chain's direct emissions. However, this research shows that the key to decarbonizing the salt-chlor-alkali chain lies in the electrification of heat generation processes, and in efficiency improvements of its power consumption. The indirect emissions caused by power consumption are modeled in a relatively simple and rough manner, and as a consequence, the effect of both identified measures is subject to large uncertainty in this investigation.

Implications of the results

The findings of this investigation underscore the multi-actor nature of the research problem; robust strategies for decarbonization of the salt-chlor-alkali production chain only exist when industry actors and policymakers both act and cooperate.

In the salt manufacturing industry, the key opportunity lies in the electrification of its heat processes by means of the implementation of mechanic vapor recompression technology, in combination with the adoption of electric boilers. For the chlor-alkali industry, the key opportunity before 2030 is the large-scale implementation of zero-gap membrane electrolyzers to reduce electricity consumption. Where the measures in the first industry can significantly contribute to direct emission reductions, the measures in the second can only help to reduce indirect emissions. Under these conditions, the total abated yearly emissions in the salt-chlor-alkali chain can range between 150 and 400 kilotons of carbon dioxide, but will require chain-wide investments ranging between 100 million and 150 million euros. Although the industries themselves are in control of the technologies they invest in to meet the thresholds stipulated by the ETS, a considerable part of the speed at which the salt-chlor-alkali chain can be decarbonized is affected by external factors.

This research shows that robust strategies for the decarbonization of the salt-chlor-alkali production chain cannot be formulated by the industry alone. Without the support of the government, it may be impossible to formulate positive business cases to invest in the necessary technologies. Furthermore, even if business cases are positive, they may actually result in net increases of CO_2 emissions under certain scenarios. Although the way in which the Dutch power supply can be decarbonized is not studied in this investigation, the research shows that the carbon intensity should be reduced from approximately 120 tons of CO_2 per terajoule to approximately 30 to 60 tons per terajoule between 2016 and 2030. This research thus emphasizes the importance of lowering the carbon intensity of the

Dutch power grid, but further research is necessary in order to provide policymakers with concrete advice on how they can attain this.

The development of the Dutch energy system as a whole, and most notably the electricity sector, strongly defines the way in which the electrification of heat processes in the salt industry, and the implementation of zero-gap technology in the chlor-alkali industry can benefit decarbonization efforts. Therefore, this research can be used as an explorative inventory of the challenges and opportunities faced by stakeholders involved in the planning of this energy transition.

Recommendations for future research

Future research as a result of this investigation could focus on the exploration of the decarbonization opportunities in other subsectors of the industry, as well as the investigation of industries ‘upstream’ from the salt-chlor-alkali chain such as the plastic manufacturing industry. Furthermore, a more thorough analysis of the salt-chlor-alkali chain which identifies robust strategies for fully decarbonization by 2050 may also prove valuable. Another important aspect to analyze may be the interaction effects of the policy and technology levers, to further quantify how industry stakeholders and policymakers can collaborate. In addition, the deployed exploratory modeling and analysis techniques could provide further insights if an energy transition across the entire Dutch industrial sector were analyzed, with models analogous to the ones developed for this investigation.

Table of Contents

List of Figures

List of Tables

List of Abbreviations

CAES	Compressed air energy storage
CBS	Centraal Bureau voor de Statistiek [Central Agency of Statistics of the Netherlands]
CO_2	Carbon dioxide
DP	Decarbonization pathway
DPE	Decarbonization Pathway Exploration
ECN	Energieonderzoek Centrum Nederland [Energy Research Centre of the Netherlands]
EMA	Exploratory modeling and analysis
ETS	Emissions Trading System
MEV	Multiple effect vaporization
MIDDEN	Manufacturing Industry Decarbonization Data Exchange Network
MVR	Mechanic vapor recompression
NEa	Nederlandse Emissieauthoriteit [Dutch Emissions Authority]
NEOMS	National Energy Outlook Modeling System
PBL	Planbureau voor de Leefomgeving [Netherlands Environmental Assessment Agency]
R&D	Research and development
STEEP	Social, Technological, Economic, Environmental, Policy
XLRM	Exogenous uncertainties, Policy levers, System relationships, Performance metrics

Chapter 1: Introduction

1.1 Research background

1.1.1 A call for action to halt anthropogenic environmental impact

Globally, the climate is changing as a result of the emission of greenhouse gases caused by human activity (Hof, Brink, Mendoza & Den Elzen, 2012). The signs of climate change are unmistakable and the speed at which it is taking place puts the adaptability of societies under pressure worldwide (UNEP, 2016). In 2015, at the Paris Convention, 196 countries pledged to contribute to attaining the long-term collective goal of keeping the increase in global average temperature to well below 2°C above pre-industrial levels and aim for a maximum warming of 1.5°C (Ros & Schure, 2016). This requires an integral transformation of the energy system, which can only be attained through a long-term policy perspective, anchored in present-day developments (Faber, De Goede & Wijnen, 2016).

For the Netherlands, their climate ambitions stipulated in the Paris Climate Agreement imply that amongst others, the energy system has to be radically changed (Ros & Schure, 2016). Furthermore, current national studies show that far more stringent climate policies are necessary than the ones that are currently being pursued by the Netherlands, specifically in the industrial sector (Den Ouden, Lintmeijer & Van Aken, 2017; Van Vuuren, Boot, Ros, Hof & Den Elzen, 2017). In order to keep the emissions below the 2°C goal, the Netherlands should contribute by decreasing its own carbon dioxide (CO_2) emissions by 85 to 95 percent in 2050 compared to their 1990-level (Van Vuuren et al., 2017). For the world to collectively reach the 1.5°C objective, the Netherlands would need to decrease its own CO_2 emissions by more than 100% compared to the emissions they had in 1990 (Van Vuuren et al., 2017). For both objectives, the Dutch emissions should be reduced by about 45% to 50% by 2030 (Van Vuuren et al., 2017). This change cannot occur instantaneously and requires careful, long-term oriented, policy planning. In climate policy literature, this gradual change in the energy system is referred to as an 'energy transition' (Verbong & Doorbach, 2012).

1.1.2 Conceptualizing an energy transition

In their study on technological transitions in the context of new environmental policy plans, Geels and Kemp (2000) conceptualize transitions as evolutionary reconfiguration processes. A transition process in this regard is seen as "a socio-technological development with processes on three layers; the landscape level, the regime level and the niche level" (Geels, 2002). This influential transition theory is represented in Figure 1.

On a macro-level, also referred to as the '*landscape*', a transition requires a change in social thinking and feeling, common concerns. It may even require a shift in perception of what is right and wrong (Geels & Kemp, 2000). In the context of the energy transition, this implies an increase in concerns about climate change and the state of the environment (Ros, 2015). This societal shift is for instance reflected in the positive public reception of the Paris Climate Agreement.

The meso-level, also referred to as the '*patchwork of regimes*', is conceptualized as the existing (technical) system with power relations between different entities interacting. On this level, there is a large role for companies in decision-making, but also for the consumers who drive change through their personal preferences and behavior (Geels, 2002). In the context of changing the energy usage of the Dutch industrial sector, the different stakeholders that interact are companies operating in the chemical industry, petrochemical companies, electricity providers, agencies that monitor competitiveness, consumers who wish to continue using (cheap) energy and national interest (Ros & Schure, 2016).

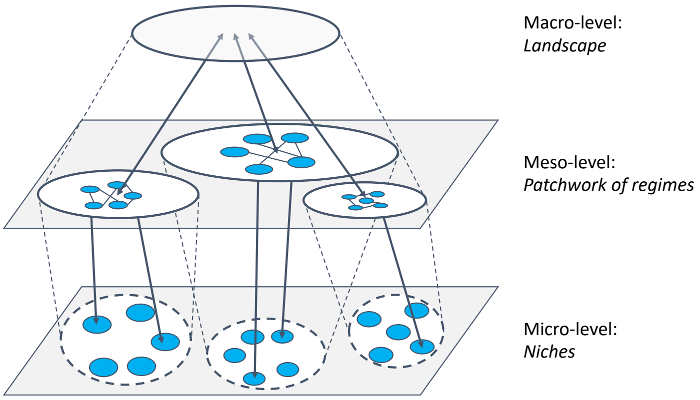


Figure 1: Multiple levels of play in transition theory

Lastly, on the micro-level, change is played out in '*niches*'. This is where new inventions and ideas are formed by the front-runners who develop innovative technologies on a small scale. From the perspective of the energy transition in industry, these niches could form at research institutes or at corporate R&D branches. Geels (2002) observes that on this level, the first applications of new technologies often come at extremely high costs. This does not only make the barriers to innovation high, but it also makes a 'spillover' from the micro-level to the meso-level unlikely.

1.1.3 The need for an energy transition in the Dutch chemical industry

Despite the goals set in the national *Energieakkoord* [Energy Agreement] (SER, 2013), and the international and even more ambitious Paris Agreement (COP21, 2015), the energy transition in the Netherlands is lagging. A 2017 study of the Central Agency of Statistics Netherlands (CBS) showed that, instead of decreasing, greenhouse gas emissions had increased by 1% in 2016 with respect to a year earlier (CBS, 2017). Moreover, these 2016 greenhouse gas emissions were only 11 percent lower than in 1990, while the court in The Hague has ruled in a climate case that emissions should be at least 25 percent lower by 2020 (Urgenda, 2015). Although net emissions from power plants have fallen between 2014 and 2016, emissions in the industrial sector had risen significantly, causing national emissions to rise (CBS, 2017).

Within the Dutch industrial sector, which comprises over 450 companies, the chemical and petrochemical industries are the main cause for these rising emission levels (NEa, 2017). The emission intensity of these subsectors is almost five times higher than that of the entire industrial sector and more than seven times higher than the emission intensity of the Dutch economy (CBS, 2017). The sheer scale of these two subsectors combined with the large variety of activities that take place within it, make it a particularly complex field for policymakers to analyze (Faber et al., 2016).

Since the start of 2018, the newly installed Dutch government has been revising its *Energieakkoord*, the revisions of which are formulated in the larger *Klimaatakkoord* [Climate Agreement]. Where the 'old' Energy Agreement lay the focus on production efficiency, the 'new' Climate Agreement will aim its attention at emission reduction strategies. Although the discussions for the Climate Agreement are well underway, an unambiguous picture of concrete reduction options per company and per subsector is still lacking (PBL, 2018).

The Dutch consultative economy, which is stooled on the principle of consensus-based decision-making, by nature adopts a multi-actor perspective to tackle policy dilemmas. Due to the complex nature of the challenge of an energy transition across the industrial sector, it is important that the policymakers involved are not only aware of their own goals, actions and dilemmas, but also of those of the other actors involved in the policy arena. Thus, from the perspective of the client of this investigation, it is important to closely investigate what decarbonization strategies industry stakeholders themselves perceive, and how the government can play a role to support these strategies.

1.1.4 The MIDDEN project

In order to be able to investigate and substantiate climate policies in the industrial sector, a close collaboration between government agencies, research institutions and private companies is crucial (Schoots et al., 2017). As such, the Energy Research Center of the Netherlands (ECN) and the Netherlands Environmental Assessment Agency (PBL) have introduced the development of a new knowledge network; the Manufacturing Industry Decarbonization Data Exchange Network (MIDDEN).

Through the MIDDEN project, energy researchers hope to gain practical knowledge about CO_2 reducing technologies through collaboration with the companies involved in the industrial sector (PBL, 2018) – or more specifically, the Dutch companies involved in the European Union Emissions Trading System (ETS). This knowledge network thus supports and facilitates decision-making in the specification of concrete CO_2 reduction steps in the Climate Agreement. Furthermore, by centralizing the data on industrial processes while sharing it with stakeholders, the ECN and PBL intend to conduct system integration studies and realize plant- and company-specific decarbonization roadmaps.

The aim of MIDDEN is to set up a comprehensive database of the industrial sector by acquiring information about processes and technological developments on the level of all Dutch production plants involved with the ETS. The total duration of MIDDEN is estimated to be covered over the span of several years, and this research serves as one of the pilot projects for the creation of the knowledge network.

1.1.5 The Dutch salt and chlor-alkali manufacturing industries

This research will be conducted as part of the MIDDEN project and will be centered around the Dutch salt and chlor-alkali manufacturing industries. The Dutch chlor-alkali industry is closely intertwined with the salt industry, as chlor-alkaline products are obtained from the electrolysis of brine (salt dissolved in water). In the Netherlands, salt production is conducted by three companies: AkzoNobel (84%), Frisia Zout (12%) and Nedmag (4%) (NLOG, 2016). Together, they produce about 6.6 million tons of salt yearly (NLOG, 2016), making the Dutch the ninth salt producer worldwide. Moreover, there are three chlor-alkali plants that together produce 847 kilotons of chlorine yearly, along with 932 kilotons of caustic soda and 24 kilotons of hydrogen (EuroChlor, 2017). These plants are located in Botlek and Delfzijl (AkzoNobel, 89% of production), and in Bergen op Zoom (Sabic, 11% of production).

Although there is clear data available on the production levels of the industries involved in the salt-chlor-alkali production chain, there is little centralized data about the industrial processes that are involved, and about the direct and indirect emission levels of specific industries. Nonetheless, salt production is commonly known as an industry with extremely high energy intensity (Worrel, Phylipsen, Einstein & Martin, 2000). The chlorine production industry is heavily reliant of electricity (EuroChlor, 2010), which in turn makes the associated carbon dioxide (CO_2) emissions directly dependent on the coal-fueled (32%) and gas-fueled (46%) Dutch electricity production sector (CBS, 2017). Furthermore, chlorine (and by extension salt) is a key raw product in an ever-expanding range of industrial applications. The Dutch industrial sector accounts for over 25% of the country's CO_2 emissions, half of which are caused by the chlorine-dependent and growing chemical industry (NEa, 2017). Thus, in the light of the MIDDEN project, there is a high need to assess these two upstream industries, identify their respective contributions to national CO_2 emissions, evaluate optimization opportunities and examine possible alternative technologies that can support decarbonization.

1.2 Research problem

1.2.1 Problem statement

Although the Dutch public and private sector are well aware of the energy intensity of a wide variety of industrial processes on a high level of aggregation, process-specific knowledge is lacking (Koelemeijer, Koutstaal, Daniëls & Boot, 2017a). Specifically, for the salt production industry, the only publicly available knowledge exchange network between industry, research institutions and government regulators is NLOG, a platform through which AkzoNobel, Nedmag and Frisia's production levels are monitored (NLOG, 2016). The chlor-alkali manufacturing industry is monitored by EuroChlor, a sector group of the European Chemical Industry Council (EuroChlor, 2017). The Dutch Emissions Authority (NEa) monitors the greenhouse gas emissions of all companies operating in the industrial sector, but these numbers are aggregated at a company level and reveal no information about industry-specific processes (NEa, 2017). In general, very little data is shared about the precise technologies deployed along the salt and chlor-alkali production lines, which prevents monitoring capabilities from a governmental perspective, slows down innovation from a research perspective and limits efficiency-boosting opportunities from the industry perspective. The Ministry of Economic Affairs released a study in 2016 which showed that the digitization of data on industry processes is extremely valuable to maintaining the competitiveness of the Netherlands while exploring cleaner technologies in industrial processes. Thus, a big challenge in planning the energy transition in the Dutch industrial sector is the collection and exchange of quantitative industry-specific data to support and substantiate decision-making around climate policy.

Secondly, even if they are well-documented and quantitatively substantiated, energy transitions are extremely complex to plan and formulate due to the world's increasing interconnectedness and interdependence (Verbong & Doorbach, 2012). The impulsiveness of certain socio-political aspects causes uncertainty to increase rapidly over the time scale (Kwakkel & Pruyt, 2015). On top of this, practical policy implementation effects such as path-dependency and lock-in risks may cause initial winning strategies to fail over the long run (Kwakkel, Haasnoot & Walker, 2016). These factors together have led to the notion of 'deep uncertainty', which is defined as a condition in which analysts and decision-makers studying a certain system cannot agree on its possible futures or model structures, the likelihood of associated future states and on the desirability of different possible outcomes (Lempert, Popper & Bankes, 2003; Agusdinata, 2008). This notion is certainly applicable to the case at hands; a few authors have made attempts at identifying robust and adaptive energy transition policies in a deeply uncertain world (Lempert & Schlesinger, 2000; Pruyt, Kwakkel, Yucel & Hamarat, 2011). Nonetheless, current research on robust energy policy is mostly from the policymaker's perspective. Due to the multi-actor nature of an energy transition in the industrial sector, it is valuable to study the transition opportunities from an industry perspective too. This multi-actor perspective allows a policymaker to gain clear insights into what measures are desirable to the industry and allows for the identification of realistic and feasible decarbonization pathways. Hence, there is a high need for innovative approaches that account for deep uncertainty to assist decisionmakers in making quantitatively informed policy decisions.

1.2.2 Research gaps

As was elucidated in section 1.2.1, process-specific knowledge on the Dutch salt and chlor-alkali production industries is not centrally maintained. The companies involved in these industries do not wish to share their production process information for fear of giving crucial information to their competitors (Ministry of Economic Affairs, 2016). This causes a strong information asymmetry and leads to a knowledge gap specifically difficult to tackle for researchers and policymakers. Thus, the first research gap identified is:

> *Research gap 1: Lack of process-specific data in the Dutch salt and chlor-alkali manufacturing industries to support decision-making about CO_2 reducing technologies*

Secondly, a lot of research seems to be focused solely on the cost-effectiveness of a transition to a cleaner, more carbon-neutral Dutch industrial sector (Schoots et al., 2017; Koelemeijer, Daniëls & Boot, 2017b). A particular worry of both the industry sector and government regulators seems to be the effect of climate regulation on production costs and by extension, on their international competitive advantage (Koelemeijer et al., 2017a). Little quantitative analysis exists on how the implementation of a specific (innovative) industry process can affect the way in which the industry changes as a whole, and specifically the attractiveness of industry process under consideration. Precisely this type of analysis allows for the identification of decarbonization pathways within the Dutch industrial sector. Furthermore, present-day models seem to overlook the effect of deep uncertainty in planning the energy transition in the industry sector in the Netherlands. Thus, the second research gap identified is:

> *Research gap 2: Lack of consideration of the effects of deep uncertainties in long-term energy transition policymaking from the perspective of the salt and chlor-alkali manufacturing industries*

1.2.3 Scientific and societal relevance

Investigating the carbon footprint of the salt and chlor-alkali manufacturing industries, whilst critically reflecting upon certain energy-intensive processes, can contribute to the Dutch efforts of decarbonizing its industrial sector. Additionally, a thorough analysis that includes the uncertainties and different perceptions of stakeholders of the system under study is necessary may provide insights as to what strategies can best be adopted and avoided in planning an energy transition in the salt and chlorine industries on a national level.

Quantitative model-based research that aims to understand the effect of decarbonizing the Dutch salt production energy on its energy transition is extremely relevant from both a scientific and a social perspective. Table 1 shows the main functions of such research from a scientific and social perspective.

Table 1: Scientific and social relevance of research

Scientific relevance:

- Strengthen the energy transition planning field with model-based decision-making methods in the challenge of decarbonizing efforts in the salt and chlorine production industries in the Netherlands
- Provide insight into the ability of model-based decision-making in long-term strategic planning

Social relevance:

- Evaluate the relevance of decarbonization pathways in the salt and chlor-alkali manufacturing industries in planning a transition away from a fossil-fuel dependent society
- Provide insights into the governance of the complex grand challenge of the energy transition in the Dutch industrial sector

1.3 Research scope

1.3.1 Research objective

The objective of this research is to study and identify key ways through which the salt and chlor-alkali manufacturing industries can be decarbonized by 2030 in support of the ambitions set out by the Dutch government. The specific processes that are at play on multiple levels of aggregation in the industries are studied, whereupon emission reduction measures are analyzed from both the perspective of the industry as well as the perspective of policymakers.

Thus, this research aims to identify strategies that lower the emission levels of the two industries, while characterizing their vulnerabilities and evaluating the tradeoffs among them. By identifying robust strategies for decarbonization, recommendations on how to decarbonize the Dutch salt-chlor-alkali chain are provided to policymakers and industry stakeholders. The obtained insights of this research feed into a large study of the Dutch industrial sector for research clients PBL and ECN.

1.3.2 Research question and strategy

The preliminary literature study, the problem statement and the identified knowledge gaps lead to the to the following main research question:

What are robust strategies to decarbonize the Dutch salt and chlor-alkali manufacturing industries in light of a deeply uncertain energy transition, analyzed until 2030?

In order to answer the main research question, the research can be divided into two distinct phases of research, with a separate research question in each. During the initial phase (Phase A), the salt and chlor-alkali industries will be studied and possible decarbonization pathways will be identified. In the second phase (Phase B), the system and identified opportunities for decarbonization will be conceptualized in a model, whereupon the space of possible futures will be explored and robust strategies can be determined that enable the decarbonization of the salt and chlor-alkali manufacturing industries. The research steps across these phases are presented in Figure 2.

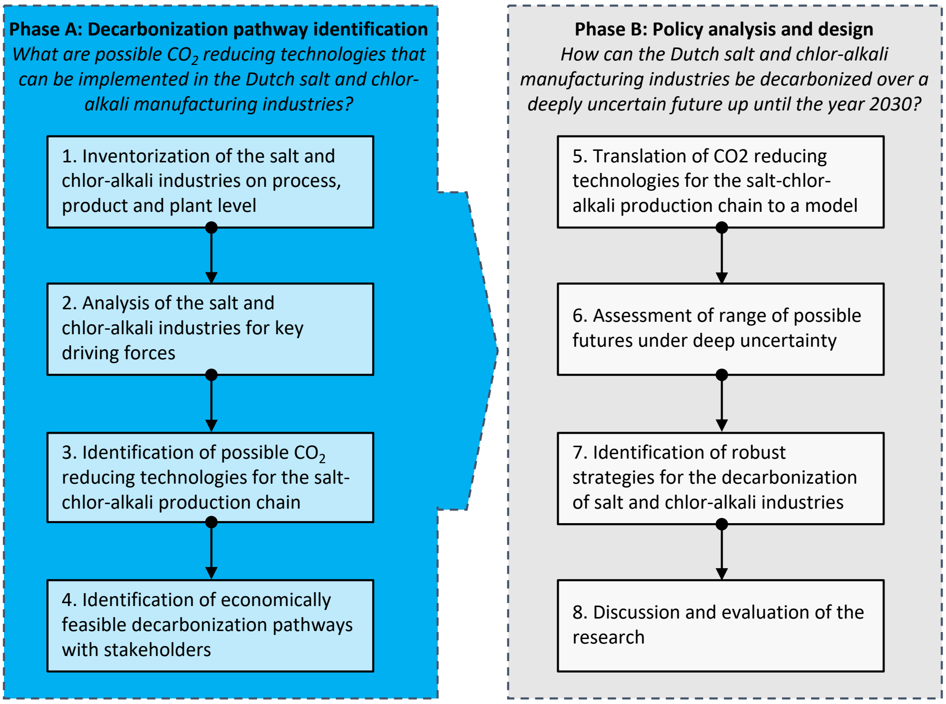


Figure 2: Research strategy

Chapter 2: Methodology

2.1 Conceptual framework

The transition theory of Geels and Kemp (2000) discussed in Section 1.1.2 form the basis for the conceptual model of this study. They argue that a transition in the socio-technical regime can be set into motion if there are enough powerful signals coming from the landscape level that there is a need for change and that enough innovative solutions have been developed successfully on the niche level. These signals on the macro-level and developments in the micro-level together can cause a change in practice, on the regime level (Ros, 2015).

Thus, in order to study an energy transition in the Dutch chemical sector, and specifically in the salt-chlor-alkali production chain, a close examination of developments on the macro-level and micro-level is necessary. Robust strategies for decarbonization can be identified by evaluating how the decisions of the stakeholders involved affect both the landscape developments, as well as the technological niches.

In this study, two scientific frameworks are identified that help to examine the signals on the macro-level on the one hand, and the developments in the micro-level on the other. As such, by combining the insights gained about the salt-chlor-alkali production chain within these two frameworks, the system under study can be conceptualized and analyzed. In Figure 3, the conceptual framework shows how this research will investigate developments on a landscape level by means of a STEEP analysis (Bartel et al., 2007), and changes on a micro-level by means of a plant-process-product analysis (Bradfield et al., 2005). These two scientific frameworks are further elucidated below.

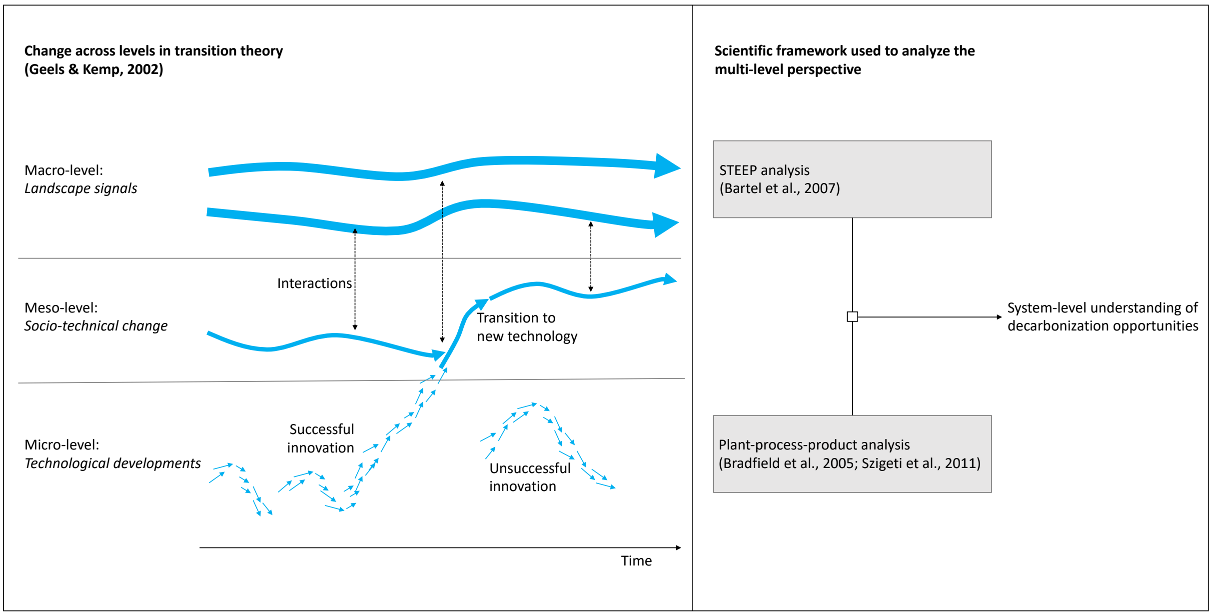


Figure 3: Conceptual framework

2.1.1 STEEP analysis

STEEP (Societal, Technological, Economic, Environmental, Political) analysis is a method used in business studies and policy literature to identify external factors that affect an industry or organization (Bradfield et al., 2005; Szigeti et al., 2011). STEEP analysis is defined by Szigeti et al. (2011) as an "audit of an organization's environmental influences with the purpose of using this information to guide strategic decision-making". This method allows to look for relevant aspects in global trends that impact how a system under consideration can be affected over time across multiple dimensions. As such, it helps to obtain a comprehensive overview of current and future opportunities and threats faced by an organization or industry (Szigeti et al., 2011).

The STEEP framework allows for the analysis of the system from multiple perspectives, and thus allows for this study to account for the multi-actor nature of the research problem. By identifying key driving forces at play on a societal, technological, economic, environmental and political level, policy and technology levers can be identified that enable change in the system under study. As such, by identifying the decision levers that affect the salt and chlor-alkali industries, the robustness of decarbonization strategies can be evaluated.

2.1.2 Plant-process-product analysis

In order to adequately conceptualize the industries under consideration, a 'plant-process-product' analysis is conducted (Bartel et al., 2007). This type of analysis is used in energy efficiency studies of the industrial sector (Wees et al. 1998, Dijkstra et al., 2009), and allows for a thorough inventory to be made of the key aspects in the industry under consideration.

On a plant level, data is collected about the companies, locations, the local energy infrastructure, the production capacities, year of construction, greenhouse gas emissions, relevant local developments, planned investments, employment, turnover and the current trade position. By compiling this data together, one can gain insight into how valuable and feasible certain investments are from the perspective of the company running the plant.

On the process level, a thorough description of the individual steps necessary to manufacture a certain product is necessary. This allows for the identification of inefficiencies across the industrial process. Furthermore, it allows for a modular breakdown of the industrial processes involved in manufacturing, which is valuable when modeling changes and investments across the industrial process. Within the considered manufacturing industries, a wide range of data will be gathered including process flow schemes, physical and energetic inputs and outputs, chemical formulas, emissions, necessary temperatures and pressure levels of individual process steps. This data can give insight into how the end-to-end manufacturing chain is set up, and how a change within an individual step of the process will affect the manufacturing chain.

On the product level, country-level data will be collected on the outputs sold by the manufacturing industry under consideration. As such, an extensive description of the products, production volume, their applications, recycling possibilities, product markets, trades and prices will be given. This gives policy analysts insight as to how valuable the different resulting products are to the industry stakeholders, and how changes in the supply and demand of the product will affect the industry.

2.2 Research framework

The research framework that is used for this study is shown in Figure 4. The figure makes a distinction between different stages throughout the study, and how different research activities contribute to the subsequent stages in the study. It also shows in a modular flow scheme how the different datasets and modeling systems deployed relate to each other, and how they together allow for the formulation of robust strategies to decarbonize the salt and chlor-alkali manufacturing industries.

The research framework is closely related to the research strategy set out in Section 1.3.3. The initial phase in Figure 2, the exploration decarbonization pathways, encompasses all steps taken during the literature study and the empirical research. The second phase of Figure 2 – the policy analysis and design – consists of the research methods deployed in the model design and data analysis.

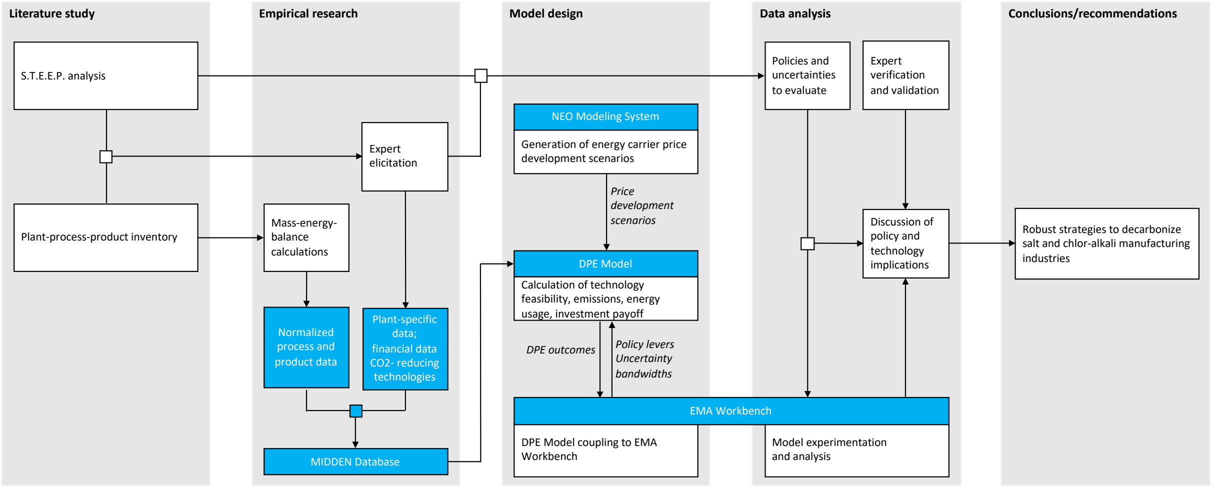


Figure 4: Research framework

The different empirical and analytical research methods deployed are further elucidated in Sections 2.3, 2.4 and 2.5. As such, the study is broken up into chapters that closely follow the research flow described in the research framework. Chapters 3 and 4 will consist of the literature study and empirical research conducted on the Dutch salt and chlor-alkali industries respectively; in Chapter 5 this study will elaborate on the modeling work; Chapters 6 and 7 comprise the analysis, verification and validation of possible decarbonization strategies; and lastly in Chapters 8, 9 and 10 this study will reflect on the research findings and identify robust strategies for the decarbonization of the salt-chlor-alkali production chain.

2.3 Empirical research

2.3.1 Mass- and energy-balance calculations

Mass- and energy-balances are an application of the law of conservation of mass and the law of conservation of energy (or often more specifically the first law of thermodynamics) to the analysis of physical systems. The technique is valuable in the study of manufacturing processes and is widely applied in chemical and industrial engineering when observing manufacturing processes. Since the laws apply across any system or subsystem within an end-to-end manufacturing process, it allows one to determine how different manufacturing processes are set up, and to gain insights into where energy is being lost or what happens to waste products across a manufacturing process. This technique is applied during the study of the salt and chlor-alkali industries across the multiple levels of aggregation that it is investigated at.

2.3.2 Expert elicitation

Throughout the course of this study, numerous experts have been consulted to gain insights into the way in which the Dutch salt and chlor-alkali industries function and what strategies are effective to reduce the CO_2 emissions of these industries. Contact with these experts was set up through the MIDDEN internship at PBL. Attention was paid to contacting a wide variety of stakeholders involved with the salt-chlor-alkali production chain – ranging from researchers from advisory bodies and universities to decision makers in the private and public sector. Below is the list of experts consulted:

- Luc Boot – Coordinating Advisor at the Dutch Council for the Environment and Infrastructure
- Marc Marsidi – Researcher at Netherlands Organisation for Applied Scientific Research (TNO)
- Marit van Hout – Researcher at Netherlands Environmental Assessment Agency (PBL)
- Niki Lintmeijer – Senior Consultant Energy & Sustainability at Berenschot
- Reinier Gerrits – Head of Unit Energy and Climate at Association of the Dutch Chemical Industry (VNCI)
- Remko Ybema – Manager External Affairs Energy at AkzoNobel Specialty Chemicals
- Rob Stikkelman – Director Center for Port of Innovation Rotterdam at TU Delft
- Sikke Klein – Technology Manager Energy at AkzoNobel Industrial Chemicals
- Ton van Dril – Senior Specialist at Energy Research Centre of the Netherlands (ECN)
- Wiek Kleijne – Business Manager R&D and Innovation at AkzoNobel Specialty Chemicals

In various meetings, e-mail exchanges and seminars, these experts were consulted to improve, verify and validate the analysis steps and findings that this study has produced. The various meetings during which these experts were consulted by the author are enumerated in the References section.

2.3.3 MIDDEN database

The data collected while inventorying and analyzing the Dutch salt and chlor-alkali industries will be placed into the MIDDEN database. The MIDDEN data template is set up in such a way that it contains information about the current production processes, alternative technological options and the conditions that need to be fulfilled to implement these options. The database per industry consists of five different datasets, as shown in Table 2. For the MIDDEN database, data is collected for individual plants. This allows one to take into account the specific characteristics of (unique) industrial processes and products. The description of the processes contains information on energy and material flows, costs, requirements, and greenhouse gas emissions. The specific location of a plant can determine possibilities for local collaboration and infrastructure connecting plants.

Table 2: Overview of datasets in MIDDEN database

Dataset	Description
Plant data	Plant-specific information, such as the plant name, address, the number of employees and its registered yearly emissions.
Technology characteristics	Information on (potential) industrial production processes. This includes data on energy and material flows and investment costs.
Current plant configuration	Information on the current production processes of companies, such as the production capacity and the capacity utilization.
Commodity data	Data on commodities that are not plant- or process-specific. The commodities include energy carriers, materials, products and waste products.

The data collected for the MIDDEN database allows for a thorough, bottom-up analysis of decarbonization strategies. Furthermore, it allows for a reasoning about decarbonization pathways from the perspective of the industry, as a thorough knowledge of the specific manufacturing industry processes.

2.4 Model design

2.4.1 Exploratory Modeling and Analysis Workbench

Exploratory modeling is a research methodology that uses mathematical or computational models to analyze complex systems, particularly policy problems involving deep uncertainty (Bankes, 1993). The fundamental idea of exploratory modeling is that the implications of multiple a priori hypotheses about a system can be explored by means of computational experiments (Agusdinata, 2008). A single computational experiment can be defined as a single run of a mathematical model using one single set of assumptions. Hence, a series of computational experiments that form a set of models can allow one to explore the plausibility of different model outcomes. Exploratory modeling allows to search across this set of models using optimization algorithms, and for the sampling over the models using the computational design of experiments and global sensitivity analysis techniques (Kwakkel & Haasnoot, 2017). Due to the complexity of the system under interest, and the deep uncertainty at play in policy planning around a transition in the Dutch energy system, this research methodology is particularly valuable in determining robust policies to decarbonize the salt and chlor-alkali industries.

This study makes use of the Exploratory Modeling and Analysis (EMA) workbench (Kwakkel, 2017), a python-coded package that allows for the deployment of exploratory modeling techniques on models developed in various environments. The EMA workbench performs computational experiments on existing models to analyze complex and uncertain systems. With this modeling method, reliable insights can be gathered on ensembles of plausible scenarios, through which robust decarbonization strategies can be identified.

The workbench makes use of three key ideas; the XLRM framework, the deployment of simulation models as if they are a function, and robustness frameworks (Kwakkel, 2017). The XLRM framework (Lempert et al., 2003) consists of four elements, as shown in Figure 5;

- Exogenous uncertainties (X) – factors outside the control of decision-makers that influence the system of interest
- Decision levers (L) – the set of possible near-term actions decision-makers can deploy to influence the system of interest
- System relationships (R) – the existing causal links between elements within the system of interest that may be directly or indirectly dependent on both X and L

- Performance metrics (M) – the standards that decision-makers use to rank and order the desirability of outcomes of the system of interest

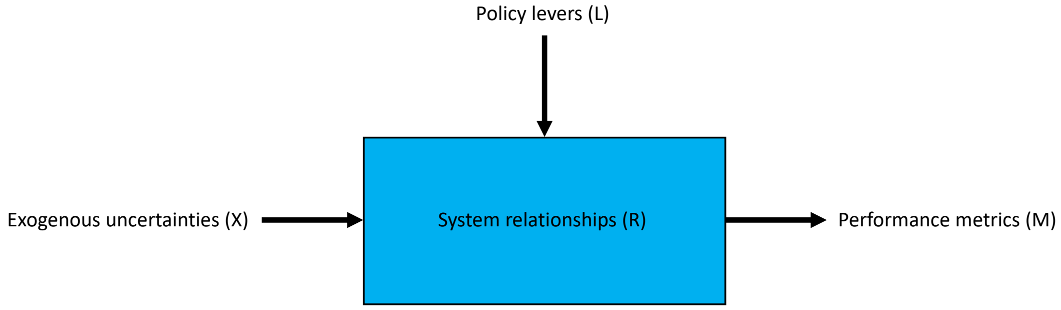


Figure 5: XLRM framework

Secondly, by running a model as if it were a function f, one can conceptualize the running of computational experiments by means of the XLRM notation as $M = f(X, L)$. The EMA workbench allows for precisely this conceptualization and can run experiments with input variables X and L to evaluate the desirability of outcomes of the modeled system M. In this study, the EMA workbench will conduct computational experiments on a model that uses the data collected for the MIDDEN database on the salt and chlor-alkali manufacturing industries. This model is further explained in Section 2.3.2.

Thirdly, the EMA workbench consists of a large range of classified robustness metrics including generation of policy options, generation of states of the world, vulnerability analysis, robustness evaluation (Kwakkel, 2017).

2.4.2 Decarbonization Pathway Exploration Model

For each manufacturing industry considered, an Excel-based model was built that incorporates the data from the MIDDEN database and allows for the assessment of the impact of developments in the Dutch energy system on technological options for decarbonization. Amongst others, the model calculates the net present value (NPV), the internal rate of return (IRR), the abated energy use and the abated direct and indirect CO_2 emissions, of pre-determined decarbonization options in the industry under consideration. This allows for the analysis of the attractiveness of different decarbonization options in the salt and chlor-alkali production industries. To distinguish between the different models used throughout this investigation, this central model will be referred to as the *Decarbonization Pathway Exploration model* (DPE model).

DPE Model

Exogenous uncertainties (X)	**Decision levers (L)**	**System relationships (R)**	**Performance metrics (M)**
NEOMS pricing scenario Price natural gas Price electricity Price biomass CO2 intensity power generation Discount rate Production variation Yearly efficiency gain Year of investment decision	Technology levers Policy levers Gas tax Reduction of CO_2-intensity of power generation	MIDDEN database structure Plant data Technology characteristics Current plant configuration Commodity data Industry-level aggregation Mass balances Energy balances Cash flow formulae NPV formulae IRR formulae	Direct emission change Indirect emission change Total emission change Internal rate of return of DP Net present value of DP Yearly production level

Figure 6: Overview of DPE model according to XLRM framework

In order to be coupled to the EMA Workbench, the DPE model has a sheet structured according to the XLRM framework. This sheet contains the exogenous uncertainties (X), policy levers (L) and performance metrics (M) relevant for experiments with the DPE model. These are discussed at depth in Chapter 5. An overview of the key model inputs, uncertainties, levers, relationships and performance metrics are shown in Figure 6.

2.4.3 National Energy Outlook Modeling System

The National Energy Outlook Modeling System (NEOMS) is the modeling system used by the ECN and PBL to make energy projections and policy evaluations (Van der Welle et al., 2017). As such, the NEOMS has been the backbone to quantitative energy policy advice to the Dutch government for over 20 years (ECN, 2016). The total modeling system encompasses 12 different modules (sub-models) that allow for detailed calculation of energy-related outcomes across 22 sub-sectors such as energy demand, supply, emissions, technology uptake, investments, costs and prices. An overview of the NEOMS is shown in Figure 7.

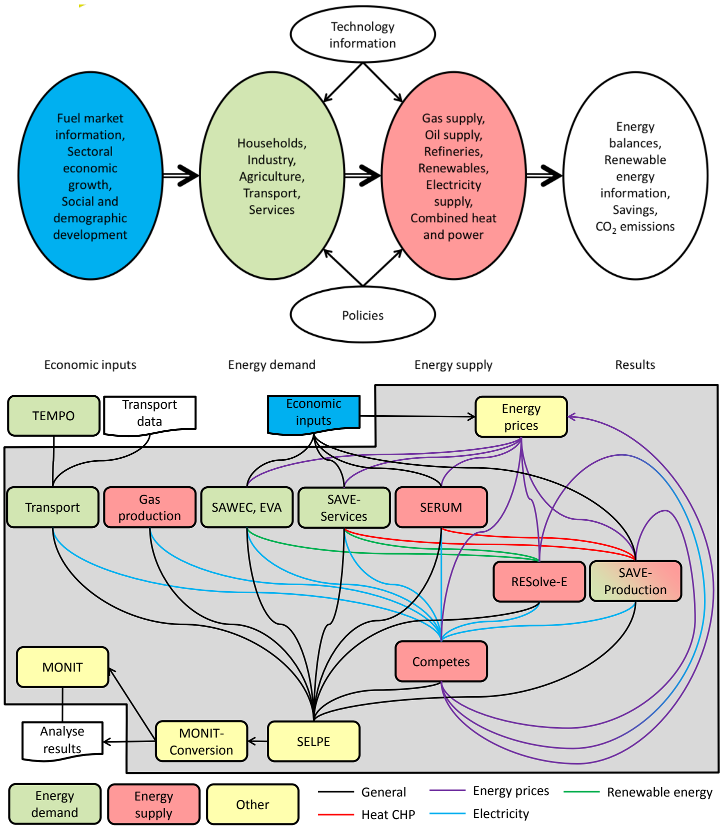


Figure 7: Data and information flows across sub-models in the NEOMS

Two sub-models in the NEOMS are of particular interest to this study:

- SAVE-production – calculates the energy demand of the industrial sector and the sectoral implementation of combined heat and power generation.
- COMPETES – calculates the centralized electricity production in the Netherlands, based on sectoral demand and on the sectoral implementation of combined heat and power plans.

These two sub-models together allow for the simulation of energy carrier prices and account for feedback effects within the Dutch energy system. The data gathered from these simulations will be used as price development scenarios which can then be used in the DPE model, in combination with the relevant data from the MIDDEN database, as shown in Figure 6.

2.5 Reflection on deployed methods

The data collection methods discussed in Sections 2.1, 2.2 and 2.3 are summarized in an overview in Table 3. For each research step identified in Section 1.3.3, the research method, corresponding data sources and associated strengths and limitations are presented. The identified limitations in each of the used methodologies are addressed with extra attention throughout the course of this study.

Table 3: Overview of research methods

Research step	Research method	Research data	Strengths/imitations
1. Inventorization of the salt and chlor-alkali industries on process, product and plant level	Literature review; desk research; energy and mass balance calculations	Reports on the Dutch industrial sector, theory on specific industry processes. *Sources:* scientific articles via Web of Science, ResearchGate and TU Delft library catalogs; publicly available reports of government advisory institutes and ministries.	A theoretical background is necessary to gain a broad view of the state of the industries and allows for an identification of the main forces at play in the field. It may prove difficult to quantify some key processes as stakeholders prefer to keep key information to themselves; certain assumptions or decisions on data aggregation will need to be made.
2. Analysis of the salt and chlor-alkali industries for key driving forces	Desk research; stakeholder analysis; S.T.E.E.P. framework (Social, Technological, Economic, Environmental and Political forces)	Documentation on Dutch energy and industrial sectors; innovation reports; *Sources:* communiques from ministries (Economic Affairs, Environment and Infrastructure), reports from VNCI (Dutch Chemical Industry Association), scientific publications on Dutch and European industrial sector	The S.T.E.E.P. framework, often used by decision-makers and policy analysts, helps to structure and identify the main mechanisms that influence and change the industry sector. Due to the multidisciplinary nature of this research, it is difficult to acquire a complete overview of the existing literature. Experiences in practice may prove different from the theories in literature.
3. Identification of possible CO_2 reducing technologies for the salt-chlor-alkali production chain	Literature review; desk research; discussions Dutch energy policy experts.	Innovation reports, qualitative and quantitative information on state of technologies, information on industry process patents; cogeneration theory. *Sources:* scientific articles; patent databases; reports from Dutch Emissions Authority (NEa); (energy) policy experts from PBL, ECN, TU Delft	It is valuable to combine knowledge from theory and practice when exploring possible options for future development. A variety of data sources can be conflicting or inconsistent. Reports and/or involved stakeholders may favor certain decarbonization opportunities over others for no rational reason.
4. Identification of economically feasible decarbonization pathways with stakeholders	Expert elicitation; inventory of functional and technical lifespan of industry processes	Findings and assessments of research steps 1, 2 and 3; input about key driving forces, uncertainties, effects of changes. *Sources:* industry experts from AkzoNobel; (energy) policy experts from PBL, ECN, TU Delft.	Expert elicitation allows for the combination of qualitative stakeholder insights and quantitative scientific information. It can also lead to new observations of both the state of the industry and possible future developments. The industry stakeholders may be biased towards cheap, short-term oriented solutions. Furthermore, most information from the interviews is qualitative and difficult to translate to a model.

Table 3 (continued): Overview of research methods

Research step	Research method	Research data	Strengths/imitations
5. Translation of CO_2 reducing technologies for the salt-chlor-alkali production chain to a model	Desk research; model development; model evaluations with energy policy experts	Findings and assessments of research steps 1 to 4; quantitative data from the literature review and from the discussions with experts. *Sources:* experts from PBL, ECN and TU Delft.	A model that incorporates data collected in steps 1 to 4 can be used to simulate possible developments of the Dutch energy system. Model review with model experts may be necessary.
6. Assessment of range of possible futures under deep uncertainty	Desk research; exploratory modeling; EMA workbench use; model evaluations with energy policy experts.	Exploratory modeling and analysis literature (authors such as Bankes, Bryant, Groves, Lempert); findings and assessments of previous research steps. *Sources:* experts from PBL, ECN and TU Delft.	Exploratory modeling theory suggests to systematically explore the consequences of uncertainties. The EMA workbench allows for the search and sampling over an ensemble of system models that are plausible. This supports reasoning on the full set of outcomes that lay ahead in the Dutch industrial sector.
7. Identification of robust strategies for the decarbonization of salt and chlor-alkali industries	Desk research; EMA workbench use; open exploration; decision support; model evaluations with energy policy experts.	Open exploration literature (authors such as Haasnoot, Herman, Kasprzyk, Jaxa-Rosen, Kwakkel, Walker, Watson); findings and assessments of previous research steps. *Sources:* experts from PBL, ECN and TU Delft.	The open exploration approach in exploratory modeling is stooled upon the systematic sampling through the decision and uncertainty space. This allows for the identification of robust strategies in planning a transition in industry.
8. Discussion and evaluation of the research	Assessment of findings of research steps 6 and 7.	Findings and assessments of previous research steps.	A critical review of the research process and deployed research methods is elementary in a scientific study.

Chapter 3:
The Dutch salt manufacturing industry

3.1 Plant–process–product inventory

3.1.1 Salt manufacturing in the Netherlands

At present, in the Netherlands, salt production is conducted by three companies: AkzoNobel, Frisia Zout and NedMag. These companies operate on four different salt production facilities and across 8 different salt extraction locations throughout the Netherlands. Together, they produce about 6.6 megatons of salt yearly. As per January 1st 2017, there were 16 extraction licenses and no exploration licenses in force for rock salt (NLOG, 2017). Furthermore, there was one request for production being processed (NLOG, 2017).

Table 4: Salt extraction and production numbers 2016

Rock salt extraction locations	Salt extracted [kton] (NLOG, 2017)	Associated plant	Salt produced [kton]
Twenthe-Rijn Twenthe-Rijn (uitbreiding) Twenthe-Rijn (Helmerzijde)	1,300 830 320	AkzoNobel Delfzijl	2,500
Adolf van Nassau II Adolf van Nassau II – uitbreiding	1,400 1,600	AkzoNobel Hengelo	3,000
Barradeel Barradeel II	450 430	Frisia Zout Harlingen	880
Veendam	270	NedMag Veendam	270
		Total	**6,600**

Note that in Table 4, only eight of the seventeen extraction licenses are shown. This is because at those extraction locations, no rock salt was mined in 2016. This is because although the operators have already been granted extraction licenses, they do not need to produce more salt in the years to come. Although AkzoNobel has been granted a rock extraction license at Isidorushoeve, the salt extraction under the Ganzenbos (Adolf van Nassau II and Adolf van Nassau II – uitbreiding) is presently achieved at such a rate that it is not necessary to open another extraction facility elsewhere.

Salt manufacturing is an energy-intensive process. For every megaton of salt produced in the Netherlands, over 1.6 PJ of heat energy is required, together with 71 GWh of electricity, producing a total of 130 kilotons of direct CO_2 emissions (see calculations in appendix A). The associated CO_2 emissions per production plant are shown in Table 5.

Although the heat generation may differ across the different salt production plants in the Netherlands, the overall salt production process is relatively similar across different plants. These different processes are discussed in the subsequent section.

Table 5: CO_2 emissions of salt production plants

Production plant	**CO_2 emissions [kton/year] (NEa, 2017)**	**Share of CO_2 emissions**	**Share of production**
AkzoNobel Hengelo	291	53%	37%
AkzoNobel Delfzijl	181	33%	46%
Frisia Zout Harlingen	2	0%	13%
NedMag Veendam	76	14%	4%
Total	**550**		

3.1.2 Salt manufacturing process

Salt in the Netherlands is produced by means of extraction from rock salt from salt caverns. This rock salt, also known as halite, is the mineral natural form of sodium chloride (NaCl). For every gram of salt, over sixty percent is chlorine (Cl^-) and almost 40 percent is sodium (Na^+). In its natural mineral form, it generally contains a range of impurities (e.g.: magnesium-, calcium- and iron ions) and occasionally other evaporate deposit minerals (e.g.: sulfates, halides and borates). The rock salt deposits have been formed hundreds of millions of years ago by the evaporation of epeiric seas, and thus lie deep underground (depths ranging between 350 and 1500 meters). For geological reasons, salt is produced in the northeast and east of the Netherlands; this is where the salt deposits of Zechstein and Trias lay. Upon extraction, the salt is processed so that it meets market demands.

The salt manufacturing process can be conceptualized as a series of sub-processes:

1. Steam generation
2. Salt extraction
3. Brine purification
4. Vaporization
5. Centrifugation
6. Treatment

These sub-processes are outlined below. More quantitative background information, calculations and derivations are presented in Appendix A.

Steam generation

Heat energy is generated in the form of steam, which for salt production is produced at a temperature of about 150 to 180 °C and a pressure of 3 to 4 bar (Holtkamp, 2011). The salt production plants in Hengelo, Delfzijl and Veendam produce their steam in on-site combined heat and power (CHP) plants (AkzoNobel, 2018; NedMag, 2016). CHP technology, also known as cogeneration, refers to the use of a heat engine to produce useful heat (in the form of steam) and electricity simultaneously. The heat engines of AkzoNobel and NedMag are both fueled with natural gas, which as it combusts create CO_2 emissions. This study's calculations reveal that 99.7% of all CO_2 emissions in the salt production industry originate from the steam generation that occurs at the different CHP installations. Nonetheless, the cogeneration plants used in the salt production industry are extremely efficient; AkzoNobel's CHP plants in Delfzijl and Hengelo have efficiencies above 85% and are about 25% more efficient than the Dutch national average (De Buck & Afman, 2011).

Interestingly, although Frisia Zout is responsible for about 13% of salt production in the Netherlands, its CO_2 share is minimal. This is due to the fact that their heat energy to produce steam originates from a waste incineration plant as opposed to a cogeneration plant. This waste incineration plant is known as the *Reststoffen Energie Centrale* (Rest material energy station), or REC. The REC has a high energy production efficiency at about 70%, where the average waste incineration plant in the Netherlands only has an efficiency of 30% (OMRIN, 2016).

Just as Frisia Zout, AkzoNobel's salt production plant in Hengelo too imports some of the steam it uses from third parties (RVO, 2013). In addition to the use of its combined heat and power facility, AkzoNobel Hengelo is supplied with steam generated at Twence, a nearby waste incinerator. Via a 2.2-kilometer-long insulated overhead line between Twence and AkzoNobel, 4 bar of superheated steam from Twence is delivered (AkzoNobel, 2018). Furthermore, AkzoNobel Hengelo also imports steam from the pyrolysis plant Empyro. This plant produces oils from wood chips. The waste heat the plant produces is used to produce steam, which is supplied to AkzoNobel's salt plant. Since 2015, Empyro has been supplying 3-8 tons of steam to AkzoNobel per hour. By using Empyro's steam, AkzoNobel was able to reduce its natural gas consumption by 3,000,000 m^3 per year and thus achieve a CO_2 reduction of 5,880 tons (AkzoNobel, 2018).

Salt extraction

In the Netherlands, salt is extracted from the ground by means of solution mining. In this process, a borehole is drilled into an underground salt layer, whereupon fresh water is forced down that whole under high pressure, 17 bar (Warren, 2016). The salt dissolves, turning the fresh water into brine and creating a cavern in the salt layer. Upon saturation, which occurs when the brine contains about 25 weight percent (wt%) of salt (Strucker, 1994; Sedivy, 2006), the brine is pumped out of the ground, and transported by pipeline to a purification installation.

The solution mining process is powered by large electric pumps, that are used to generate the high-pressure levels needed for the fresh water to be pumped down. Estimations of pumping energy needed are based on the depth of the solution-mined salt layer, as well as the length of the solution mining piping system. In Delfzijl, for example, the solution-mining facility is connected to the salt production plant with a complex network of pipelines, that are approximately 20 km in length (Klein & Ybema, interview 1, 2018). In this study, based on calculations and discussions with experts, about a quarter of all electricity used in the end-to-end process is attributed to the solution mining process.

Brine purification

The raw brine subsequently undergoes a purification process where the impurities are removed through a series of reactions. In the Netherlands, the most commonly occurring impurities in solution mined brine are sulphates, calcium salts and magnesium salts (Warren, 2016). These impurities are precipitated with chemicals and removed by a series of complex and confidential chemical processes. Based on calculations in this study, the brine purification process produces approximately 150 kilotons of waste chemicals per year across the Netherlands. These waste chemicals – which consist mostly of barium sulphate, calcium carbonate and magnesium hydroxide – are commonly stored in the empty salt caverns that are a result of the solution mining process (Klein & Ybema, interview 1, 2018).

One must note that the NedMag salt production plant does not produce sodium-based salts, but rather magnesium-based salts. Hence the brine purification process is different but is not explicitly considered within this study.

Vaporization

The purified brine, which consists of roughly a quarter of its weight as salt and three quarters fresh water is subsequently vaporized in order to isolate the salt. Different vaporization processes exist and are used in parallel at the different salt manufacturing facilities. Nonetheless, all purified brine is vaporized until it becomes a large salty slurry which contains approximately 10% water (AkzoNobel, 2018).

The principal technology used to vaporize the brine is multiple effect vaporization (MEV). This technology makes use of the fact that a solution's boiling point lowers as the surrounding pressure is lowered with large vacuum pans. By connecting multiple vacuum pans in series and generating different pressures to each other, the evaporated water from one vacuum pan can be used to heat the next. The efficiency gain from this technology is considerable; MEV facilities are at least twice as efficient as single effect vaporizers; which means that the deployment of MEV technology halves the steam energy demand (Strucker, 1994).

MEV facilities are relatively costly to invest in but require little maintenance and age slowly. More effects imply higher investment costs but are also more efficient. Across all salt production facilities, multiple effect vaporization occurs with three to five connected vacuum pans (Klein & Ybema, interview 1, 2018).

The brine evaporation process is very energy intensive; it uses 95% of the total heat energy consumption in the end-to-end salt production process.

Centrifugation

The slurry, containing approximately 90% salt, is centrifuged in large drums to remove residual water and prevent salt crystallization (Sedivy, 2006). The resulting salt contains roughly 2.5% moisture (Bakker, 2011). The large salt centrifuges used in the salt production facility in Hengelo can process 50 tons of salt per hour (AkzoNobel, 2018).

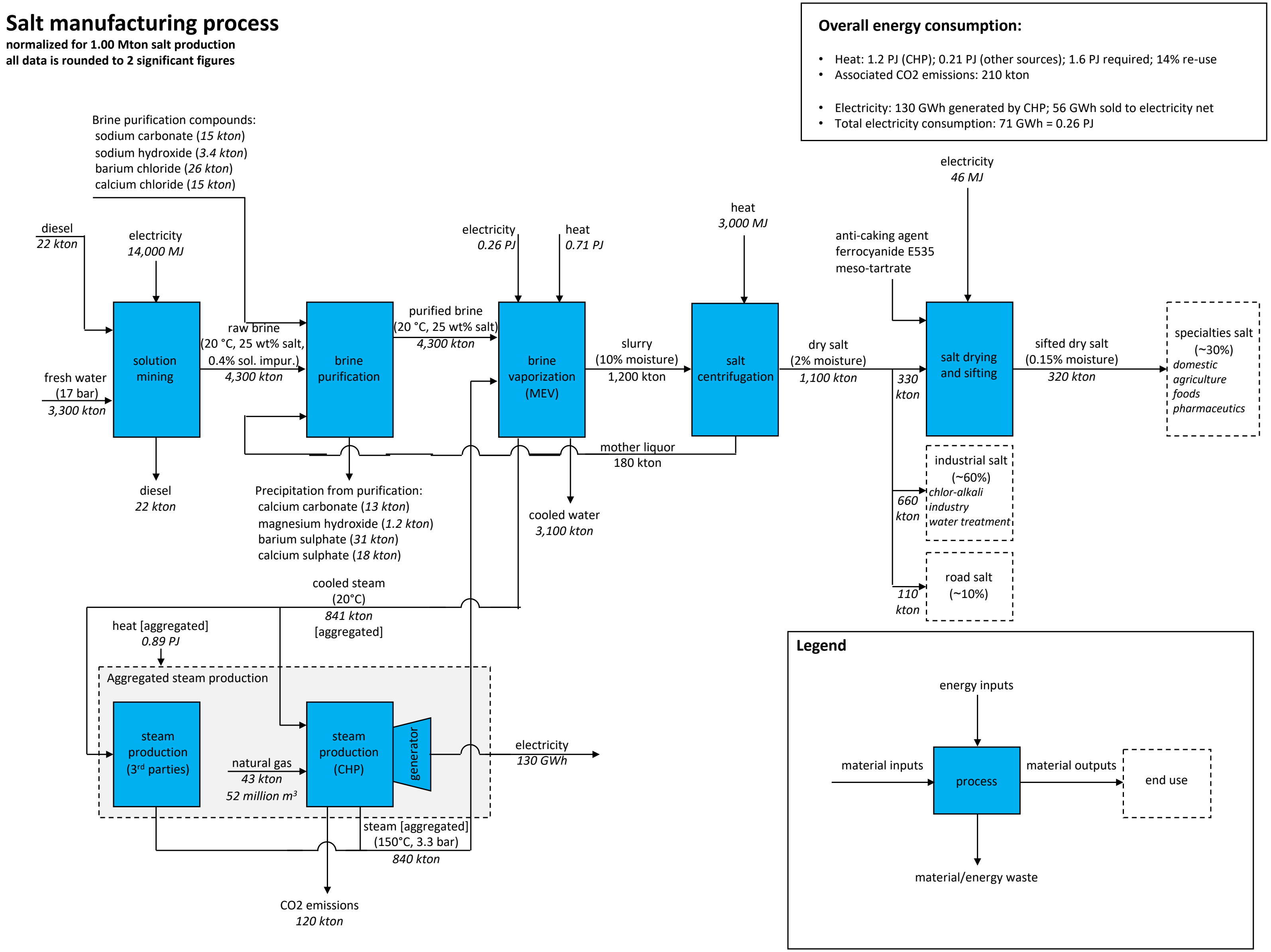
Across the Dutch salt manufacturing industry approximately 80% of all centrifuged salt is used for industrial purposes (see Section 3.1.3). The remaining 20% is treated further (Klein & Ybema, interview 2, 2018).

Treatment

The remaining salt is stripped of the residual water and worked up to dry salt with large rotary sifting machines. These machines use little electrical energy but require some heat energy to ensure the treated salt has a humidity level lower than 0.1% (Bakker, 2011).

The sifted salt is supplemented with an anti-caking agent to prevent the formation of lumps, and to ensure easy transport and packaging. Commonly used anti-caking agents in the salt manufacturing industry include ferrocyanide E535 and meso-tartrate (AkzoNobel, 2018).

An overview of this end-to-end process is shown in Figure 8. A more detailed explanation of the salt manufacturing process, including calculations, derivation and assumptions made, can be found in Appendix A.



Overall energy consumption:

- Heat: 1.2 PJ (CHP); 0.21 PJ (other sources); 1.6 PJ required; 14% re-use
- Associated CO2 emissions: 210 kton

- Electricity: 130 GWh generated by CHP; 56 GWh sold to electricity net
- Total electricity consumption: 71 GWh = 0.26 PJ

Figure 8: Salt manufacturing process

3.1.3 Salt products

Salt is used for the chlor-alkali industry, various metal industries, agriculture and animal husbandry, the food industry, road salt, the pharmaceutical industry and for consumption. The products generated by the salt manufacturing industry can loosely be categorized across four categories: industrial vacuum salt, specialties salt, off-spec salt and magnesium-based salt, as shown in Table 6.

The chemical industry is the largest salt consumer using almost four fifths of the total production in the Netherlands. This industry converts the salt mainly into chlorine and caustic soda which, in turn, are indispensable to the paper and pulp industry, the petrochemical industry, organic synthesis and glass production. 90% of the salt produced in AkzoNobel’s plant in Hengelo is used in the chlor-alkali industry – at AkzoNobel’s membrane electrolysis plant in Botlek (Klein & Ybema, interview 2, 2018).

Specialties salt is high quality, dry-sifted salt, used predominantly for human consumption. This is salt that is both directly sold to consumers, as well as salt that is used in the food industry and in water softening. The quality of this salt is closely monitored, as strict specific requirements for the different products within this product category. As a consequence, specialties salt is the most expensive type of sodium-based salt, as can be seen in Table 6.

Off-spec salt is salt that, just like specialties salt, has been dry sifted. Due to errors in the production chain this salt does not meet specified or standard requirements needed for human consumption; neither can it be re-processed to upgrade it to specialties salt (Bakker, 2011). This type of salt does however meet the environmental requirements for other applications such as road salt and is mostly used as such.

The magnesium- and calcium-based salts form a separate category in the salt manufacturing industry. These salts have a much higher market value, as they are used in very specific industrial processes such as the production of refractory bricks for coating cement and steel furnaces, sustainable bleaching technologies and the cosmetic industry.

Table 6: Salt products in the Netherlands

Product category	**Market value [€/ton] (Brinkmann et al., 2014)**	**Mass share in market**	**Product examples**
Industrial salt	57	79%	Electrolysis salt, pharmaceutical salt, food salt, feed salt
Specialties salt	60	10%	Table salt, nitrite pickling salt, water softening salt
Off-spec salt	46	7%	De-icing salt, road salt, dishwasher salt
Other salts	150	4%	Magnesium chloride, calcium chloride, magnesium oxide, magnesium hydroxide

3.2 STEEP analysis

3.2.1 Society and the salt manufacturing industry

Dutch society has a long history with the salt manufacturing industry. The first underground caverns were discovered in 1886 in Delden, Overijssel. The *Koninklijke Nederlandse Zoutindustrie* (Royal Dutch Salt Industry) was the first company to exploit these caverns shortly after (Paar, 2010). This company later became a founding member of AkzoNobel's salt branch (AkzoNobel, 2018). Throughout the twentieth century, salt became an increasingly relevant product in the chemical industry, both for the Netherlands and neighboring Germany. By 1994, three companies were involved in the Dutch salt manufacturing industry; Frima B.V. (present day Frisia Zout B.V.) near Harlingen; Biliton Delfstoffen (present day NedMag Industries) near Veendam and AkzoNobel B.V. near Hengelo and Delfzijl.

By 2018, over 750 people nationwide are directly employed in the salt manufacturing industry, and almost 3000 are indirectly involved with the industry (NedMag, 2018; AkzoNobel, 2018). Due to the salt mining concessions and the salt manufacturing facilities lying in rural low populated areas, the salt manufacturing industry has proved to be an important source of economic activity in all four industry locations. Both companies operating in the plants' respective areas, as well as research institutes and universities have become closely involved with the activities in the salt manufacturing industry. In Hengelo, for example, AkzoNobel has formed strategic partnerships with Twence and Empyro, by which its steam generation process is made more sustainable (RVO, 2013).

3.2.2 Technological opportunities in the salt manufacturing industry

As of 2018, a wide range of new technologies is under development that may provide opportunities in terms of efficiency, cost reduction or sustainability of the salt manufacturing industry. These different emerging technologies are categorized across a series of categories deployed in other technological studies of the chemical industry (VNCI, 2018; Den Ouden, Lintmeijer & Van Aken, 2017; Deloitte, 2012); sustainable heat generation, efficiency and electrification, and circularity and recycling. These different developments are discussed below.

Sustainable heat generation
Since the beginning of the 21st century, a great number of different technologies have been rising that allow for more sustainable generation of heat (Dombi, Kuti & Balogh, 2014). According to a study of the Dutch Association of the Chemical Industry, these include biomass boilers, electric boilers and geothermal heat supply (VNCI, 2018).

Biomass boilers generate steam by burning wood chips, logs, pellets, or other similar organic material. The capital cost of installing a biomass boiler is a multiple of that of a fossil fuel-fired boiler (Dombi, et al. 2014). Although the combustion of biomass also generates CO_2 emissions, biomass is considered a carbon-neutral form of energy because the amount of CO_2 released from the combustion process is later re-absorbed by new plants and trees that are planted in the biomass industry. Although this philosophy is increasingly questioned in the literature (Ros, 2015; Vuuren et al., 2017), biomass boilers are nonetheless seen as a technology through which steam generation in the chemical industry can be made more sustainable (VNCI, 2018).

An electric boiler is a device that uses electrical energy to boil water, rather than through the combustion of a fuel source. State-of-the-art industrial electrical boilers convert electrical energy to thermal energy with efficiencies up to 99% (Den Ouden, et al., 2017). Capital expenditures for electric boilers are relatively low, and upon installation, the electric boilers can easily and rapidly be deployed.

Thus, this technology offers industries flexibility, and allows them to operate at times of low electricity prices, thus reducing the factory's dependence on gas-fired boilers or a CHP (Deloitte, 2012).

Geothermal heat generation refers to the production of steam using thermal energy stored inside the Earth's crust. Although geothermal energy is not yet ready in 2018 to be implemented as a new source for steam generation, experts predict it will be available before 2040 (Deloitte, 2012). A study by the Netherlands Organisation for Applied Scientific Research showed that the in the north-east of Groningen and the north-west of Friesland geothermal energy may be used to generate low-temperature steam (temperatures up to 150°C). The salt manufacturing plants in Delfzijl and Harlingen are located precisely in these respective areas, and so this may prove to have a high potential for sustainable heat generation after 2030 (Boxem, Veldkamp, & Van Wees, 2016).

Efficiency and electrification

In the salt manufacturing industry, different technologies exist that allow for further efficiency gains. Furthermore, experts consider the electrification of certain industrial processes to play an increasingly important role in transitioning towards a more CO_2 neutral industry (Ros & Schure, 2016).

The vaporization of brine can be made more efficient by the installation of more elaborate Multiple-Effect Vaporizers (MEVs) (Westphal et al., 2012). A general rule of thumb observed is that for each extra effect added in a multiple effect vaporization system, a 10% efficiency gain is made. A trade-off is that the investment costs are higher for each extra effect. In Europe, the maximum amount of effects deployed in the salt manufacturing industry is eight (Westphal et al., 2012).

A new technology that is used to vaporize the brine is Mechanical Vapor Recompression (MVR). MVR technology is an energy recovery process in which low pressure water vapor that has evaporated from the brine is recompressed to higher temperatures and pressures and used as a heat source to vaporize more brine (Den Ouden et al., 2017). Since new steam is generated from vaporized brine, the necessary steam inputs of MVR are about 95% lower than that of MEVs. Although MVR requires substantial amounts of electrical energy for the recompression of vapor, the total electric and heat energy required for MVR technology is about half of that of a 5-effect MEV (Westphal et al., 2012).

In the Dutch salt manufacturing industry, upon removing water through vaporization and centrifugation, industrial salt is transported to chlor-alkali plants where it is re-mixed with water to be used in electrolysis (Brinkmann et al., 2014). As such, the vaporization is solely necessary due to the higher transport costs of brine. This is a consequence of strict regulations that were imposed on the chlor-alkali manufacturing industry in the early 2000s, upon which a chlorine plant in Hengelo was closed (Klein & Ybema, interview 2, 2018). If more brine were to be used directly in the chlor-alkali industry, less brine would have to be vaporized, leading to a considerable gain in efficiency in the salt manufacturing industry. This may prove especially interesting for the salt production plant in Delfzijl, which is closely linked AkzoNobel's nearby chlor-alkali production plant.

Circularity and recycling

The large underground salt caverns provide a lot of opportunities for the salt manufacturing industry. The thick permeable salt layer in which these caverns are nested are unreactive and thus offer many opportunities for temporary and permanent storage of a wide range of substances (Paar, 2010).

Up until today, Dutch salt caverns are mostly used for fossil fuel reserve storage. After the oil crisis in 1973, the Netherlands pledged to build up an oil supply large enough to sustain the country for three months, in the event of international tensions or war (Nijland, 2014). Furthermore, partly due to the liberalization of gas markets in recent years, there is an increasing interest in the storage of natural gas in salt caverns in the Netherlands (Klein & Ybema, interview 1, 2018). In 2010, ten caverns were prepared for the storage of natural gas in Hengelo (Paar, 2010).

Other resource storage opportunities are under development and gaining increasing interest. In 2017, Dutch natural gas infrastructure company Gasunie has invested in the development of a new hydrogen production and storage system in Nedmag's empty salt caverns (Tissink, 2017). It hopes this can offer an answer to the volatile supply of sustainable electricity (Nedmag, 2018). The hydrogen is produced using solar power and stored in the underground caves, along with natural gas. The gas can be pumped back up at will to be converted back into electricity with a fuel cell. As such, the hydrogen cavern thus functions as a large renewable battery. The hydrogen can also be missed with natural gas or serve as a raw material for the chemical industry (Tissink, 2017).

The hydrogen storage technology being deployed is similar to that of carbon capture and storage (CCS). CCS is the process of capturing waste carbon dioxide from point sources such as fossil fuel power plants and storing the CO_2 such that it does not enter the Earth's atmosphere. Various studies predict that CCS technology will become financially viable as a decarbonization strategy in the European chemical industry as of 2035 (VNCI, 2018; Berhout, 2015).

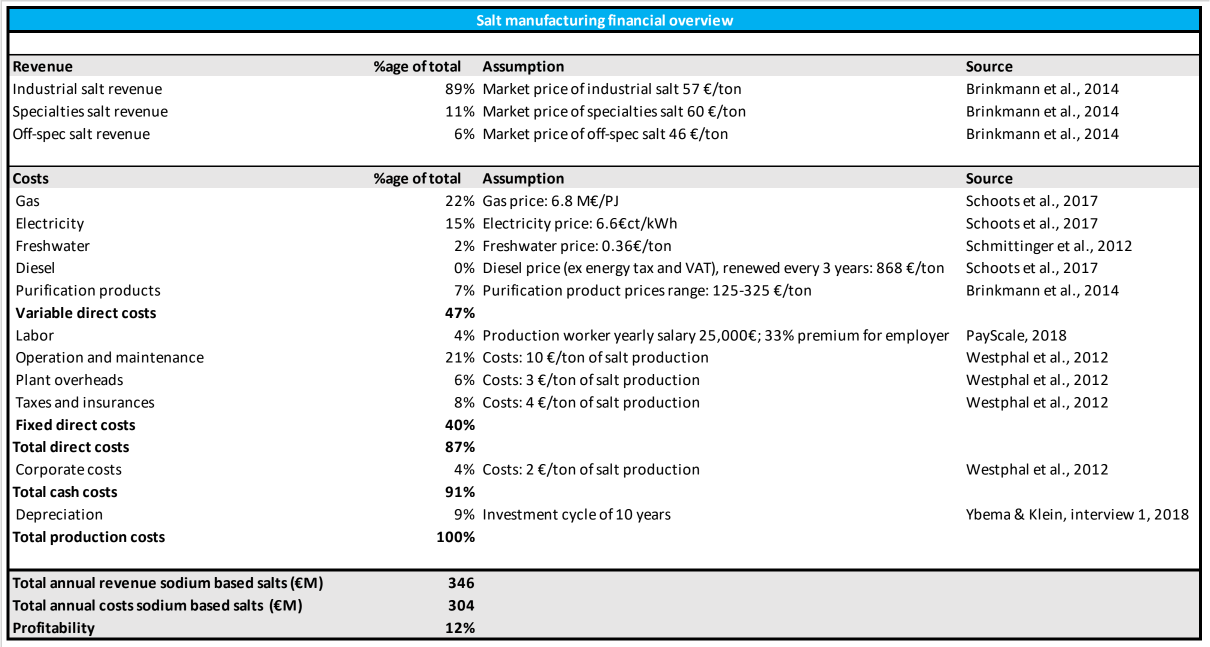
Salt caverns in neighboring Germany have also been used for Compressed Air Energy Storage (CAES) (Klein & Ybema, interview 1, 2018). CAES is a relatively new technology in which ambient air is compressed and stored under pressure in an underground cavern during periods of electricity surplus. When extra electricity is required, the pressurized air is heated and expanded in an expansion turbine through which new electrical energy is produced. Although this technology is unlikely to be ready by 2030, it may prove to become an interesting technology to invest in in the longer term (VNCI, 2018).

3.2.3 Economic analysis of the salt manufacturing industry

The total turnover of the salt manufacturing industry in the Netherlands is estimated to be around 466 million euros. The sodium-based salt manufacturing plants in Hengelo, Delfzijl and Harlingen together account for approximately 346 million euros, whereas the magnesium-based salt plant in Veendam has a turnover of roughly 120 millions euros (NedMag, 2018). Cost estimations of magnesium-based salt production are beyond the scope of this study.

Figure 9 shows that the largest source of income for the sodium-based salt industry is the manufacturing of industrial salt. Due to the fact that the Dutch industrial salt is solution-mined, purified through a patented series of steps and vacuum-evaporated, this salt is known to have extremely high purity within the European market (AkzoNobel, 2018). Moreover, the figure emphasizes the fact that the salt-manufacturing industry is extremely energy intensive; almost 40% of the total costs within the industry are attributed to gas and electricity expenses.

From this financial overview, one can see that the industry is extremely dependent on the prices of its energy sources. A small variation in gas or electricity prices will have a direct effect on the company's incurred costs. As a whole, the salt manufacturing industry is relatively low on capital costs and makes marginal profits. AkzoNobel however considers its salt manufacturing branch as an essential business unit in its Specialty Chemicals business area; the extreme high purity levels of their industrial salt is a boundary condition for their competitive advantage in the downstream chlor-alkali manufacturing industry (Klein & Ybema, interview 2, 2018).



Salt manufacturing financial overview			
Revenue	**%age of total**	**Assumption**	**Source**
Industrial salt revenue	89%	Market price of industrial salt 57 €/ton	Brinkmann et al., 2014
Specialties salt revenue	11%	Market price of specialties salt 60 €/ton	Brinkmann et al., 2014
Off-spec salt revenue	6%	Market price of off-spec salt 46 €/ton	Brinkmann et al., 2014
Costs	**%age of total**	**Assumption**	**Source**
Gas	22%	Gas price: 6.8 M€/PJ	Schoots et al., 2017
Electricity	15%	Electricity price: 6.6€ct/kWh	Schoots et al., 2017
Freshwater	2%	Freshwater price: 0.36€/ton	Schmittinger et al., 2012
Diesel	0%	Diesel price (ex energy tax and VAT), renewed every 3 years: 868 €/ton	Schoots et al., 2017
Purification products	7%	Purification product prices range: 125-325 €/ton	Brinkmann et al., 2014
Variable direct costs	**47%**		
Labor	4%	Production worker yearly salary 25,000€; 33% premium for employer	PayScale, 2018
Operation and maintenance	21%	Costs: 10 €/ton of salt production	Westphal et al., 2012
Plant overheads	6%	Costs: 3 €/ton of salt production	Westphal et al., 2012
Taxes and insurances	8%	Costs: 4 €/ton of salt production	Westphal et al., 2012
Fixed direct costs	**40%**		
Total direct costs	**87%**		
Corporate costs	4%	Costs: 2 €/ton of salt production	Westphal et al., 2012
Total cash costs	**91%**		
Depreciation	9%	Investment cycle of 10 years	Ybema & Klein, interview 1, 2018
Total production costs	**100%**		
Total annual revenue sodium based salts (€M)	**346**		
Total annual costs sodium based salts (€M)	**304**		
Profitability	**12%**		

Figure 9: Financial overview of the Dutch sodium-based salt manufacturing industry

Salt production in Hengelo and Delfzijl is part of AkzoNobel's Specialty Chemicals chemical branch. At the end of March 2018, this branch was sold to the American private equity company Carlyle, but the sale has not yet been completed (Verbraeken, 2018). The transaction will be finalized by the end of 2018. Although it is unlikely that this private equity firm is going to radically change the business management of the salt industry, this causes an increase in uncertainty surrounding the future of salt production in the Netherlands (Klein & Ybema, interview 1, 2018).

3.2.3 Environmental analysis of salt manufacturing industry

Apart from the greenhouse gas emissions attributed to the salt manufacturing industry, the industry has some other effects on the living environment that require careful consideration. These are briefly elucidated below.

Soil subsidence

Upon the salt extraction from thick underground salt layers, large underground salt caverns are formed. These salt caverns are often cylindrical in shape, over 100 meters in diameter, and have heights varying from 30 to 550 meters depending on the depth of the salt layer (Paar, 2010).

The salt caverns in Delfzijl and Harlingen, which are at depths ranging from 1,500 to 3,000 meters below the ground have extremely large volumes (over 4 million cubic meters – the size of three football stadia). These caverns have shown to be causing slight soil subsidence at the Earth’s surface. Due to the extreme pressures that occur at these depths, it has been shown that there is a direct relationship between the volume of salt extracted from the cavern and the soil subsidence on the ground level (Warren, 2016). In Delfzijl, soil subsidence levels have been recorded to range between 1 and 2 mm per year (Paar, 2010). In Harlingen, although amount of salt extracted is much lower than in Delfzijl, soil subsidence ranges between 4 and 5 cm per year. The affected area at the ground level is about 3 km in diameter.

Although soil subsidence levels are closely monitored by the *Staatstoezicht op de Mijnen* (State Supervision of the Mines, SSM) it is unclear whether this soil subsistence will remain constant, or whether it will increase or decrease. Underground solution mining activities have been associated with moderately strong earthquakes on numerous occasions worldwide – in France, the United States, China, and in Iraq (Foulger, Wilson, Gluyas, Julian & Davies, 2017). These earthquakes are postulated to have occurred after periods of high water injection rates and have caused damage to buildings and infrastructure in the surrounded areas (Foulger et al, 2017).

Furthermore, dozens of unstable salt caverns have been identified by the SSM (Paar, 2010). In 1991 a salt cavern collapsed in Hengelo, creating a hole at ground level of dozens of meters of diameter and a few meters deep (Reijm, 2016).

Brine leakages

As the solution mined brine flows to the surface, it is pumped from the mining concessions to the salt processing factories across a complex network of pipelines of up to 50 kilometers in length. Due to the corrosive nature of brine, the transport pipelines have been seen to cause major leakages throughout the years (Verbraeken, 2018).

Between 2014 and 2016, over 130 tons of salt have leaked into the environment at the salt mining concessions in Hengelo (Reijm, 2016). This caused trees to drop their leaves and profitable agricultural fields to be cleared for numerous years. Incidentally, AkzoNobel, who were responsible for the damages done have repaired and covered all damages. In May of 2018, following a brine leakage at Nedmag's concession in Veendam, there were worries about the quality of the regional drinking water, but these worries proved to be unfounded (Nauta, 2018).

Nonetheless, monitoring remains extremely difficult and the leakages are a risk taken for granted in the salt manufacturing industry. The leaks are often discovered by local residents. AkzoNobel's two mining facilities in Hengelo and Delfzijl together have had a total of 19 brine leakage incidents on the transportation pipelines between 2015 and 2017 (Verbraeken, 2018).

Blanket fluid spills

Not only the brine is known to have spilled in neighboring environments: diesel, that is used as a blanket fluid in the solution mining process, is also reported to spill into the environment. In 2016, 11,000 liters of diesel spilled into the environment following a major leak at one of the boreholes in Hengelo (Bakker, 2016). This fluid spill was reported almost 11 months after it occurred and led to severe damage of surrounding agricultural crops.

Other chemical spills

The salt caverns are used for storage of waste chemicals from the salt manufacturing industry. Furthermore, some salt caverns are known to store natural gas and nitrogen. In Germany, crude oil is stored in salt cavities at Amtsvenn, just across the border at Enschede. That oil storage began to leak heavily in 2014 and led to major environmental damage (Reijn, 2016). Although no cases of chemical spills have been reported in the Netherlands, it remains an environmental risk of the salt manufacturing industry.

3.2.4 Political analysis of salt manufacturing industry

The companies involved in the salt industry need to comply with the legal rules of the mining legislation, but also with laws and regulations in the field of working conditions and the environment. Of interest are the *Mijnbouwwet* (Mining Act), *Mijnbouwbesluit* (Mining Decree), *Mijnbouwregeling* (Mining Regulations), the *Besluit algemene regels milieu mijnbouw* (General Environmental Mining Decree), the *Wet algemene bepalingen omgevingsrecht* (Environmental Provisions Act) and the *Arbeidsomstandighedenwet* (Working Conditions Act) (AkzoNobel, 2018).

On January 8, 2018, an earthquake with a magnitude 3.4 on the Richter scale occurred at Zeerijp, in the northern province of Groningen. As a result, the Dutch SSM sounded alarm and the highest level of the ‘measurement and control protocol was reached’ – the intervention level (code red) (SSM, 2018). The Dutch State Supervision of Mines advised the Minister of Economic Affairs and Climate to reduce gas production significantly for the safety of the inhabitants of Groningen. Within three months, the Dutch government pledged to halve gas production by 2022, and completely end Dutch gas production by 2030. This has caused not only the Dutch public perception of gas to change radically, it has also made interest groups more critical of any type of mining activities in the Netherlands (Verbraeken, 2018).

This rapid political shift is likely to have a direct effect on the salt manufacturing industry. Although the long-term hazards of salt solution mining are known to have a far smaller impact than that of gas fracking (Foulger et al., 2017), it may prove difficult for the companies involved in the salt industry to acquire new licenses for salt extraction. This may impact their long-term salt production levels. Furthermore, AkzoNobel’s salt manufacturing plants are fired on Groninger gas, and stakeholders in the salt industry have stated that this political swing has caused them to consider a more rapid transition to more sustainable sources of steam generation (Klein & Ybema, interview 1, 2018).

Apart from the political developments around gas production and a change in perception of the dangers of mining activities, the SSM has also tightened its supervision of the salt production industry following a series of brine, oil and chemical leakages between 2014 and 2016 (Verbraeken, 2018). This may cause extra maintenance costs within the salt manufacturing industry, which further inhibits capital investments into new technologies that would make the industry more sustainable.

3.3 Alternative technologies to decarbonize industry

3.3.1 Electric boilers

Electric boiler technology for small-scale industrial processes has existed for numerous years, but their deployment in the chemical industry has only recently become attractive due to lower investment costs, the increased temperatures at which they can generate steam, and the low electricity prices in the Netherlands (VNCI, 2018).

In an electric boiler, electricity runs through a heating element, which heats water via a heat exchanger. The water is heated hot enough until it boils, upon which saturated steam can be transported to the necessary plant facility. Electric boilers require little equipment to be installed, and as such their investment costs are substantially lower than other sustainable steam generation technologies (Ros & Schure, 2016). Furthermore, once placed, the maintenance costs of electric boilers are relatively low, as (bio-)fuel-heated boilers need periodic refurbishment of their tubing systems (RVO, 2013).

Table 7: Technological specification of electric boilers
(Krebbekx et al., 2015; VNCI, 2018; Koelemeijer et al., 2017a)

Parameter	Value	Units
Unit of main output	1	GJ steam
Investment cost per unit main output	15,000	€
Operating and maintenance cost per unit main output	6.00	€
Refurbishment interval	10	years
Electricity requirements per unit main output	1.1	GJ
Water inputs per unit main output	0.38	ton
Capacity of single unit (on full utilization)	20	TJ/year

According to industry stakeholders (Klein, e-mail, 2018; Lintmeijer, interview, 2018), the placement of electric boilers in salt manufacturing plants will reduce the plant’s dependence on its combined heat and power plant. The low electricity prices in the Netherlands not only make investments in electric boilers interesting, they also make the deployment of on-site CHPs less attractive. Table 7 gives an overview of the main relevant parameters for the conceptualization of this technology in the MIDDEN dataset.

3.3.2 Mechanic vapor recompression

Mechanic vapor recompression (MVR) technology is a relatively novel alternative technology to multiple effect vaporization. The MVR technology can be deployed to vaporize the brine. In the MVR technology, steam cools as it heats the brine via heat exchangers, whereupon the cooled steam is re-compressed. This recompression causes an increase in pressure and in temperature. This allows it to be again to further vaporize the brine. This technology thus allows the latent heat of low-pressure steam to be maintained within the system, and leads to considerable efficiency gains (Krebbekx, Lintmeijer, Den Ouden & Graafland, 2015). Although the amount of electricity needed per tonne of vaporized brine is higher than that of multiple effect vaporization, the savings in steam demand for MVR make the technology financially attractive in countries with low electricity prices (Westphal et al., 2012).

As such, MVR is an energetically and economically attractive way to work up low pressure steam to high pressure steam so that it can be fed back into the industrial steam infrastructure. In combination with a combined heat and power (CHP), this offers possibilities for greater flexibilization (Krebbekx et al., 2015).

Table 8: Technological specification of mechanic vapor recompression (Krebbekx et al., 2015; Westphal et al., 2012)

Parameter	Value	Units
Unit of main output	1	ton 90% brine
Investment cost per unit main output	25,200	€
Operating and maintenance cost per unit main output	1260	€
Refurbishment interval	5	years
Steam requirements per unit main output	0.04	GJ
Electricity requirements per unit main output	0.67	GJ
Brine (25%) inputs per unit main output	3.6	ton
Water output per unit main output	2.6	ton
Capacity of single unit (on full utilization)	600	kton/year

The installation of mechanic vapor recompression facilities in salt manufacturing plants is seen by industry specialists as the most cost-effective investment to rapidly decarbonize the salt manufacturing industry (Klein & Ybema, interview 1, 2018). By lowering the demand for high pressure steam, the utilization of on-site CHPs will directly be lowered, which directly lowers CO_2 emissions. An important aspect to investigate is the extent to which the increased electricity demand increases the indirect emissions of the salt manufacturing industry, and whether the net change in CO_2 emissions is still negative. Table 8 gives an overview of the main relevant parameters for the conceptualization of this technology in the MIDDEN dataset.

Chapter 4:
The Dutch chlor-alkali manufacturing industry

4.1 Plant–process–product inventory

4.1.1 Chlor-alkali manufacturing in the Netherlands

Chlorine is produced by the electrolysis of salt. The laws of chemistry define that for every ton of chlorine that is produced, about 1100 kg of caustic soda is also produced, together with 28 kg of hydrogen (EuroChlor, 2018). This product combination is often referred to as one electrochemical unit (ECU). Although caustic soda and hydrogen can easily be produced in other ways, chlorine cannot. As such, the chlorine production industry is inseparable from the production industries of caustic soda and hydrogen, and thus, production plants that produce these products are together referred to as the chlor-alkali manufacturing industry.

Chlorine is obtained in the Netherlands at three locations, by means of membrane electrolysis of undried vacuum evaporated salt dissolved in water. Table 9 shows the location of the chlorine production facilities across the Netherlands, as well as their production numbers. With over 800 kilotons of chlorine produced in 2016, the Netherlands is the fourth largest chlorine producer of Europe. The chlorine production plant in Botlek is the largest membrane electrolysis facility of Europe, and second largest of all production facilities.

Table 9: Chlor-alkali production in the Netherlands

	Production in 2016 [kton] (EuroChlor, 2017)		
Site	**Chlorine**	**Caustic soda**	**Hydrogen**
AkzoNobel Botlek	640	700	18
AkzoNobel Delfzijl	120	130	4
Sabic Bergen op Zoom	90	100	2
Total	**850**	**930**	**24**

As can be seen from Table 9, the Dutch chlorine production industry is dominated by AkzoNobel; they produce almost 90% of chlorine in the Netherlands, three quarters of which is produced in the chemical industry park in Botlek. Sabic (formerly known as General Electrics) is responsible for the remaining 10% of Dutch chlorine production, which it uses in the production of plastics – predominantly polycarbonates.

Table 10: CO2 emissions of chlor-alkali production plants

Production plant	CO_2 emissions (kton/year) (NEa, 2017)	Share of CO_2 emissions	Share of production
AkzoNobel Botlek	133	72%	75%
AkzoNobel Delfzijl	27	15%	14%
Sabic Bergen op Zoom	24	13%	11%
Total	**184**		

From Table 10, one can see that the chlor-alkali industry too, just as the salt manufacturing industry, is energy intensive. For every megaton of chlorine produced in the Netherlands, almost 3.5 PJ of heat energy is required, together with 3000 GWh of electricity, producing a total of 210 kilotons of direct CO_2 emissions.

The indirect CO_2 emissions are much higher due to the extreme proportions of electricity used by the chlor-alkali manufacturing industry, and due to the proportion of Dutch electricity that is generated with the help of fossil fuels. As a comparison, the Botlek production plant uses as much electricity as all households in the city of Utrecht (Joulz, 2016). Table 11 shows the estimated electricity usage and calculated indirect CO_2 emissions of the chlor-alkali plants in the Netherlands. Thus, in considering strategies to lower the emissions of the chlor-alkali industry, serious considerations must be made about technologies that also help to reduce indirect emissions.

Table 11: Indirect CO_2 emissions of chlor-alkali plants in 2016

Production plant	**Electricity usage in 2016 [PJ]**	**Indirect CO_2 emissions in 2016 [kton/year]**
AkzoNobel Botlek	6.1	1,100
AkzoNobel Delfzijl	1.2	230
Sabic Bergen op Zoom	0.9	170
Total	**8.2**	**1,540**

Note that the indirect emissions in Table 11 are estimated using the emission intensity factor calculated for the National Energy Outlook (Schoots et al., 2017). The emission intensity factor used is roughly 0.137 tons of CO_2 per GJ of electricity produced, as can be seen in Appendix D. By using this value to estimate the indirect emissions of the different plants of the chlor-alkali industry, the individual plants are each assumed to obtain their electricity from the Dutch power grid, and not through specific power suppliers. Although such an assumption is a simplification of reality, it is commonly deployed in studies to gain insight in the indirect emissions caused by an industry (Koelemeijer et al., 2017a; Werkhoven, 2018; VNCI, 2018; Marsidi & Wetzels, 2018).

4.1.2 Chlor-alkali manufacturing process

The central aspect in the chlor-alkali manufacturing process is the electrolysis of sodium chloride (NaCl). This may be acquired using several different techniques. Worldwide, roughly three distinct production methods are in use in the chlor-alkali production industry; membrane electrolysis, mercury-based cell electrolysis and diaphragm electrolysis. In the Netherlands, all chlor-alkali production is conducted via membrane electrolysis.

This central aspect in the chlor-alkali production chain is surrounded by a series of sub-processes that allow for the right proportions of sodium chloride and caustic soda to flow into the electrolyzer at one time. As such, the chlor-alkali manufacturing process can be conceptualized as a series of sub-processes:

1. Steam generation
2. Caustic soda preparation
3. Brine preparation
4. Electrolysis
5. Caustic soda processing
6. Hydrogen processing
7. Chlorine processing

These sub-processes are outlined below. More quantitative background information, calculations and derivations are presented in Appendix B.

Steam generation

Low-temperature steam is needed in the chlor-alkali production industry for the processing of caustic soda. Similar to the steam generation process of the salt manufacturing industry, the steam that is required for this process must have a temperature of approximately 150°C and a pressure of 3 to 4 bar (Schmittinger et al., 2012). This steam is generated through on-site and off-site CHP plants. In Botlek, AkzoNobel uses an on-site CHP to generate its steam. The Sabic chlor-alkali plant in Bergen-op-Zoom also produces its steam with an on-site CHP.

In Delfzijl, on the other hand, the steam is generated at three different sources; a third of the required steam comes from Eneco's converted biomass power station Bio Golden Raand (BGR); another third is from the gas-fired CHP plant Delesto, which is fully owned by AkzoNobel; the rest of the steam is generated at the waste incineration plant EEW Energy from Waste Delfzijl. The large CHP plant Delesto is also used by multiple other industrial plants of the Delfzijl chemical cluster (AkzoNobel, 2018), and due to its size it has a higher efficiency compared to smaller on-site CHPs – almost 90% (Klein & Ybema, interview 2, 2018). As such, the direct CO_2 emissions attributed to chlor-alkali production in Delfzijl is a complex issue, as it is not directly individually monitored by the NEa, and estimates were made for this study (see Appendix B).

Caustic soda preparation

From the electrolysis process, some of the 32% caustic soda that is formed is sent back to a dilution chamber. Here, it is combined with dilution water and depleted to 30% caustic soda. This 30% caustic soda serves as one of the material inputs for the electrolysis process, during which more concentrated 32% caustic soda is produced. Waste heat originating from the electrolyzers is also used to heat the depleted caustic soda to the required 90°C (Schmittinger et al., 2012).

As such, there is a constant circular flow of depleted and replenished caustic soda between these dilution chambers and the electrolyzers.

Brine preparation

From the electrolysis process, 17% depleted brine is sent back to be processed and replenished to 23% concentrated brine. In this process, the depleted brine must be treated and dechlorinated using large pumps, hydrochloric acid and a small portion of 32% caustic soda (Brinkmann et al., 2014).

The dechlorinated depleted brine is subsequently combined with dilution water and industrial salt. This new mixture is heated again to 90°C using waste heat energy originating from the electrolyzers. This process requires a substantial amount of heat (approximately half of all waste heat produced at the electrolyzers goes to heating the newly formed concentrated brine). In Delfzijl, this step in the brine preparation process is slightly different: the dechlorinated depleted brine is combined with directly concentrated brine from the salt production industry in Delfzijl and vaporized again with an MEV facility to form 23% concentrated brine.

Lastly, the newly concentrated brine is passed through resins to remove traces of calcium, magnesium and other metals which are harmful to the membranes in the electrolyzers.

Electrolysis

Inside an electrolytic cell, two separate chambers are separated by a membrane; the first contains a positive anode and the second contains a negative cathode, as can be seen in Figure 10.

For the production process, heated 23% concentrated brine (containing sodium chloride ions) is injected into the second chamber. Chloride ions Cl^- are oxidized at the anode – they lose electrons, to form chlorine gas $Cl_{2(g)}$. Thus, the reaction that occurs at the anode is:

$$2\,Cl^- \rightarrow Cl_{2(g)} + 2\,e^-$$

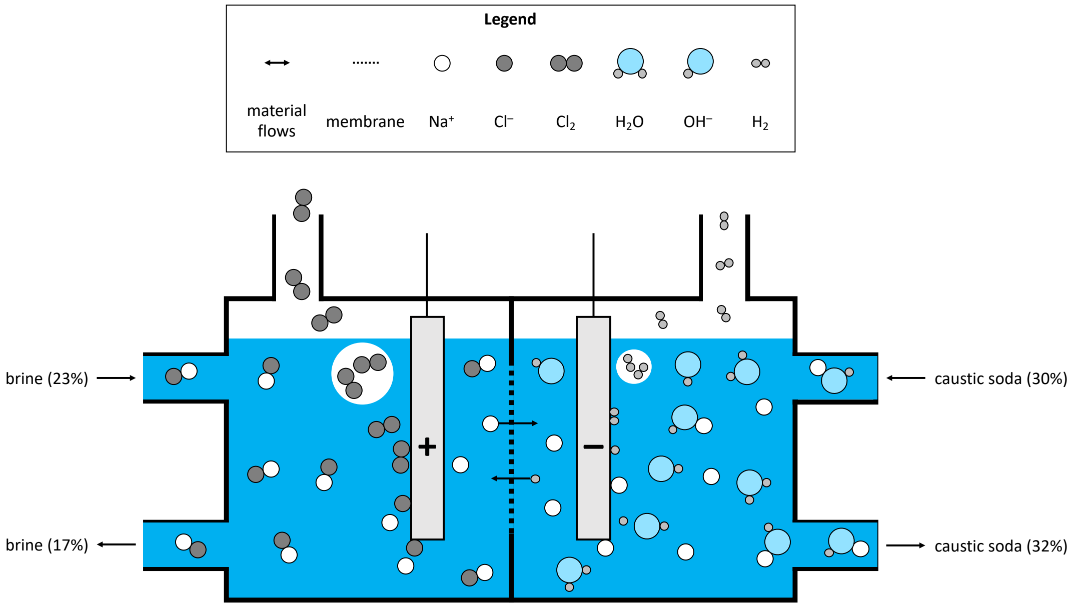


Figure 10: Overview of chemical reactions in electrolytic membrane cell

Meanwhile, at the cathode, caustic soda solution $NaOH_{(aq)}$ is fed into the second chamber. This solution is a mixture of sodium hydroxide NaOH and water H_2O. The hydrogen ions H^+ in the water are reduced at the cathode – they gain electrons, to form hydrogen gas $H_{2(g)}$, while releasing hydroxide ions OH^- into the solution. Thus, the reaction that occurs at the cathode is:

$$2\,H_2O + 2\,e^- \longrightarrow H_{2(g)} + 2\,OH^-$$

The membrane is permeable to positive ions such as H^+ and Na^+, but not to negative ions such as Cl^- and OH^-. Thus, while these redox reactions occur, Na^+ ions move from the anode to the cathode chamber where they combine with OH^- to form extra caustic soda solution. This causes the brine concentration to decrease in the first chamber and the caustic soda concentration to increase in the second. To keep the nonspontaneous redox reaction in balance, the depleted 17% brine and concentrated 32% caustic soda are drained from their respective chambers and are replaced equal amounts of 23% brine and 30% caustic soda.

The overall reaction of the membrane electrolysis process, depicted in Figure 10, can thus be described with the following equation:

$$2\,NaCl + 2\,H_2O \longrightarrow 2\,NaOH_{(aq)} + H_{2(g)} + Cl_{2(g)}$$

Due to resistance across the induced current between the anode and the cathode, useful energy is lost and a considerable amount of heat is produced. The smaller the distance between the anode and the cathode, the smaller the resistance. Since 2012, new cell designs have incorporated so called ‘zero-gap technology’, which minimize the distance between the anode and the cathode, allowing for lower energy losses (Garcia-Herrero et al., 2018, Brinkmann et al., 2014). This technology, however, has relatively high capital costs. In the Netherlands, only the Botlek chlor-alkali makes use of the zero-gap technology. About 10 out of the 30 electrolyzers in Botlek have the zero-gap technology implemented (Klein & Ybema, interview 2, 2018). All other electrolytic cells still use finite gap technology.

Caustic soda processing

About nine tenths of the 32% caustic soda that is drained from the electrolytic cells is sent back to the caustic soda preparation step. The remaining caustic soda is processed to produce high concentration 50% caustic soda to meet market demands (Brinkmann et al., 2014).

The 32% caustic soda is upgraded to 50% caustic soda through multiple effect evaporation. In terms of process steps, this technology is identical to the MEV of brine explained in Section 3.1.2. The exact conditions for caustic soda vaporization are explained in Appendix B. This process requires a considerable amount of heat energy; approximately 80% of the total steam demand for the chlor-alkali manufacturing industry is used for this vaporization (Schmittinger et al., 2012).

In Botlek and in Bergen-op-Zoom, the caustic soda is vaporized using two vacuum pans connected in series, whereas in Delfzijl, four vacuum pans are connected in series (Klein & Ybema, interview 2, 2018). As such, the MEV process in Delfzijl is about 20% more efficient than on the other two locations.

Hydrogen processing

Due to the high temperatures in the electrolyzers, the hydrogen gas captured from the electrolysis process is mixed with large amounts of steam (Brinkmann et al., 2014). The steam and hydrogen gas mixture (approximately 75% steam, 25% hydrogen gas) is cooled such that the water condenses and pure hydrogen gas is left (Schmittinger et al., 2012). Subsequently the hydrogen gas is compressed using large electric pumps and transported along pipelines to end-users within the chemical clusters where the various plants operate.

Chlorine processing

The chlorine gas captured upon electrolysis, just like the hydrogen gas, is also mixed with steam due to the high temperatures in the electrolyzers (approximately 20% steam, 80% chlorine gas) (Brinkmann et al., 2014). The chlorine is cooled to remove the largest proportion of steam. Subsequently, it is dried using highly concentrated sulphuric acid; whereupon it is compressed and liquified with large electric pumps (Schmittinger et al., 2012).

An overview of the chlor-alkali end-to-end manufacturing process is shown in Figure 11. A more detailed explanation of the chlor-alkali manufacturing process, including calculations, derivation and assumptions made, can be found in Appendix B.

Chlor-alkali manufacturing process

normalized for 1.00 Mton chlorine production
all data is rounded to 2 significant figures

Overall energy consumption:

- Heat: 1.89 PJ from CHP; 3.4 PJ in; 2.3 out; 81% re-use
- Associated CO2 emissions: 210 kton

- Electricity: 280 GWh from CHP; 2800 GWh from electricity net
- Total electricity consumption: 3,000 GWh = 11 PJ

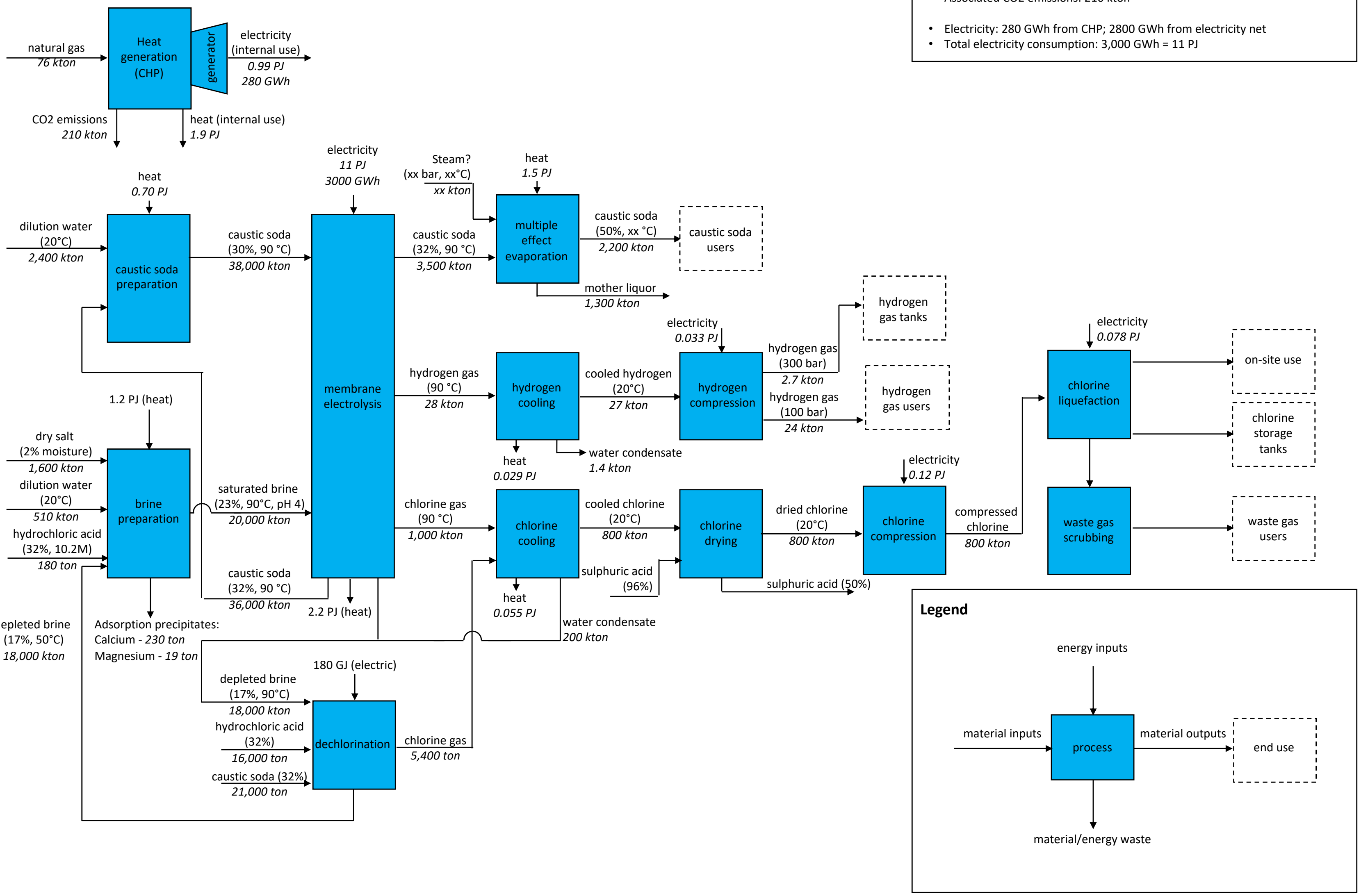


Figure 11: Chlor-alkali manufacturing process

4.1.3 Chlor-alkali products

The chlor-alkali industry has three distinct products, which each have separate applications and industries in which they are used. An estimated 55% of European chemical production depends on chlor-alkali products (EuroChlor, 2018). Table 12 shows the different main usages of the different products resulting from the chlor-alkali manufacturing industry. Below, a further explanation is given as to the application of the products across different industries.

Table 12: Chlor-alkali products in the Netherlands

Product	Market value (€/ton) (Brinkmann et al., 2014)	Mass share in market	Main usages
Chlorine	264	31%	Production of plastics (PVC, Teflon, etc.), MCA production
Caustic soda (50%)	165	68%	Organic chemical production, paper and pulp industry, food industry, metal industry, water treatment, bleach
Hydrogen	2340	1%	Petrochemical industry, fertilizer production, electronics industry, fuel source

Chlorine

Chlorine, commonly known as a disinfectant for drinking water and swimming pools, has a large amount of applications in the chemical industry. About two thirds of all chlorine in Europe is used in the production of plastics such as polyvinylchloride (PVC), poly-urethanes, epoxy-resins and neoprene (EuroChlor, 2018). In the Netherlands, this proportion lays even higher; about 80% of all chlorine produced in the Netherlands is used the plastics manufacturing industry by companies including Shin-Etsu, Hexion, Huntsman, Lyondell, Covestro, Teijin and Lubrizol (Stikkelman, interview, 2018). Sabic's chlor-alkali production facility is fully vested in the production of plastics. These plastics are derived from different chlorine products – chloromethanes (CM) and ethylene dichloride (EDC) – which are manufactured on-site within the chlor-alkali manufacturing plants of AkzoNobel and Sabic. Nonetheless, the production costs of CM and EDC are minor and are therefore not included within the scope of this investigation.

The remaining chlorine is used in the production of monochloroacetic acid (MCA), which in turn is used for pesticide production, the production of medical drugs and dyes. As such, approximately 85% of all produced medicines make use the chlor-alkali production industry, as well as 25% of all medical equipment (EuroChlor, 2018). Furthermore, half of the chemicals used to protect crops and to sustain food production and quality are based on the chlor-alkali industry.

A negligible proportion of chlorine produced in the Netherlands is used for other disinfecting purposes such as water treatment (AkzoNobel, 2018). Nonetheless, even within this application, chlorine has a high impact; 90% of all European drinking water is made safe with the help of chlorine (EuroChlor, 2018).

Caustic soda

Just as chlorine, caustic soda is widely used across a wide range of different industrial processes. Almost a third of caustic soda produced is used as reactant in the production of organic chemicals. Approximately 15% of produced caustic soda is used by the paper and pulp industry.

Caustic is essential too in the food industry (approximately 6% of total production), in water treatment (5%), in the process of refining aluminium from bauxite (4%), in detergent and soap manufacturing (4%), as a bleach mainly in the textile sector (3%), in the production of mineral oils (2%) and in the synthesis of rayon, a synthetic fibre (2%). The remaining production of caustic is attributed to many more applications, such as rubber recycling, acid neutralization and the pharmaceutical industry.

4.2 STEEP analysis

4.2.1 Society and the chlor-alkali manufacturing industry

The chlor-alkali production industry has played an important role in Dutch society since the end of the Second World War and the growth of the Dutch chemical industry. AkzoNobel had mercury electrolysis plants for chlor-alkali production in Hengelo and Delfzijl since the 1930s and opened its third mercury electrolysis plant in Botlek in 1961 (AkzoNobel, 2018). In the late 1980s, General Electrics (present-day Sabic) opened a membrane electrolysis plant in Bergen-op-Zoom. The Dutch chemical industry's heart lay by the port of Rotterdam, whereas the raw material needed to produce chlorine, salt, could predominantly be found in underground salt layers in the east (Hengelo) and northeast (Delfzijl) of the Netherlands. As such, chlorine was transported by train throughout the Netherlands. The demand for chlorine was so great that the Dutch chlorine industry also exported their product to Germany and Sweden by train. By the 1970s, AkzoNobel, the Netherlands' largest chlorine producer, transported over 300,000 tonnes of chlorine per year (Beukers & Van den Tweel, 2006).

In the 1990s, following increasing concerns from environmental organizations and regulation measures on chlorine transport in neighboring countries, Dutch public opinion on chlorine transport changed (Beukers & Van den Tweel, 2006). Furthermore, the polluting effects of mercury and diaphragm electrolysis methods were becoming increasingly apparent. Dutch Emission Guidelines introduced in the late 1990s stipulated all chlorine production processes must be switched to mercury free processes by 2010, while new mercury electrolysis processes could no longer be started. As regulation of chlorine production and chlorine transport tightened, multiple chlorine production facilities were closed down; Solvay Chemie (in Herten) closed in 1999, and AkzoNobel's mercury electrolysis facilities were closed in Hengelo and Delfzijl by 2002. By 2006, AkzoNobel halted its chlorine production in Hengelo completely, leaving three chlorine production facilities in the Netherlands (Botlek, Delfzijl and Bergen op Zoom). By 2018, chlorine transport occurs incidentally between Botlek and AkzoNobel's chlorine plant in Germany, despite strong public opposition.

Nationwide, the chlor-alkali manufacturing industry employs approximately 1,000 people in 2018 (Klein & Ybema, interview, 2018; Sabic, 2018). Indirect employment is estimated on 3,000 people (AkzoNobel, 2018; Sabic, 2018).

4.2.2 Technological opportunities in the salt manufacturing industry

As of 2018, a series of innovative technologies is under development that may provide opportunities in terms of efficiency, cost reduction or sustainability of the chlor-alkali manufacturing industry. These different emerging technologies are categorized across a series of categories deployed in other technological studies of the chemical industry, as in Section 3.2.2. These different developments are discussed below.

Sustainable heat generation
Steam generation is, just as with the salt manufacturing industry, the core source of CO_2 emissions. As such, the different technologies discussed in Section 3.2.2 are equally applicable here.

Another relevant note on geothermal heat generation is that a study of the Netherlands Organisation for Applied Scientific Research showed that there is a potential for geothermal steam generation in the east of the province of Zeeland, precisely where Sabic's chlor-alkali production plant is located

(Boxem, Veldkamp, & Van Wees, 2016). This may prove to be an interesting technology to invest in after 2030, when the experts deem that the technology will be ready for implementation (VNCI, 2018).

Efficiency and electrification

Just as with the MEV technology for brine, the efficiency of MEV vaporization of caustic soda increases by about 10% for each extra effect that the vaporization process passes through. Investment costs for MEV facilities for caustic soda are considerably higher; because of its irritant and corrosive nature extra safety regulations are in place for the multiple effect vaporizers. Furthermore, caustic soda has a higher boiling point, so energy costs for both steam generation as well as for the vacuum pumps are considerably higher than those of brine vaporization (Brinkmann et al., 2014). It is not cost-effective to have more than five vacuum pans for the vaporization of caustic soda (Schmittinger et al., 2012). The vaporization process may, in the long run, also be made more efficient by deploying Mechanic Vapor Recompression. Due to the higher steam temperature requirements, the MVR technology is estimated to be ready for implementation in caustic soda vaporization after 2030 (Klein & Ybema, interview 2, 2018), and thus falls beyond the scope of this investigation.

Membrane cell designs are refined and optimized continually in the competitive chlor-alkali industry (O'Brien, Bommaraju & Hine, 2007). In 2005, the so called 'zero-gap technology' was developed. With this technology, the distance between the anode and cathode is minimized as they are placed very closely to the membrane wall. This technology has become widely adopted since 2010 (Klein & Ybema, interview 2, 2018), but due to the high investment costs, chlor-alkali plants that had switched to membrane electrolysis before 2005 are struggling to catch up. The zero-gap technology is said to be deployed partially AkzoNobel's chlor-alkali plant in Botlek since 2017, thus realizing significant energy savings (AkzoNobel, 2017); the energy usage of their chemical processes was said to have been reduced by 10%.

Although chlor-alkali plants are preferably operated at maximum capacity because of their high capital intensity, it is theoretically relatively easy to vary the production of chlorine (Stikkelman, interview, 2018). This can be done by lowering or increasing the amount of current that is passed through the electrolysis cells. This then automatically leads to less or more electricity consumption. By increasing the production flexibility of an electrolysis plant, production can be increased when electricity prices are low, and decreased when prices are high. This is known as 'peak-shaving'. To increase the flexibility of an electrolysis plant, the overall production capacity and storage capacity of raw products must be increased, which requires high capital investments. In countries with low electricity prices, marginal costs of the implementation of peak-shaving technology are therefore much higher than in countries with high electricity prices (Krebbekx, Lintmeijer, Den Ouden & Graafland, 2015).

Circularity and recycling

The hydrogen that is generated from the chlor-alkali process is sold within the chemical clusters where it is produced. Hydrogen, when coupled to clean energy production, is seen by experts as a necessary energy carrier to facilitate the energy transition (Koelemeijer et al., 2017a). AkzoNobel aims to build new hydrogen gas facilities to further increase the production of gas. In the long-run, the chemical industry sees a positive business case for the deployment of hydrogen gas in the transport sector, while using it to balance the electricity grid and heating buildings. Large but relatively simple adaptations of the existing gas infrastructure are a boundary condition and are estimated to become reality as of 2030. The hydrogen that is currently produced in the chlor-alkali industry can help the testing of pilot projects for this long-term structural change.

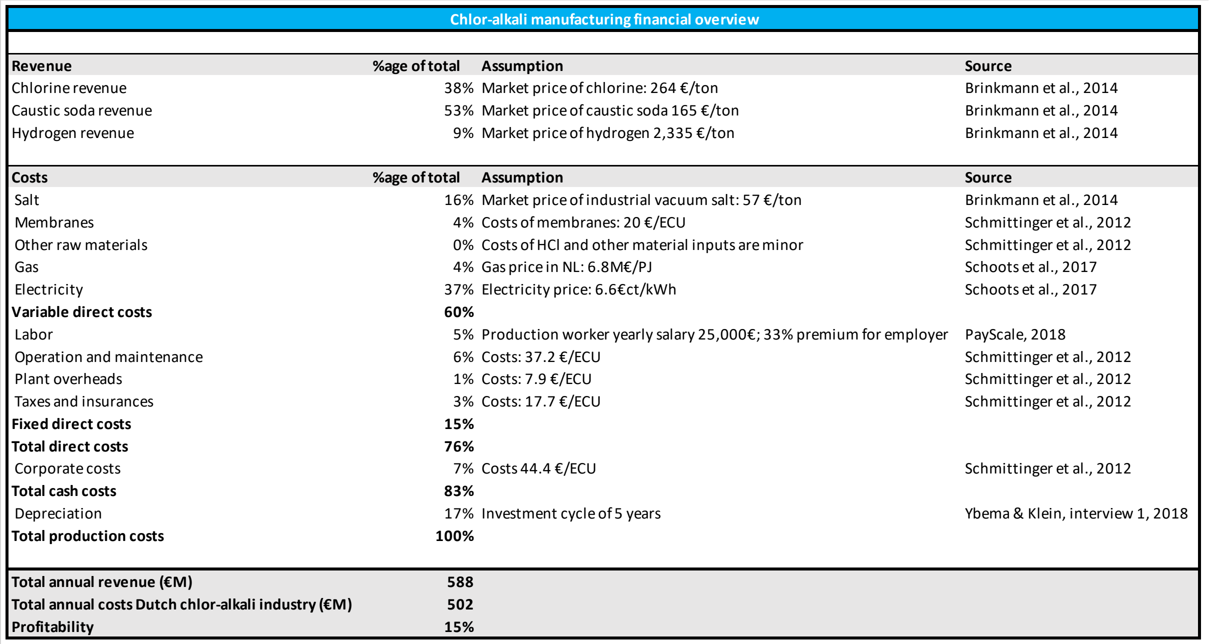
Sustainability across the product chain

Chlorine is used as a building block for the production of plastics worldwide. While plastics' intended useful life is typically less than a year, the material lives on for centuries – thus having a detrimental impact on the environment. New technologies are increasingly investigating alternatives to plastics across its wide range of uses. There is a rapidly growing 'green building' movement that has developed a large number of successful alternatives to PVC production. As these technologies develop further and their production costs decline, this may have an effect on the chlor-alkali industry. PVC production may also be regulated more strongly, which will push the development of alternate technologies even further. Nonetheless, experts involved in the chemical industry believe that the demand for chlorine is likely to keep steadily increasing until the year 2050 (Kleijne, email, 2018).

4.2.3 Economic analysis of the chlor-alkali manufacturing industry

The Dutch chlor-alkali industry makes an annual revenue of approximately 588 million euros per year, roughly 450 of which are obtained at AkzoNobel's chlor-alkali plant in Botlek. Although much of the public, political and media attention is centered around the production of chlorine, it is interesting to note that the national revenue for caustic soda is about 40% more than that of chlorine. The underlying reason is the fixed ratios between chlorine, caustic soda and hydrogen in the chlor-alkali industry.

On the costs side, it is interesting to observe that the chlor-alkali industry, just like the salt industry, is energy- and resource dependent. Roughly 41% of total production costs are spent on electricity and gas. When depreciation is not taken into consideration, the chlor-alkali manufacturing industry spends almost half of its total cash costs on electricity (Brinkmann et al., 2014). This shows the extent of dependence of Sabic and AkzoNobel on the electricity prices which are determined predominantly on the European market.



Chlor-alkali manufacturing financial overview

Revenue	**%age of total**	**Assumption**	**Source**
Chlorine revenue	38%	Market price of chlorine: 264 €/ton	Brinkmann et al., 2014
Caustic soda revenue	53%	Market price of caustic soda 165 €/ton	Brinkmann et al., 2014
Hydrogen revenue	9%	Market price of hydrogen 2,335 €/ton	Brinkmann et al., 2014

Costs	**%age of total**	**Assumption**	**Source**
Salt	16%	Market price of industrial vacuum salt: 57 €/ton	Brinkmann et al., 2014
Membranes	4%	Costs of membranes: 20 €/ECU	Schmittinger et al., 2012
Other raw materials	0%	Costs of HCl and other material inputs are minor	Schmittinger et al., 2012
Gas	4%	Gas price in NL: 6.8M€/PJ	Schoots et al., 2017
Electricity	37%	Electricity price: 6.6€ct/kWh	Schoots et al., 2017
Variable direct costs	**60%**		
Labor	5%	Production worker yearly salary 25,000€; 33% premium for employer	PayScale, 2018
Operation and maintenance	6%	Costs: 37.2 €/ECU	Schmittinger et al., 2012
Plant overheads	1%	Costs: 7.9 €/ECU	Schmittinger et al., 2012
Taxes and insurances	3%	Costs: 17.7 €/ECU	Schmittinger et al., 2012
Fixed direct costs	**15%**		
Total direct costs	**76%**		
Corporate costs	7%	Costs 44.4 €/ECU	Schmittinger et al., 2012
Total cash costs	**83%**		
Depreciation	17%	Investment cycle of 5 years	Ybema & Klein, interview 1, 2018
Total production costs	**100%**		

Total annual revenue (€M)	**588**
Total annual costs Dutch chlor-alkali industry (€M)	**502**
Profitability	**15%**

Figure 12: Financial overview of the Dutch chlor-alkali manufacturing industry

Another important cost aspect in the chlor-alkali industry is the trade-off between expenditures on high quality industrial salt and the refurbishment of membranes. The membranes used in electrolysis are very expensive and there is a high business interest to keep them in the best possible quality (Klein & Ybema, interview 1, 2018). The higher the purity of the salt, the longer the membranes can be used, and the lower the expenditures on the membranes. Higher purity salt, however has higher costs too (Schmittinger, 2012). In the European salt market, AkzoNobel's industrial salt is of extreme high quality, which gives it a competitive advantage over other chlor-alkali manufacturers (Stikkelman, interview, 2018). In terms of cost-efficiency, AkzoNobel believes its salt manufacturing plants are in the top 5%, whereas its chlor-alkali manufacturing plants are in the top 15% (Klein & Ybema, interview 2, 2018).

Due to the high overall costs in the chlor-alkali manufacturing industry – total expenses are estimated at 502 million euros per year – the profitability of the industry is relatively low. As a consequence, capital investments are difficult to make and innovation within the industry is hampered by uncertainty around gas and electricity prices (Klein & Ybema, interview 2, 2018).

Just as the salt branch of AkzoNobel Specialty Chemicals, the chlor-alkali branch was sold to the American private equity company Carlyle in March 2018. New investments in its chlor-alkali plant in Botlek are planned for 2021 to upscale production levels (Verbraeken, 2018b). This investment in the largest chlor-alkali plant in the Netherlands will further lower costs of production and raise the annual revenue of the industry.

4.2.4 Environmental analysis of chlor-alkali manufacturing industry

Apart from the CO_2 emissions attributed to the chlor-alkali manufacturing industry, the industry has some other effects on the living environment that require careful consideration. These are briefly elucidated below.

Chlorine spills

Chlorine is a hazardous chemical, and human exposure to high concentrations of chlorine can cause permanent damage or even be fatal. Furthermore, if chlorine spills into the environment, this can have detrimental effects on living organisms. Since the implementation of strict regulations on chlorine production the limiting of chlorine transportation in 2001, the number of incidents involving chlorine leaks has fallen rapidly (Du Pré, 2018). Between 2010 and 2018, only five chlorine spills were reported, only one of which affected humans; in 2011 two workers became unwell after a lightning strike caused a small chlorine gas leak in AkzoNobel's plant in Botlek.

Following a series of earthquakes in 2014 in the northern provinces of the Netherlands, a government investigation confirmed that there is no higher risk for external safety based on expectations for the Delfzijl Chemicals Park. AkzoNobel's plant in Delfzijl was deemed to be earthquake resistant by independent experts (Verbraeken, 2018a). As such, there is no higher risk of chlorine spills in Delfzijl than in other Dutch chlor-alkali plants.

Other emissions

Other pollutant outputs which may occur in the chlor-alkali industry include chlorates, bromates, sulphate, heavy metals, sulphite, organic compounds and halogenated organic compounds and spent acids from the chlorine drying (Brinkmann et al., 2012). Nonetheless, all of these emissions are minor and closely monitored by regulators. The mercury and diaphragm electrolysis techniques are far more polluting, and so the Dutch chlor-alkali industry is seen as having a relatively low impact on its environment (Paar, 2010).

4.2.5 Political analysis of chlor-alkali manufacturing industry

Despite the fact that chlorine trains were largely banned in the Netherlands as of 2006, AkzoNobel and the Dutch government signed a covenant in which it was determined that incidental transport for the maintenance of factories would still be possible (Verbraeken, 2018a). AkzoNobel now has one production line for chlorine in Rotterdam-Botlek. If it does not run – for example due to major maintenance – occasional transports from Germany are needed to meet the demand for chlorine. This is seen by industry stakeholders as a consequence of strict regulations on chlorine storage (Klein & Ybema, 2018). If AkzoNobel were allowed to store chlorine on its chlor-alkali plant site, it could build up reserves to reduce the dependence of transports from Germany.

In 2018, a new agreement was formulated between the government and AkzoNobel to completely get rid of chlorine transportation by 2021. Instead of building extra chlorine storage facilities, the government supported AkzoNobel's investment in a second chlor-alkali plant in Botlek (Verbraeken, 2018b). As of 2021, a second, fully independent chlor-alkali plant will be operational in Botlek. This plant is projected to have an annual production capacity of 150 kilotons of chlorine and will be fitted with the best available technologies in the chlor-alkali industry. Although in absolute sense, chlorine production will increase as a consequence of these developments, political and public opposition to chlorine production is likely to decline (Stikkelman, interview, 2018). The 'chlorine trains' had become such a politicized issue that this compromise between AkzoNobel and the government is seen as a positive development for all involved stakeholders (Boot, interview, 2018).

Apart from political developments around the transport and storage of chlorine, the new Dutch government has put more emphasis on its sustainable agenda. In their coalition agreement, the cabinet pledged to shut down or structurally rebuild all five coal-fired power stations by 2030. The two eldest (and most polluting) coal-fired power stations will be shut down by 2025, whereas the remaining three will be converted into biomass-fired power stations (Hofs, 2018a). This political decision is likely to have serious implications for the carbon-footprint of the power generation industry. Preliminary model calculations show that the CO_2 intensity of power generation is reduced by half by 2025 (Koelemeijer, Daniëls & Boot, 2017b). With the chlor-alkali industry being one of the prime consumers of electricity in the Dutch industrial sector, this development is likely to affect its indirect emissions. Although no regulation exists on indirect emissions, studies show that including indirect emissions within the coverage of an emissions trading scheme can help further reduce CO_2 emissions as a whole (Shim & Lee, 2016). Industry stakeholders believe it is plausible that such schemes develop prior to 2030, which can have a severe impact on the chlor-alkali manufacturing industry (Kleijne, email, 2018; Lintmeijer, interview, 2018).

4.3 Alternative technologies to decarbonize industry

4.3.1 Electric boilers

Because the steam pressure and temperature requirements of the vaporization of caustic soda are in the same range as that of brine vaporization, electric boilers too can be deployed in the chlor-alkali manufacturing industry. As such, electric boilers are seen to be a feasible technology that can help the chlor-alkali lower its CO_2 emissions by 2030. The specific parameters relevant for electric boilers are given in Table 7 in Section 3.3.1.

4.3.2 Biomass boilers

Biomass boilers, just like electric boilers, form a more sustainable source of steam generation. Biomass boilers can generate high pressure steam at temperatures up to 200°C, which is largely sufficient for the chlor-alkali manufacturing industry (VNCI, 2018). Biomass is the collective name for a wide range of wood types; it can include pellets, chips and logs. Biomass is considered a carbon-neutral form of energy, as the amount of CO_2 released by burning biomass is later re-absorbed by the plants that are grown for the biomass industry. Furthermore, biomass prices are generally more stable than those of other energy carriers such as gas and electricity (Ros & Schure, 2016).

The technology of industrial biomass boilers is very similar to that of regular gas-fired boilers. By burning biomass, water is heated via a heat exchanger which eventually boils to form steam. After passing through the brine vaporization process, cooled or condensed steam can be passed back into the biomass boilers where it can be heated again. Loss of water throughout this circular process is compensated by adding treated fresh water. The treated water in the piping system is periodically refreshed to avoid corrosion.

Biomass boilers are more expensive than electric boilers but have lower operating and maintenance cost (VNCI, 2018). State-of-the-art biomass boilers have efficiency rates ranging between 85% and 90% (Schoots et al., 2017). Due to the fact that the biomass is combusted in large chambers, biomass boilers require a substantial amount of space to be installed.

Industry stakeholders (Kleijne, e-mail, 2018; Lintmeijer, interview, 2018) believe that the placement of biomass boilers in chlor-alkali manufacturing plants can help it reduce its CO_2 emissions. Although they foresee that the placement of electric boilers will be financially more attractive, the diversification of steam generation processes is attractive as it decreases a plant's dependence on the prices of a single energy carrier. Since biomass has a relatively stable price, biomass boilers remain an interesting alternative technology to consider when evaluating technologies to decarbonize the chlor-alkali manufacturing industry. Due to the fact that it is more capital intensive than electric boilers, the industry stakeholders do not see it as a viable technology alternative for the salt manufacturing industry. Table 13 gives an overview of the main relevant parameters for the conceptualization of this technology in the MIDDEN dataset.

Table 13: Technological specification of biomass boilers
(Koelemeijer, 2017a; VNCI, 2018)

Parameter	Value	Units
Unit of main output	1	GJ steam
Investment cost per unit main output	50,000	€
Operating and maintenance cost per unit main output	3.47	€
Refurbishment interval	10	years
Electricity requirements per unit main output	1.1	GJ
Water inputs per unit main output	0.38	ton
Capacity of single unit (on full utilization)	25	TJ/year

4.3.2 Zero-gap membrane electrolyzers

Zero-gap membrane electrolyzers consist of an electrolytic cell where the anode and the cathode are placed extremely close to the membrane wall that separates them; the distance between the electrodes is less than or equal to 1 mm (Brinkmann et al., 2014). Minimization of the distance between the electrodes leads to a minimization of the voltage drop across the electrolyte, and thus saves electric energy. However, with the minimization of electrode distance, bubbles are more likely to be entrapped between the membrane wall and the electrodes, which causes the voltage drop to increase again. This is avoided by special coating of the membrane with a porous inorganic material (O'Brien et al., 2007). The development of this coating layer has caused zero-gap technology to become widely adopted across the European chlor-alkali industry as of 2005 (Brinkmann et al., 2014).

Although the chlor-alkali's direct emissions are not lowered by the zero-gap technology, it has a serious influence on its electricity usage, and thus helps to reduce indirect emissions. Since the indirect emissions of the chlor-alkali industry are considerably higher than the direct emissions, this alternate technology seems promising in reducing the net emissions of the Netherlands as a whole (Klein & Ybema, interview, 2018).

Since the electricity savings from zero-gap electrolyzers are considerable, the technology is financially attractive as a long-term investment for companies in the Dutch chlor-alkali industry. However, due to the fact that AkzoNobel and Sabic had changed from diaphragm and mercury electrolyzers to the more expensive membrane electrolyzers prior to 2005, they had been unable to further invest in the zero-gap technology once it became available. A change from finite gap electrolyzers to zero-gap electrolyzers requires considerable new investments, and would require the writing off of previous considerable investments in the finite gap electrolyzers (Klein & Ybema, interview, 2018). Furthermore, the maintenance costs of the membranes themselves, as well as those of the coating layer are considerable (Schmittinger et al., 2012).

Table 14: Technological specification of zero-gap membrane electrolyzers (Brinkmann et al., 2014; Schmittinger et al., 2012)

Parameter	Value	Units
Unit of main output	1	ton 80% chlorine
Investment cost per unit main output	102,000	€
Operating and maintenance cost per unit main output	15,300	€
Refurbishment interval	5	years
Electricity requirements per unit main output	6.7	GJ
Brine 23% inputs per unit main output	17	ton
Caustic soda 30% inputs per unit main output	32	ton
Heat output per unit main output	1.6	GJ
Caustic soda 32% output per unit main output	33	ton
Hydrogen 25% output per unit main output	0.09	ton
Brine 17% output per unit main output	15	ton
Capacity of single unit (on full utilization)	28	kton/year

Dutch chlor-alkali industry specialists see the implementation of zero-gap electrolyzers as the most serious investment in their industry until 2030 (Kleijne, email, 2018). As such, not only the chlor-alkali's direct emissions, but also its considerable indirect emissions can be reduced. Table 14 gives an overview of the main relevant parameters for the conceptualization of this technology in the MIDDEN dataset.

4.3.3 Capacity increase to utilize peak-shaving production

When a chlor-alkali plant deploys peak-shaving production, it adapts its production levels to the electricity prices. This is potentially not only financially interesting but can also help making the production of chlorine more sustainable by making direct use of the electricity generated from renewable sources (Krebbekx et al., 2015).

Table 15: Technological specification of capacity increase to deploy peak-shaving technology (VNCI, 2018; Den Ouden et al., 2017)

Parameter	Value	Units
Unit of main output	1	ton 80% chlorine
Investment cost per unit main output	480,000	€
Operating and maintenance cost per unit main output	48,000	€
Refurbishment interval	5	years
Electricity requirements per unit main output	6.1	GJ
Brine 23% inputs per unit main output	17	ton
Caustic soda 30% inputs per unit main output	32	ton
Heat output per unit main output	1.5	GJ
Caustic soda 32% output per unit main output	33	ton
Hydrogen 25% output per unit main output	0.09	ton
Brine 17% output per unit main output	15	ton
Capacity of single unit (on full utilization)	28	kton/year

Increasing production when electricity prices are low and reducing production when electricity prices are high requires larger storage capacities to ensure product delivery with clients. Chlorine storage capacity is strictly regulated in the Netherlands, so flexible operation of a chlor-alkali plant is only possible for short periods of time without influencing the constant supply to chlorine customers. Thus, the number of hours that peak-shaving can be applied depends on the amount of storage capacity and on the extra production capacity.

AkzoNobel has already closely investigated peak shaving and formulated a business case for the implementation of the technology (Klein & Ybema, interview 2, 2018). Upon the construction of their second independent chlor-alkali plant in Botlek as of 2021, AkzoNobel can supply dozens of megawatts of interruptible flex power with for their new chlorine plant (Verbraeken, 2018b). The costs for flexible operations are mainly determined by possible investments in extra capacity and ICT, which are necessary to make flexibility possible. Once the extra capacity is available and the operating system of the plant has been set up in such a way that flexible operation is possible, the further costs for flexible operation are mainly for ICT and adjustment of procedures. The costs and other relevant parameters for the implementation of this technology are estimated for the MIDDEN database and shown in Table 15.

Chapter 5:
Model conceptualization

5.1 System relationships

5.1.1 MIDDEN database structure

With the help of the empirical research outlined in Chapters 3 and 4, all existing processes of the salt and chlor-alkali manufacturing industry were quantified and mapped into the MIDDEN database for each specific plant. An overview of the process-level data that was mapped into the MIDDEN database is shown in Appendix C. Furthermore, the identified alternate technologies that can help to reduce both direct and indirect CO_2 emissions were also mapped into the MIDDEN database.

Each existing and alternate technology is mapped into the *Technology characteristics* dataset of the MIDDEN database (see Table 2), and all data on material flows, energy flows and investment costs are normalized per unit of main output of the specific process. This standardized approach enables modelers to easily investigate the effect of the deployment of a certain technology for a certain process. Furthermore, it allows for future researchers to expand the existing dataset with new technologies relevant to the industry under consideration. Lastly, it allows for multiple technologies to be deployed for a certain process in parallel.

Figure 13 and Figure 14 give a modular overview of the technology characteristics for the salt and chlor-alkali manufacturing industries respectively. The figures show how for a specific process within the industry under consideration, different technologies are used to produce the outputs generated by the process step. For example, in Figure 13, the vaporization process (Step 4) contains three currently deployed technologies and one alternate technology, each of which are quantified in the technology characteristics dataset.

This modular approach also allows to distinguish between different technologies deployed at different plants, in order to be able to formulate plant-specific material and energy flows. It also allows for multiple technologies to be deployed for a certain process in parallel at a given plant. For a process p, the total amount of a main output produced y at a given plant a is equal to the sum of outputs x generated by the different technologies deployed for the process t. Hence:

$$y_{a_p} = \sum x_{a_{p_t}}$$

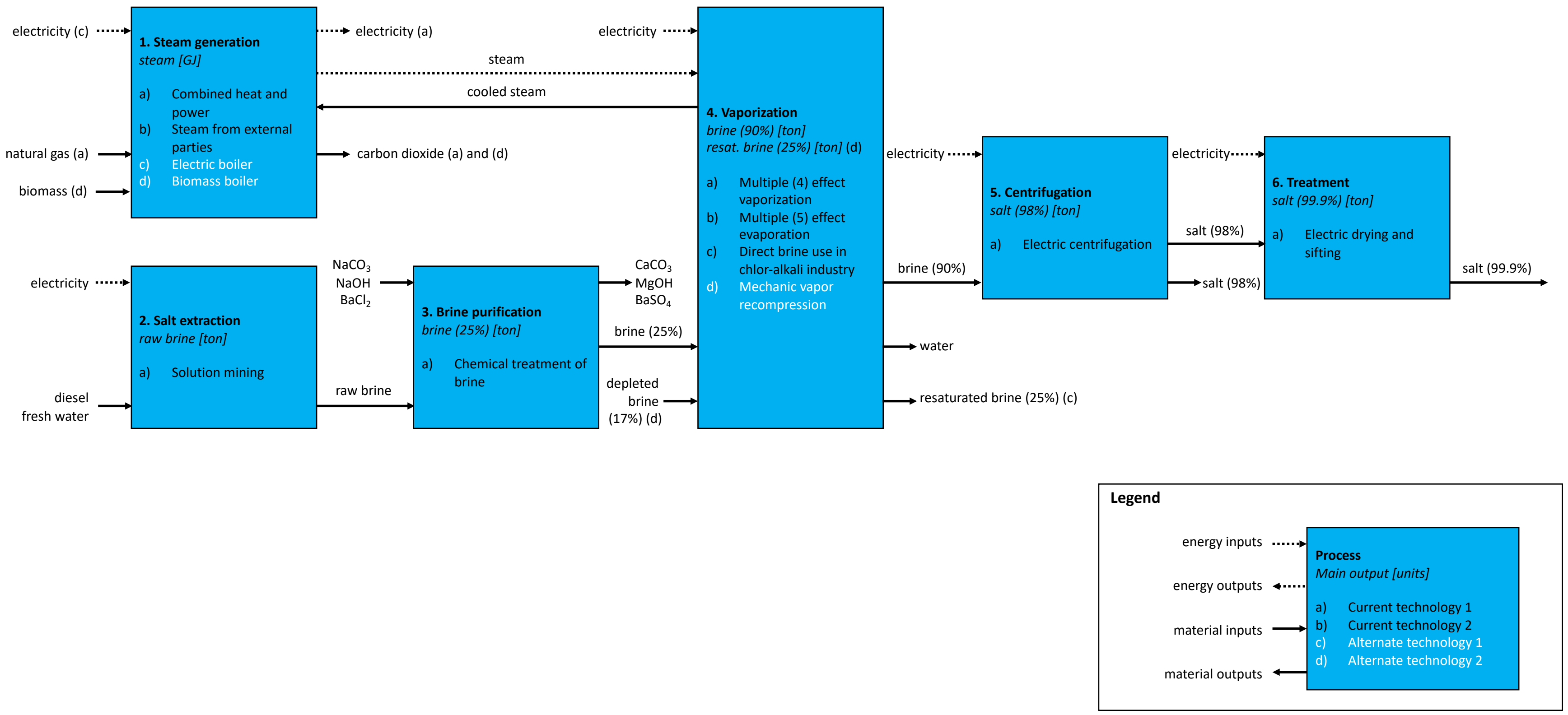


Figure 13: Modular overview of MIDDEN dataset for salt manufacturing industry

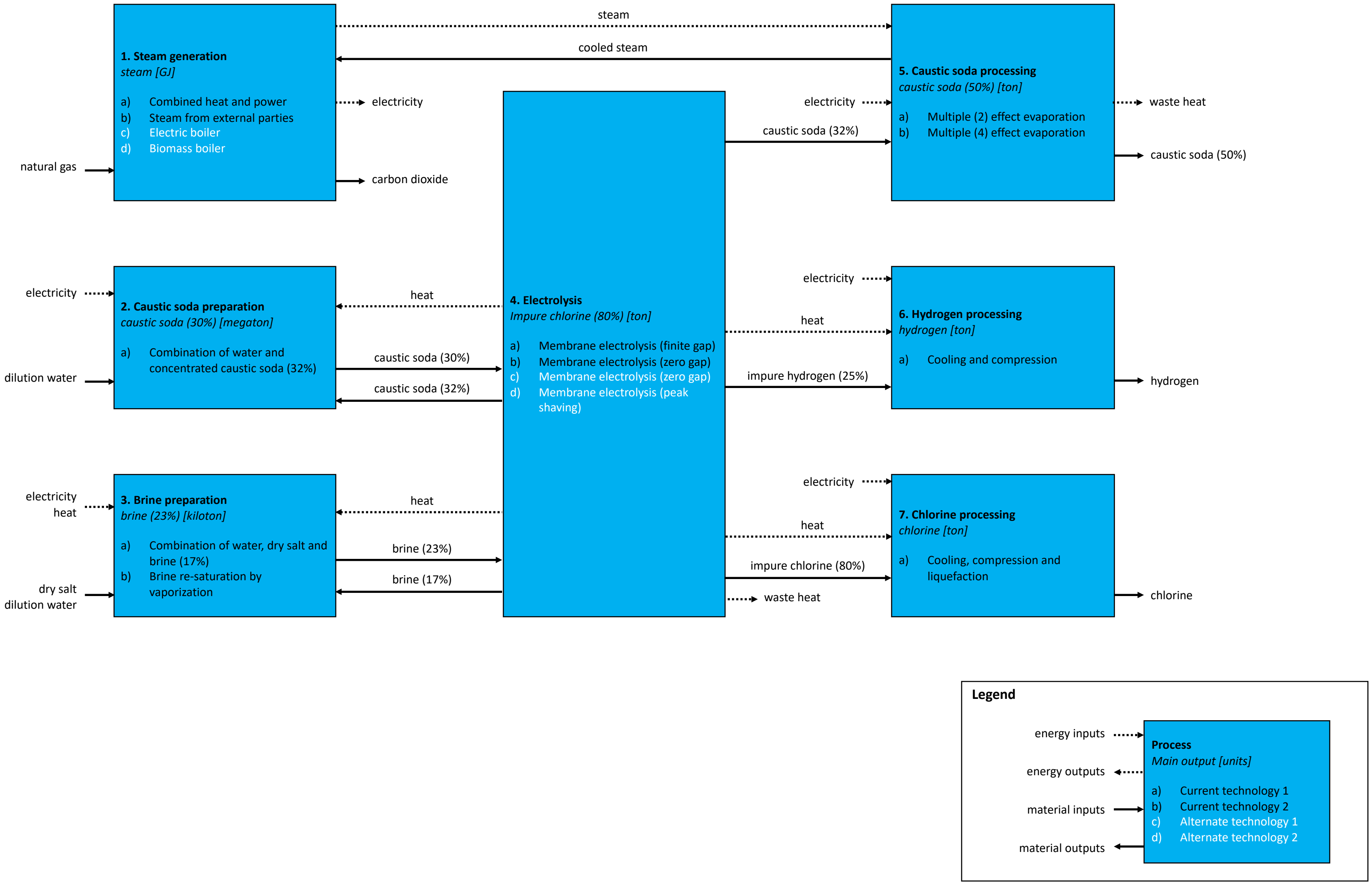


Figure 14: Modular overview of MIDDEN dataset for salt manufacturing industry

For instance, the salt manufacturing plant in Hengelo produces part of its steam using an on-site CHP, while it imports the rest from a waste incineration plant and a pyrolysis plant as was discussed in Section 3.1.2. As such, in the *Current plant configuration* dataset, the amount of steam generated for AkzoNobel Hengelo is 3.05 PJ/year at its CHP, and 0.53 PJ/year by third parties. Using the above formula, and the notation deployed in Figure 14, this can be written as:

$$\begin{aligned} y_{a_p} &= \mathrm{steam}_{\mathrm{Hengelo}_1} \\ &= \sum x_{a_{p_t}} \\ &= x_{\mathrm{Hengelo}_{1(a)}} + x_{\mathrm{Hengelo}_{1(b)}} \\ &= 3.05\ \mathrm{PJ/year} + 0.53\ \mathrm{PJ/year} \end{aligned}$$

The overall plant configuration is thus constructed in a similar manner, where the *Current plant configuration* dataset specifies how much of a certain main output each of the technologies in a process produces annually.

Each of the main output production numbers, in turn is dependent on three variables, that form the inputs to the *Current plant configuration* MIDDEN dataset, as shown in Table 16. The *Current plant configuration* and *Technology characteristics* datasets together form the inputs used in the DPE Model.

Table 16: MIDDEN input parameters used for process-level specification of outputs generated per plant

Technology parameter	Description	Units
NUMBER	The amount of facilities of a certain technology deployed at a plant	Integer value
CAPACITY	The quantity of main output the facility can produce in a year	PJ/year or kton/year
CAPACITY UTILIZATION	The proportion of the year during which the facility is active and producing the main output	[100%]

5.1.2 Industry-level aggregation

In order to analyze the identified decarbonization pathways on the industry level, the plant-specific data of the MIDDEN database is aggregated. Although the DPE model can simulate the effects of the decarbonization pathways on a plant level too, the industry perspective is chosen for the scope of this investigation. This is done by summing the total production number for each technology across all plants under the industry under consideration.

Referring to the notation used in Table 16, one can see that the total production per technology is defined as the sum of the product of the technology number, its capacity and its capacity utilization across all plants:

$$\mathrm{TOTAL\ PRODUCTION} = \sum \mathrm{NUMBER} \times \mathrm{CAPACITY} \times \mathrm{CAPACITY\ UTILIZATION}$$

5.1.3 Mass and energy balances

To analyze the impact of an alternative technology on the material and energy flows within an industry, the DPE model imposes mass and energy balance restrictions on the system under consideration. This means that if an alternate technology produces a certain amount of a main output, the existing technology will automatically produce less of that main output. This is done by lowering the capacity utilization of the technology that is already in place. The DPE model automatically lowers the capacity utilization of the most energy-intensive (and by consequent cost-intensive) to balance the mass and energy flows of the industry under consideration.

For example, if the steam generation process in the Botlek chlor-alkali plant is partially replaced by electric boilers, the capacity utilization of the CHP is lowered, which has effects on the net gas consumption, net electricity production and net CO_2 emissions of the Botlek plant. The DPE model uses these mass and energy balances to calculate the future gas and electricity consumption costs based on the scenarios generated (see Section 5.2.1).

5.1.4 Yearly efficiency gains

The modeling system assumes that the salt and chlor-alkali manufacturing industries autonomously will become more efficient over time, regardless of whether the industry makes investments in certain alternate technologies. A study of DNV GL on energy efficiency in the manufacturing industry showed that the chemical industry annually gains approximately 0.5% in energy efficiency across its processes (Brems, Steele & Papadamou, 2016). Consequently, the DPE model assumes consumption of energy carriers such as gas and electricity is reduced by 0.5% of that of the previous year. These efficiency gains are subject to uncertainty, as is elucidated further in Section 5.2.4.

5.1.5 Cash flows

The DPE model calculates the change in energy carrier consumption for each year between 2016 and 2035. These changes in consumption levels can lead to extra revenues or expenditures, based on projected price scenarios of the respective energy carriers. These yearly extra revenues and expenditures are summed together to generate the cash flows. As such, the future cash flows generated by an investment into an alternate technology can be calculated based on projected prices of energy carriers.

5.1.6 Net present value

A central aspect in this simulation model is the calculation of the net present value (NPV) of an alternate technology. The NPV is a financial tool often used in capital budgeting to analyze the profitability of a projected investment. It is defined as the difference between cash proceeds (the present value of future revenues) and cash costs (present value of future costs). Hence, it is calculated based on the project investment duration, the expected cash flows during the project execution and the discount rate.

This is described in the following formula:

$$\mathrm{NPV} = \sum_{t=0}^{N} \frac{CF_t}{(1+r)^t}$$

where:

N	is the duration of the projected investment
CF_t	is the cash flow after period t; i.e. the difference between project-related incomes and expenses
r	is the discount rate – also known as the yield requirement; which indicates the ‘time value of money’ as a percentage per period

The NPV gives an indication of the financial attractiveness of an alternative technology option from a company perspective, as can be seen in Table 17.

Table 17: Net present value implications

Situation	Financial implication	Decarbonization implication
$NPV > 0$	The investment adds value	The project is feasible
$NPV < 0$	The investment diminishes value	The project is unfeasible
$NPV = 0$	The investment neither adds nor diminishes value	Other (strategic, political) criteria may determine project feasibility.

By calculating the NPV of alternate technology combinations for the year that it is simulated to be implemented in, the DPE model will allow the user to determine whether the industry under consideration will adopt a certain combination of alternate technologies.

Combined with the relations described in Sections 5.3.1 to 5.3.3, the DPE model thus simulates the effects on emissions, and whether the salt and chlor-alkali industries can meet the targets stipulated by the Dutch government.

5.1.7 Internal rate of return

The internal rate of return (IRR) on an investment is defined as the interest rate at which the net present value of all cash flows on an investment is equal to zero. The IRR is used in capital budgeting as a metric to account for the time preference for money and investments. The IRR allows companies to rank potential projects by the overall rate of return, rather than their net present values.

In the energy and material intensive industries where capital investments are difficult to make, the companies involved wish to invest in technologies with the highest possible IRR. Thus, the IRR is an important and useful metric to determine the financial attractiveness of different investment possibilities in a combination of alternate technologies.

The IRR is defined by the following relationship:

$$0 = \sum_{t=1}^{N} CF_t \times \frac{1-(1+\mathrm{IRR})^{-n_t}}{\mathrm{IRR}} \times (1+\mathrm{IRR})^{-\sum_{q<t} n_q} + CF_0$$

where:

N	is the duration of the projected investment
CF_t	is the cash flow after period t; i.e. the difference between project-related incomes and expenses
n	is the number of cash flows

The IRR cannot be derived analytically and is solved through trial and error. Microsoft Excel contains an IRR()-function, which is deployed in the DPE model to find the IRR of the alternate technology investments under consideration.

5.2 Exogenous uncertainties

In order to explore the space of possible futures set out by the system relations in the DPE model, computational experiments can be run with the EMA workbench while varying the values of specific model inputs. For each computational experiment, values within the uncertainty range of the specified uncertainties are randomly generated. An overview of the defined uncertainty ranges and used parameter references for the EMA workbench is shown in Table 16. In the following paragraphs, further explanation is given for the choice of the specified uncertainties, and the determination of their ranges.

Table 18: Uncertainty ranges deployed for DPE model experimentation

Uncertainty	EMA parameter	Uncertainty range	Baseline conditions	Units
Price and CO_2-intensity scenarios	`price_scenario`	1 – 6	1	Integer value
Discount rate	`discount_rate`	0.025 – 0.125	0.04	[100%]
Production levels	`production_uncertainty`	0.85 – 1.15	1.00	[100%]
Yearly efficiency gains	`efficiency_gain`	0.0015 – 0.0085	0.005	[100%]

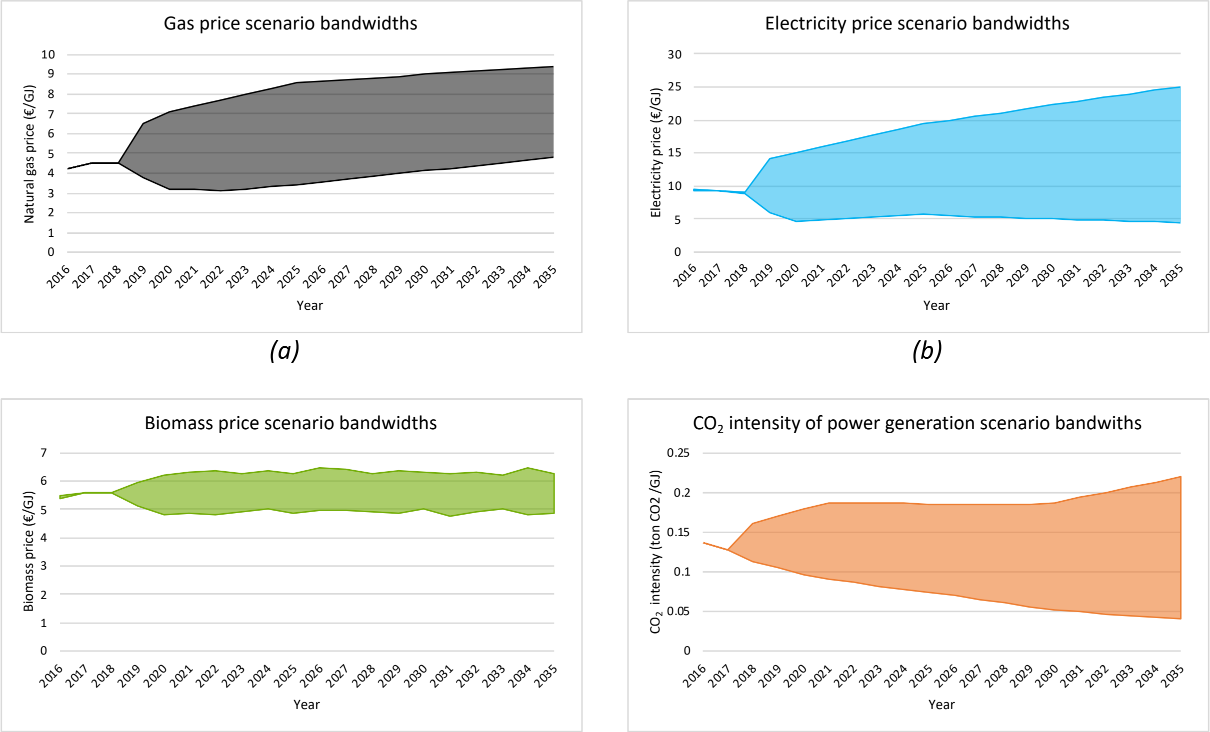
5.2.1 NEOMS price scenarios

From the National Energy Outlook Modeling System, a series of possible future scenarios were generated for gas, electricity and biomass price development, as well as the evolution of the CO_2 intensity of power generation. The NEO Modeling System accounts for the feedback effects of the prices of different energy carriers on each other, as well as the developments within the Dutch market as a whole. The NEO Modeling System has generated a total of 6 possible scenarios. These scenarios together define a subset of the uncertainty space that the salt and chlor-alkali manufacturing industries face.

Figure 15 shows the bandwidths of gas, electricity and biomass prices as well as the projected CO_2 intensity of power generation between 2016 and 2035 according to the NEOMS. One must note that each simulated plausible scenario is formed by a specific combination of price developments of the energy carriers as well as the CO_2 intensity of power generation. Hence, each simulated scenario can be seen as a combination of four lines within the bandwidths of Figure 15 (a), (b) (c) and (d). A total overview of the deployed pricing scenario combinations can be found in Appendix D.

For each model run, the DPE model assumes a certain price and CO_2 intensity scenario. The EMA workbench generates a random number between 1 and 6, which leads to one of the six scenarios generated by the NEO modeling system to define the development of energy carrier prices and the CO_2 intensity of power generation.

A similar approach to scenario uncertainty was adopted in a scientific study of the geopolitical impact of shale gas, where price scenarios from one model served as input scenarios for a second model (Auping, De Jong, Pruyt & Kwakkel, 2014). A further motivation of choice for these specific scenarios and the extent of their validity for the scope of this investigation is given in Section 6.3.5.



(a) *(b)*

(c) *(d)*

Figure 15: Bandwidths of gas, electricity and biomass prices and CO2 intensity across generated scenarios

5.2.2 Discount rate

The discount rate is the minimum interest rate set by the central bank for giving out loans. The discount rate in the Netherlands has been falling gradually for the period of 2012 to 2018. Although most financial predictions seem to indicate that the discount rate is likely to keep falling over time, there is a high degree of uncertainty on the discount rate in the long term. Since the discount rate is a pivotal part of the NPV and IRR calculations, it is important to take the effects of discount rate variations into account when considering the financial attractiveness of certain investments.

Between 1990 and 2016, the discount rate determined by the Central Bank in the Eurozone has fluctuated between 0.75% and 6% (RaboBank, 2016), with peaks reached during the years and aftermath of the financial crisis of 2007 and 2008, and lows reached from 2015 until 2017. A high discount rate makes long-term investments less attractive than a low discount rate. Throughout the course of this investigation, it was observed that the involved industries are very risk-averse in their investments in alternative technologies. This is because the reliability of a deployed technology is one of the most important aspects of whether a technology is attractive to invest in. New alternative technologies are always less reliable than the technologies that are already deployed across the industry on a large scale. As such, investments in new technologies are financially less attractive than for the involved industries to keep deploying the technologies they already use. As such, in the DPE model runs with the EMA workbench, the discount rate is varied at higher rates than those observed in the Eurozone, to account for the risk-averseness of the involved industries. Together with policy specialists from PBL, the discount rates for investments in the salt-chlor-alkali production chain were set between 2.5% and 12.5%.

5.2.3 Production variation

The specialists consulted throughout this research seemed to indicate that the market for salt, chlorine, caustic soda and hydrogen is likely to remain relatively constant throughout the years (Klein

& Ybema, interview 2, 2018). Nonetheless, a variation in production will have a severe impact on the net consumption of energy carriers. This will not only impact the emissions, but also the financial feasibility of certain technological investments. The bandwidths of the production levels of the salt and chlor-alkali manufacturing industries are therefore varied between 85% and 115% of current levels.

5.2.4 Yearly efficiency gain

The gains in efficiency are likely to have effects consumption of energy carriers, and by consequence, will affect the level of the industry's CO_2 emissions and returns and expenditures on energy carriers. The yearly efficiency gain is therefore considered under the following bandwidth: 0.5% ± 0.35%. This is in concurrence with observations made in industry efficiency studies in the literature (Hasanbeigi et al., 2013; Brems et al., 2016).

5.3 Decision levers

The DPE models for the salt and chlor-alkali industries deploy two kinds of levers. The first type of levers is used to explore the effect of the implementation of the alternate technologies discussed in Sections 3.3 and 4.3. This lever type is industry-specific and is used to explore industry-specific strategies for decarbonization. The second lever type is a governmental policy lever, which applies to all industries. These two levers combined help to uncover how the Dutch government and the companies involved in the salt-chlor-alkali chain can collaborate to formulate robust strategies for decarbonization. These are further elucidated below.

5.3.1 Technology levers

For the salt manufacturing industry, the effects of investments in electric boilers and mechanic vapor recompression are investigated. Based on discussions with industry stakeholders, different levels of deployment of each of the technologies is investigated. In the DPE model, the alternate technologies can be introduced such that they fully replace the current technologies responsible for a specific process.

As such, the placement of 350 electric boilers across the 4 salt manufacturing plants would fully replace steam generation by CHP, and thus fully decarbonize the salt manufacturing industry. Similarly, the deployment of 5 mechanic vapor recompressors would fully replace all multiple effect vaporizers across all plants in the salt industry. The technology levers then refer to the degree of deployment of those technologies as a fraction of the total production within the industry process, as can be seen in Table 19. These deployment fractions have been verified as plausible scenarios with industry stakeholders.

Table 19: Technology levers used in DPE model for salt manufacturing industry

Policy lever	**EMA parameter**	**Lever values**
Electric boiler investments	`Electric_boiler_investments`	0=0%, 1=15%, 2=30% deployment
MVR investments	`MVR_investments`	0=0%, 1=40%, 2=80% deployment

Similarly, the deployment of 75 electric or biomass boilers would fully decarbonize the chlor-alkali industry and the deployment of 31 zero-gap electrolyzers would replace all existing finite-gap electrolyzers in the chlor-alkali industry. For the implementation of extra electrolyzers to allow for peak shaving, an overall capacity increase of 20% is assumed, which equates to the deployment of 8 extra electrolyzers across the chlor-alkali industry. Table 21 shows the fraction of which each of these maximum deployment levels is investigated with the technology levers in the DPE model.

Table 20: Technology levers used in DPE model for chlor-alkali manufacturing industry

Policy lever	EMA parameter	Lever values
Electric boiler investments	`Electric_boiler_investments`	0=0%, 1=25%, 2=50% deployment
Biomass boiler investments	`Biomass_boiler_investments`	0=0%, 1=25% deployment
Zero-gap investments	`Zero_gap_investments`	0=0%, 1=50%, 2=100% deployment
Peak shaving investments	`Peak_shaving_investments`	0=0%, 1=25% deployment

5.3.2 Policy levers

The policy levers in the DPE model are applied to the entire salt-chlor-alkali chain. This allows one to investigate what governmental policies can support different industries in their decarbonization efforts. The policy levers that are investigated are: the year of investment in a certain technology, the implementation of a tax on gas for the industrial sector, and the closing down of coal-fired power station.

The year in which the investment is made in a series of alternative technologies is varied between 2020 and 2025. This enables the exploration of the effects of bringing forward or delaying certain technological investments, both on the abated emissions as well as the financial feasibility of those investments. Government representatives seem to indicate that gas taxation is likely to increase considerably between 2018 and 2030. Some representatives are arguing for a 75% increase in gas tax, which will also apply to the industrial sector (Hofs, 2018b). Stakeholders interviewed for this investigation are more conservative; they predicted a maximum increase of 50% on gas tax rates (Boot, interview, 2018; Lintmeijer, interview, 2018). The DPE model therefore has policy levers that allow for the investigation of the effects of a 25% and 50% increase in gas tax, as shown in Table 21.

Lastly, as was discussed in Section 4.2.5, the current Dutch government has pledged to radically restructure the power generation industry. All five coal-fired power stations active in the Netherlands in 2018 are to be shut down or rebuilt to biomass-fired power stations by 2030 (Hofs, 2018a). Together with considerable investments in off-shore wind farms, this projected policy is projected to reduce the CO_2 intensity of power generation in the Netherlands from 0.19 to 0.05 tons of CO_2 per GJ of electricity between 2020 and 2030. Nonetheless, because this policy has not officially been put into effect, it is considered as one of possible future scenarios. By implementing it as a policy lever in the DPE model, it is possible to investigate the effect of the lowering of the carbon intensity of power generation on the indirect emissions of the salt-chlor-alkali chain.

Table 21: Policy levers used in DPE models of salt-chlor-alkali chain

Policy lever	EMA parameter	Lever values
Year of investment decision	`Investment_year`	2020–2025
Tax on gas for industrial sector	`Energy_tax`	0=None; 1=25% gas tax; 2=50% gas tax
Coal-fired power station shutdown	`Coal_plants_shutdown`	0=Current poliy; 1=Envisaged policy

5.4 Performance metrics

With the DPE model, a large variety of different variables can be investigated and tested. For the scope of this research, the performance metrics investigated include direct, indirect and total emission predictions of the industry under consideration, the total investments deployed, the internal rate of return and the net present value of the combinations of technology investments investigated. An overview of the used performance metrics is shown in Table 22. The computational experiments run by the EMA workbench on the DPE model thus allow to explore how the different interests of industry and government stakeholders can be aligned while exploring efforts to decarbonize the salt-chlor-alkali chain.

Table 22: Performance metrics used for DPE models of salt-chlor-alkali chain

Performance metric	Units	EMA parameter
Direct emissions in 2016	kton	`Direct_emissions_2016`
Direct emissions in 2030	kton	`Direct_emissions_2030`
Direct emission change	kton	`Direct_emission_change`
Indirect emissions of production plant in 2016	kton	`Indirect_emissions_2016`
Indirect emissions of production plant in 2030	kton	`Indirect_emissions_2030`
Indirect emission change	kton	`Indirect_emission_change`
Total emissions in 2016	kton	`Total_emissions_2016`
Total emissions in 2030	kton	`Total_emissions_2030`
Total emission change	kton	`Total_emission_change`
Investment cost	€	`Investment_cost`
Internal rate of return of decarbonization pathway	[100%]	`IRR`
Net present value of decarbonization pathway	€	`NPV`
Yearly production	kton salt	`Yearly_production`

Chapter 6: Model verification and validation

6.1 Overview

Verification and validation are two distinct procedures used to identify a model's relation to the actual system. Upon performing these two actions, the quality of the model and the scope and implication of the results can be identified.

When performing verification, it is assessed whether the empirical model and the data used have been correctly translated from the conceptual model. As such, with model verification, one checks whether the built model 'matches' the author's understanding of the system. Thus, the final operations of the model are checked for consistency with the underlying mathematical equations. Note that verification only says something about how the model relates to the author's understanding of the system, and it says nothing about how the model relates to the real-world system itself.

The validation process, on the other hand, is used to identify the extent to which the results of the empirical model agree with observations made in the real world, while keeping in mind the purpose for which the model was built. Richardson (2011) argues two questions dominate the validation process:

1. Is the model suitable for its purposes and the problem it addresses?
2. Is the model consistent with the slice of reality it tries to capture?

Thus, if a model is properly verified, the model validation process allows one to determine the accuracy of the conceptual model for its application. One must note that, by definition, a model can never be a full representation of reality. Therefore, the validation process is all about establishing confidence in the usefulness and soundness of a model.

If during the validation process, unsurmountable discrepancies between the conceptual model and reality are found, the model will need to be adapted to provide results that better suit its purpose and more accurately represent the slice of reality it tries to capture. This adaptation process is encompassed within the iterative process of model validation (Richardson, 2011).

In the following paragraphs, the conceptual model described in Chapter 5 will be verified and validated in line with the theory described above. The model is verified with other experts involved in the MIDDEN project, and simple calculations are made to verify whether the outcomes of the model match outcomes of the experts' understanding of the system. Lastly, the model is validated by evaluating the purpose for which it was built, and to what extent it suitably represents the aspects of reality it needs to represent to fulfill this purpose.

6.2 Verification

Although two separate DPE models were built for each of the industries investigated in this research, they have the exact same underlying calculation structure. Therefore, in verifying the models built, it only necessary to examine the underlying calculation structure of either of the models. The DPE model for the salt manufacturing industry was therefore thoroughly verified, whereupon the DPE model for the chlor-alkali industry was checked for structural consistency.

The conceptualized DPE model for the salt industry was verified together with two energy researchers from the ECN division of the Netherlands Organisation for Applied Scientific Research, Marc Marsidi and Wouter Wetzels.

Firstly, the model structure was thoroughly examined. The two researchers verified the way in which the investment in a certain technology affected the cash flows for the industry under consideration. This was done by running a simple example calculation within the large DPE model. Instead of calculating the NPV and IRR of technology investments for the industry as a whole, the DPE model was verified by focusing on a particular plant.

The effect of the implementation of a mechanic vapor recompression facility (with a capacity of 150 kilotons of brine per year) in AkzoNobel Hengelo's salt plant was investigated under the baseline conditions (Price scenario = 1, Discount rate = 4%, Production level = 100%; Yearly efficiency gains = 0.05%). The investment costs and the change in electrical and heat energy demand were calculated, whereupon an estimation the abated emissions were made. These simple hand-made calculations agreed with the resulting outputs from the DPE model.

Furthermore, the way in which the net present value and internal rate of return were calculated were thoroughly discussed and verified. The DPE model calculates future cash flows based on the prices of different energy carriers it expects, and on the change in energy consumption of the production plant under consideration. The way in which these functions were written in Excel were verified by the two energy researchers, who had built similar models to quantify investments made in alternative technologies in the paper and pulp industry.

As such, the conceptual models of the salt and chlor-alkali industries were verified to match the both the author's understanding of the system, as well as the broader understanding of the energy researchers. The model structure, as well as the way in which the output variables are calculated in the conceptual model, were deemed to be consistent with the author's and energy researchers' understanding of the system as a whole.

6.3 Validation

As was seen in Section 6.1, the validity of a model is the extent to which the model matches the real-life system, for the given purpose and within the chosen boundary. Hence, in order to determine the validity of the DPE models deployed, this research will first identify the purpose of the model and the chosen boundaries. Subsequently, it will evaluate the extent to which the identified purpose is met within the scope of the conceptualized system.

6.3.1 Model purpose

The purpose of the DPE models is closely related to the central aim of this research. The research aims to identify robust strategies to decarbonize the Dutch salt-chlor-alkali production chain in light of a deeply uncertain energy transition until 2030. Thus, the DPE models of the salt and chlor-alkali industries should produce outputs that on the one hand quantify the effect on the industries' emission levels, whilst making an estimation of the financial feasibility of explored technological investments. Lastly, the model should allow for the exploration of a wide range of possible futures in order to account for deep uncertainty in energy transition planning. Thus, the purpose of the DPE model for each modeled industry is arguably threefold:

1. Evaluate the financial feasibility of alternative technologies
2. Evaluate the effect of the implementation of alternative technologies on resulting emissions
3. Explore the plausible futures in light of a change in energy usage over time

The extent to which each of these three purposes is met is essential to evaluating the validity of the model, as well as to understanding the implications of the results of the model.

6.3.2 Model boundaries

The two deployed DPE models investigate potential changes in technologies deployed in the salt and chlor-alkali production industries between 2018 and 2030.

As such, although this research is carried out in light of MIDDEN, which encompasses more than just the salt-chlor-alkali production chain, it is important to note that the results from the DPE models only have implications for the salt and chlor-alkali industries. Although the different technologies that are investigated may also be deployed in other industries, the results of this research are not directly applicable to other industries.

An example of this can be found within the scope of this research. Although the DPE models of the salt and chlor-alkali industries both investigate the effects of the deployment of electric boilers across the two industries, the conditions for steam generation in the two industries are different. The steam needed in the chlor-alkali chain has considerably higher temperature and pressure requirements. An electric boiler deployed to generate steam in a plant in the salt industry will therefore not have the same investment costs as an electric boiler deployed in a chlor-alkali production plant and will have different energy consumption costs. Similarly, electric boilers deployed in other industries outside the scope of this research will have other energy and investment requirements.

Furthermore, this research is focused around the salt-chlor-alkali production chain meeting the emission levels stipulated by the ETS for 2030. This means that the DPE model cannot make predictions of strategies further decarbonize these industries beyond 2030. Although pricing scenarios within the DPE model may propagate beyond 2030, the model only helps to identify whether and how the production plants investigated across the salt-chlor-alkali production chain can reduce their CO_2 emissions to meet centrally agreed upon emission levels.

6.3.3 Validity of financial results

Since the DPE models are used to evaluate the financial feasibility of investments in alternative technologies, this research must carefully evaluate the extent to which the financial results produced by the DPE models are an accurate representation of reality.

All model inputs – the MIDDEN databases of the salt and chlor-alkali industries, as well as the generated pricing scenarios – have undergone the scrutiny of different stakeholders involved. The investment costs and operational and maintenance costs of the different facilities deployed across different plants were checked for consistency with reality by both policy researchers from PBL, as well as by industry experts from AkzoNobel. Although the estimated investment costs for different technologies corroborated with the expectations of the industry experts, one must be wary of the fact that these investment costs are still ballpark estimates. These figures too are subject to high uncertainty, the effect of which is not extensively investigated in this research. The substantiated investment costs from this study can, therefore, be used to estimate the effect on cash flows for industry-wide investments, but cannot be used to make precise business case projections for a company that wishes to reduce the emissions of its production plant.

Another aspect to consider is the fact that the calculations for the NPV and IRR of the different technological investments are based on a series of pricing scenarios. Although these different price scenarios originate from the Dutch national authority for energy carrier pricing projections (Schoots et al., 2017), it is uncertain whether these pricing projections are an all-encompassing representation of reality. Furthermore, all pricing scenarios deployed in the DPE model (see Figure 15) are within bandwidths deemed reasonable for possible futures but do not account for extreme pricing fluctuations in the years to come. Although the companies that make their own NPV and IRR calculations for specific technology investments are unlikely to assume extreme pricing fluctuations themselves, the relative conservativeness of these different pricing scenarios poses a limitation to the extent to which the financial calculations are an accurate estimation of reality.

Another limitation on the calculation of financial parameters in the DPE models is the discount rate. This model input is an essential part of NPV and IRR calculations. Although the EMA workbench allows for the investigation of the effects of fluctuations in the discount on financial outcomes, the discount rate is a pivotal figure on which different technology investment considerations are based. Since companies involved in the industrial sector are very risk-averse with the implementation of new technologies, the discount rate in the DPE model is assumed to be relatively high (between 2.5% and 12.5%, as discussed in Section 5.2.2). Since future cash flows are discounted at a discount rate, a higher discount rate results in a lower present value of future cash flows thus in a lower NPV. In assuming the discount rate to be relatively high, the DPE model assumes the companies in the industry to be relatively unwilling to invest in alternative technologies, which may not be a fully accurate representation of reality. Nonetheless, it helps policymakers understand and identify the financial obstacles face in their efforts to reduce CO_2 emissions in the salt-chlor-alkali production chain.

Lastly, it is important to note that in capital budgeting theory, the NPV and IRR are two separate methods used to evaluate the attractiveness of a certain financial investment. Each of the two figures has its own strengths and weaknesses. The NPV quantifies investment attractiveness in terms of real money and the financial impact on a company but requires assumptions about the discount rate. The IRR on the other hand does not require assumptions about the discount rate and only quantifies the attractiveness of an investment as a function of the internal cash flows of that particular investment. The NPV is consequently more valuable in assessing the financial impact on a firm level, whereas the IRR is a more reliable quantification of the investment attractiveness when investigating an entire industry, given that the NPV of the investment is considerable for the industry as a whole. Therefore, in this investigation, it is important to assess both the NPV and the IRR in order to adequately quantify the financial feasibility of different technological investment options.

6.3.4 Validity of emission results

The DPE models estimate the emission levels of plants involved in the salt-chlor-alkali production chain. This is done mainly through mass- and energy balance calculations and estimated yearly efficiency gains as described in Sections 5.3.2 and 5.3.3. The extent to which these calculations result in a correct representation of reality is discussed below.

The emission levels of the salt and chlor-alkali production industries were quantified through a bottom-up approach by closely looking at the deployment of CHP facilities across the different investigated plants. Through estimations of the CHP efficiency levels and their thermal and electrical capacity, and data found in the literature, it was possible to get an estimate of the current emission levels of the various plants involved. These estimates corroborated with the emission levels registered in the Dutch National Emissions Authority. As such, the emission levels of the modeled current processes provide a correct representation of reality.

The challenge in the validity of the emission results lays in the projected future emissions of the investigated industries. The energy- and mass-balance condition that is imposed within the DPE model allows for the investigation of the effect of fluctuations in production levels, efficiency changes and the investment in new technologies. However, for each of these changes, there are limitations to the extent to which the model remains an accurate representation of reality. Nonetheless, for the DPE models as a whole the energy- and mass balance calculations were compared to other calculations made by policy researchers from PBL, and these different projections align with each other.

The estimated direct emissions are mainly based on current understanding of CHP deployment across the salt-chlor-alkali production chain. This has several implications for the way in which direct emission reduction is modeled:

Firstly, the emission change based on efficiency improvements is based on a decrease in gas demand of the CHP proportional to the modeled efficiency improvement. Although on a yearly basis, this efficiency improvement has little effect on abated emissions, the resulting change in emissions by 2030 can be considerable. For the salt manufacturing industry for example, a yearly efficiency improvement of 0.5% results in a direct emission reduction of 24 kilotons of CO_2 emissions. Although this emission reduction is not sufficient for the industry to meet the emission limitations imposed by the ETS, it constitutes approximately 35% of the total required emission reduction. This corroborates with a study by Hasanbeigi et al. (2013), which estimated energy efficiency improvements across the industrial sector constitute about a third of primary energy savings. As such, the validity of total emission reductions depends for a considerable amount on the modeled effects of efficiency improvements.

Secondly, when the DPE model simulates the investment in an alternative technology, it assumes that the most expensive technology is replaced by the alternative technology, or that the capacity utilization of the more expensive technology is reduced by a percentage that keeps the mass- and energy flows constant. For example, when 40 industrial biomass boilers are implemented across the chlor-alkali industry, this affects the capacity utilization of all the CHP's in the modeled industry, due to the industry-level aggregation (see Section 5.1.2). In reality, the deployment of biomass boilers in a specific plant would cause the CHP of a specific plant to close down, instead of the utilization of all CHP's to reduce by a proportional amount. Nonetheless, from an industry perspective, this amounts to the same result and as such this aggregation is deemed acceptable for the purpose of this investigation. This approach is also used in other industry simulations of PBL and ECN (Marsidi & Wetzels, 2018).

Thirdly, the DPE model cannot simulate the effects of a step-wise replacement of plant facilities. Step-wise replacement of facilities is considered to be financially more attractive (Klein & Ybema, interview 2, 2018), because the technology investments tend to decrease over time, and because technology reliability can be tested before large-scale implementation. Nonetheless, the DPE model does simulate the effects of the implementation of combinations of technologies in parallel, as well as the extent to which a certain technology is deployed across the entire industry. Thus, the projected emission level reductions as a result of technology investments are likely to be less discrete than the model projects, but since this investigation is focused around the change in emission levels until 2030, this should not pose a serious threat to the validity of the model.

> Lastly, in the modeled industries, direct emission reductions can also be acquired as a result of the decrease in steam demand due to improvements in other processes. For example, in the salt manufacturing industry, the implementation of mechanic vapor recompressors for the vaporization of brine can significantly reduce the steam demand for the plant. This steam demand reduction however, is modeled as a steam demand reduction of the industry as a whole. In reality, this may mean that on a plant level, the deployment of the CHP is no longer financially viable. Due to the industry-level aggregations and the mass- and energy balances imposed on the model, this aspect is not considered and poses a limitation on the projected emission reductions. Nonetheless, due to the fact that the deployment of MVR is also investigated in parallel with the deployment of electric boilers, this limitation is partially resolved within the model structure.

The DPE models do not only measure the change in direct emissions, but also the change in indirect emissions of the industries under consideration. Indirect emission levels are based on the total external electricity consumption of the industry under consideration, and the CO_2 intensity of the Dutch power grid. This too has implications for the validity of indirect emissions within the deployed DPE models:

> The values of CO_2 intensity of the Dutch electricity network are based on values resulting from the National Energy Outlook modeling system. Although these values are deemed to be conservative by some experts, their accuracy and reliability have been systematically evaluated by a wide range of energy experts (Welle et al., 2018; Schoots et al., 2017). Nonetheless, the Dutch electricity net is far more volatile on a day-to-day level than on a yearly basis, and as a result, this implies a larger uncertainty on the modeled electrification of industrial processes, especially in the DPE model of the chlor-alkali industry.
>
> The fact that the chlor-alkali industry is extremely electricity-intensive and that the modeled indirect emissions have limited validity poses serious consequences for the extent to which the model portrays the way in which the chlor-alkali industry is to evolve over the years. Especially for the peak-shaving technology, in which the industry uses electricity price fluctuations to decrease electricity expenditures, it is extremely complex to model the implications this has for the indirect emissions of the chlor-alkali industry. This is because the peak-shaving technology, if implemented on a large scale, is meant to aid the smoothing of the distribution grid and increase high renewable electricity penetration (Krebbekx et al., 2015), but that this effect is not and cannot be modeled within the scope of this investigation. Applying peak-shaving only in the chlor-alkali industry is unlikely to have effects on the CO_2 intensity of electricity generation, so the effect of the implementation of this technology should be investigated with higher industry-wide models that account for daily electricity price fluctuations, and for the fluctuations in the CO_2 intensity of power generation on a daily basis. Nonetheless, for the scope of this investigation, evaluating the effects of the implementation of peak-shaving technology on indirect emissions may provide first valuable insights that can benefit the development of such more elaborate models. Therefore, although the validity of the results of indirect emissions is limited, they can provide first insights about the way in which increased dependence on the electricity grid will affect the salt-chlor-alkali production chain.

6.3.5 Validity of explored futures

The nature of this investigation is explorative, and as such the DPE models are used to explore the range of plausible futures that lay ahead for the salt-chlor-alkali production chain. Thus, the validity of the explored futures is dependent on both the validity of the DPE models themselves, as well as the validity of the deployed uncertainty ranges used as inputs in the EMA workbench. The exogenous uncertainties investigated are the price scenarios, the discount rate, the production level and the yearly efficiency gains (as was seen in Table 18). The bandwidths deployed for each of these uncertainties have been substantiated in Section 5.2. Nonetheless, to further determine the validity of these explored futures, further discussion is necessary.

The six price scenarios resulting from the National Energy Outlook modeling software have been thoroughly scrutinized by a large team of energy specialists from ECN, PBL, CBS and RVO (Welle et al., 2018; Schoots et al., 2017). Nonetheless, the extent to which these scenarios together cover all plausible futures is questionable. As can be seen in the scenario graphs in Appendix D, the modeled price scenarios are relatively stable, and although they show both increases and decreases in price levels, the predicted futures have little extreme fluctuations in prices. Therefore, although experts deem these price developments to be most plausible, the DPE model does not account for a more unstable energy carrier market. This is a limitation on the deployed model and should be accounted for when evaluating the robustness of outcomes of the DPE models.

6.4 Model validity

Having identified the boundaries of the DPE model, the direct limitations of the used models are clear and plain. Although the total scope of MIDDEN is far larger than the industries under consideration, one must be careful not to transpose the results on robust strategies for decarbonization from this research to strategies for decarbonization across other industries. On top of this, no quantitatively substantiated conclusions can be made about decarbonization strategies beyond 2030, even within the scope of the salt-chlor-alkali production chain. Nonetheless, the identified boundaries do not limit the identified purposes of the model, which makes the model suitable for the research at hands.

Although there are some clear limitations to the extent to which the financial results from the deployed DPE models are a representation of reality, they give estimates of investment costs, the NPV and IRR for various alternative technology investments. When interpreting the results of the DPE models, it is therefore important to weigh these different financial outcomes with each other in order to gain a grasp of the financial feasibility of possible investments in alternative technologies. Furthermore, it is important to realize that the financial results from the DPE models cannot be used as business case projections for individual plants; they simply give the reader an indication of industry-wide investments necessary for a certain combination of technology and policy levers.

As a whole, it is clear that the DPE model deployed for the two industries of this research has some limitations on the validity of its emission results. Nonetheless, for the purpose of investigating the effect of the implementation of certain alternative technologies across the industries on the change in emissions, the DPE model is adequate and corroborates with literature findings as well as expert judgments. For the models deployed, the validity of direct emission changes is stronger than the validity of indirect emission changes. Since the focus of MIDDEN lies in investigating direct emission reductions, the deployed model is relatively useful for its intended purpose.

Chapter 7:
Model experimentation and analysis

7.1 Experimental set-up

Using the EMA workbench, a series of experiments are set up with the DPE model to explore and identify robust strategies to decarbonize the salt and chlor-alkali manufacturing industries by 2030. Using the Excel connector of the library, experiments can be run with the DPE model using the uncertainties (X) and levers (L) defined in Sections 5.2 and 5.3, while measuring the performance metrics (M) defined in Section 5.4.

For each of the two industries considered, a separate model was coupled to the EMA workbench and separate model experiments were set up. For each model, 500 scenario runs were run in together with a full factorial design to investigate all policy combinations. For the DPE model of the salt industry, this meant $4^2 \times 3 \times 2 = 96$ policy combinations, while for the DPE model of the chlor-alkali industry, $3^3 \times 2^3 = 216$ policy combinations were investigated. Table 23 shows the total number of scenarios, policy combinations and experiments run for each of the industry models.

Table 23: Overview of experiment runs for deployed DPE models

Experimental parameter	Salt industry	Chlor-alkali industry
Number of scenarios	500	500
Number of policies	96	216
Number of experiments	**48,000**	**108,000**

Experiments conducted for the purpose of exploratory modeling are about understanding how regions in the uncertainty space (X) and the decision space (L) map to regions in the outcome space (M). In the literature (Kwakkel, 2017), two distinct approaches to investigate these mappings are discussed:

1. *Open exploration*: by sampling systematically through the decision or uncertainty space;
2. *Directed search*: by searching through the output space using a directed optimization approach.

In this research, the open exploration approach is deployed. Open exploration is suitable for this investigation because the focus of this investigation lay on the identification of robust strategies to decarbonize the salt-chlor-alkali production chain. Industry and government stakeholders involved in the Dutch climate negotiations can benefit from clearly substantiated studies of the effects of the uncertainties and possible decision levers on the range of plausible future outcomes.

In the following sections, several tools from the EMA workbench will be deployed to analyze and evaluate the explored mappings from the uncertainty and decision space to the output space. These include feature scoring, scenario discovery and dimensional stacking.

Feature scoring is a family of methods that is used to determine the importance of certain inputs to preserve data output similarity (Li, Cheng, Wang, Morstatter, Trevino, Tang & Liu, 2017). Through the selection of a subset of the original variables the dimensionality of the input data – the number of random variables under consideration – can be reduced (Jaxa-Rozen & Kwakkel, 2018). By defining a set of inputs and outputs of interest, the feature scoring toolkit conducts regressions to identify the importance of variations in input parameters on the set of outputs by calculating their normalized relative effects on the defined output space (Kwakkel, 2017). Feature scoring is conducted both on the uncertainty space as well as the decision space.

Scenario discovery is a relatively new model-based approach that is aimed at making transparent which uncertain factors influence the decision problem at hand (Kwakkel & Jaxa-Rosen, 2016). In this approach, scenarios are defined as “a set of plausible future states of the world that represent vulnerabilities of proposed policies” (Bryant & Lempert, 2010). These sets are identified by the application of data-mining algorithms with the EMA workbench and can be interpreted through structured data analysis. In this research, a relatively simple analysis will be made by visualizing the set of all plausible futures in the uncertainty and decision space and isolating the set of future states where policies fails to meet the required goals set out by this investigation, using a parallel coordinates plot from the Plotly python package.

Lastly, dimensional stacking can be described as a more visual approach to scenario discovery. Once the most important uncertainties that affect system behavior are identified, their relative multi-dimensional relations are mapped in a two-dimensional grid structured heatmap. This approach allows for the identification of mutually strengthening policy combinations, as well as areas in the decision space which lead to the unwanted output spaces.

This series of experiments and analysis steps together form the basis for recommendations for technology investments and policy considerations that ensure robust pathways towards reducing CO_2 emissions of the Dutch salt-chlor-alkali production chain.

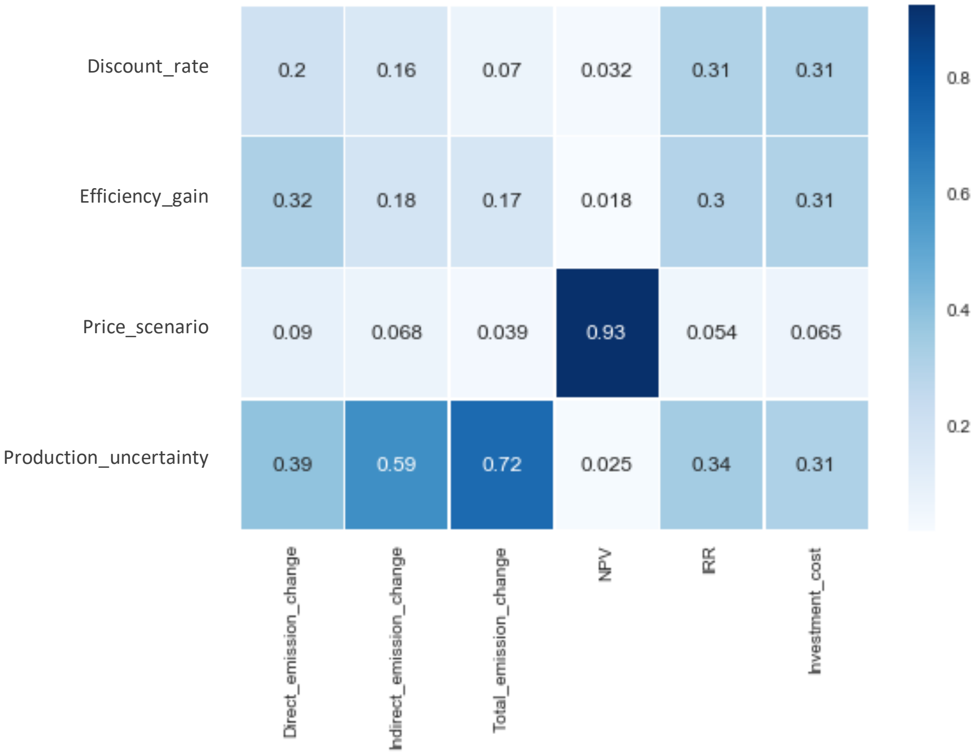
7.2 Uncertainty analysis

Using feature scoring, the influence of the uncertainty spaces defined in the DPE model is evaluated on the range out possible outcomes. Figure 16(a) and (b) show the feature scores of the uncertainty space against a set of performance metrics: changes in direct, indirect and total emissions, and the NPV, IRR and investment.

Interestingly, both feature scores produce very similar results. Figure 16(a) as well as Figure 16(b) show that the price scenarios have the strongest influence on the NPV of investment decisions. This indicates that the variation in projected energy carrier prices is a large driver for the profitability of investments. As such, the more certainty firms can have about the future of energy carrier prices, the more clear-cut their considerations will be about what technologies to invest in.

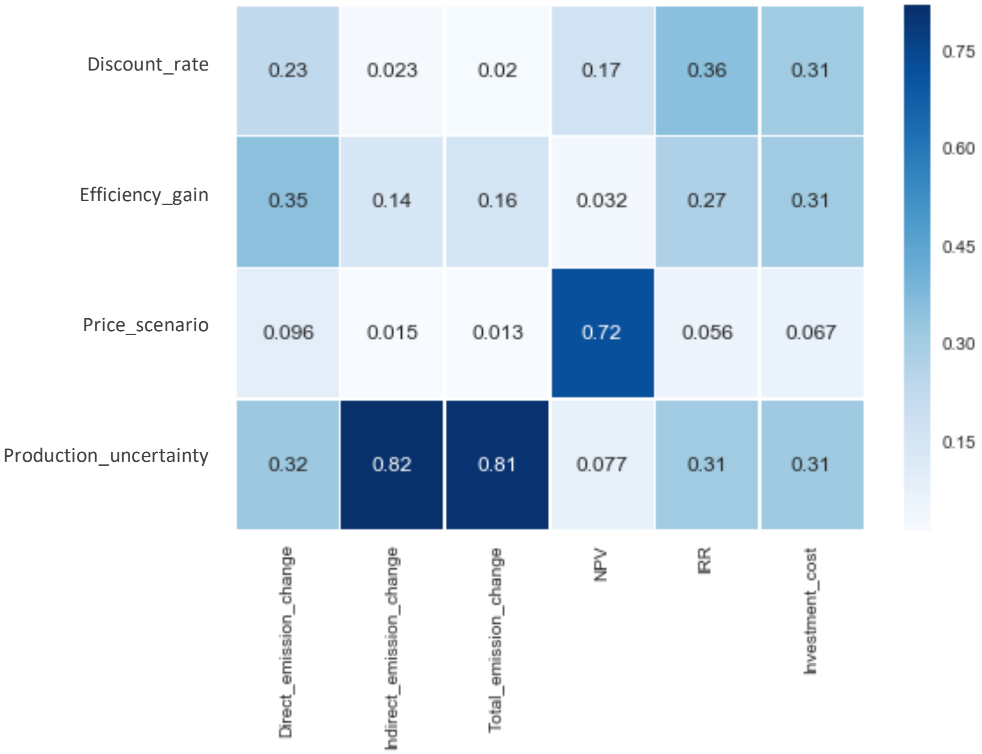
Interestingly the net present value of the technologies explored is relatively insensitive to variations in the discount rate. Although the discount rate by definition has a direct effect on the NPV, its effect is eclipsed by the effects of energy carrier price fluctuations. From the policy maker’s perspective, it is important to see that price futures therefore largely define how attractive investments in alternate technologies are. Policies aimed at restricting uncertainty on future prices of energy carriers is therefore likely to have more effect than monetary policies focused on discount rates aimed at promoting an investment climate. That said, the former is much more difficult to attain than the latter.

Another aspect that can be observed from Figure 16(a) and Figure 16(b) is that relatively small fluctuations in production levels have a strong effect on the direct, indirect and total emission changes.



	Direct_emission_change	Indirect_emission_change	Total_emission_change	NPV	IRR	Investment_cost
Discount_rate	0.2	0.16	0.07	0.032	0.31	0.31
Efficiency_gain	0.32	0.18	0.17	0.018	0.3	0.31
Price_scenario	0.09	0.068	0.039	0.93	0.054	0.065
Production_uncertainty	0.39	0.59	0.72	0.025	0.34	0.31

(a) Salt production industry



	Direct_emission_change	Indirect_emission_change	Total_emission_change	NPV	IRR	Investment_cost
Discount_rate	0.23	0.023	0.02	0.17	0.36	0.31
Efficiency_gain	0.35	0.14	0.16	0.032	0.27	0.31
Price_scenario	0.096	0.015	0.013	0.72	0.056	0.067
Production_uncertainty	0.32	0.82	0.81	0.077	0.31	0.31

(b) Chlor-alkali production industry

Figure 16: Feature scores of uncertainty spaces of investigated industries

This shows that from a government perspective, it may be interesting to think of ways to regulate the production of salt and chlorine, in order to have a direct control over the emissions the industry causes as a whole. Furthermore, uncertainty on the yearly efficiency gains of the salt and chlor-alkali industries also affects their direct, indirect and total emissions. The effect of improvement of industry efficiency on its emission levels is obvious, but the uncertainty analysis shows that it is a factor that must not be underestimated. Model calculations show that with maximum efficiency gains, the total emission reductions in the salt and chlor-alkali industries together can be up to 150 kilotons of CO_2 per year without even investing in alternate technologies.

It is also interesting to note that the direct emissions are more strongly affected by efficiency gain changes than the indirect emissions. This effect of the uncertainty of the output space can be attributed to the fact that the model experiments focus on reducing the direct emissions of the salt-chlor-alkali production chain.

The similarity between Figure 16(a) and Figure 16(b) may indicate a strong similarity between the two closely linked industries. However, it may also be an indication of the strong structural similarity between the two models that the computational experiments are run on. Further research may be necessary to uncover whether this similarity between the feature scores is attributed to the model structure, or to the way in which the modeled system functions.

7.3 Decision space analysis

Using the same strategy as was applied to the uncertainty space, it is also possible to systematically sample over the decision space. Figure 17 and Figure 18 give the feature scores of the two industries under consideration. The decision space spans both the policy lever space as well as the technology lever space. The two lever spaces are closely related and will be therefore analyzed in sequence below.

Policy space analysis
Both Figure 17 and Figure 18 show that the government's projected policy to shut down the coal-fired power plants has very large effect on the total emission change of the salt-chlor-alkali production chain. This effect is primarily acquired by the change in indirect emissions it causes, as is supported by the relatively high feature scores of the indirect emission changes of the `coal_plants_shutdown` policy lever. It may be interesting to investigate whether there are certain positive reinforcing effects between the lowering of the CO_2 intensity of power generation and the investment in technologies that are electricity-fueled rather than gas-fueled.

Where the shutting down of coal-fired power stations has a high effect on the CO_2 emission levels, the feature score charts also show that a tax on gas has a strong influence on variations in the NPV and IRR variables. A tax on gas makes the net present value of alternative technologies more attractive because of the change in projected cash inflows it causes with respect to sticking to the current technology of the plant. From the industry firm's perspective, a tax on gas causes alternative technologies to become financially more attractive, and as such they are more likely to invest in them.

Lastly, from a policy perspective, it is interesting to note that the year in which the investment occurs does have strong effects on the financial considerations such as the net present value and the internal rate of return but has little effects on the realized CO_2 reductions. Thus, it is interesting to investigate whether from the firm's perspective investment decisions are more attractive earlier than later.

Technology space analysis
Along the technology levers implemented in the two models of the two industries under consideration, some preliminary observations can be made based on the feature scores in Figure 17 and Figure 18.

For the salt manufacturing industry, shown in Figure 17, it is clear that investments in the mechanic vapor recompression technology cause the greatest changes in direct emissions of the industry. Hence, it is interesting that for the salt manufacturing industry, the best way to reduce CO_2 emissions is not by replacing the process that causes the CO_2 emissions (i.e.: replacing a CHP by electric boilers), but rather by replacing the process that causes the high demand for steam (i.e.: replacing multiple effect vaporizers by mechanic vapor recompressors).

Nonetheless, both MVR technology as well as electric boiler investments seem to have a considerable effect on the change in direct emissions. Therefore, it will be interesting to further investigate how the two technologies complement or disturb each other's' effects on CO_2 emission changes. From Figure 17, it can also be seen that their respective effects on indirect emissions is also considerable. It is therefore possible that the implementation of only one of the two technologies only increases the total emissions, whereas implementing the two technologies in parallel allows the total emissions of the salt industry to also be reduced.

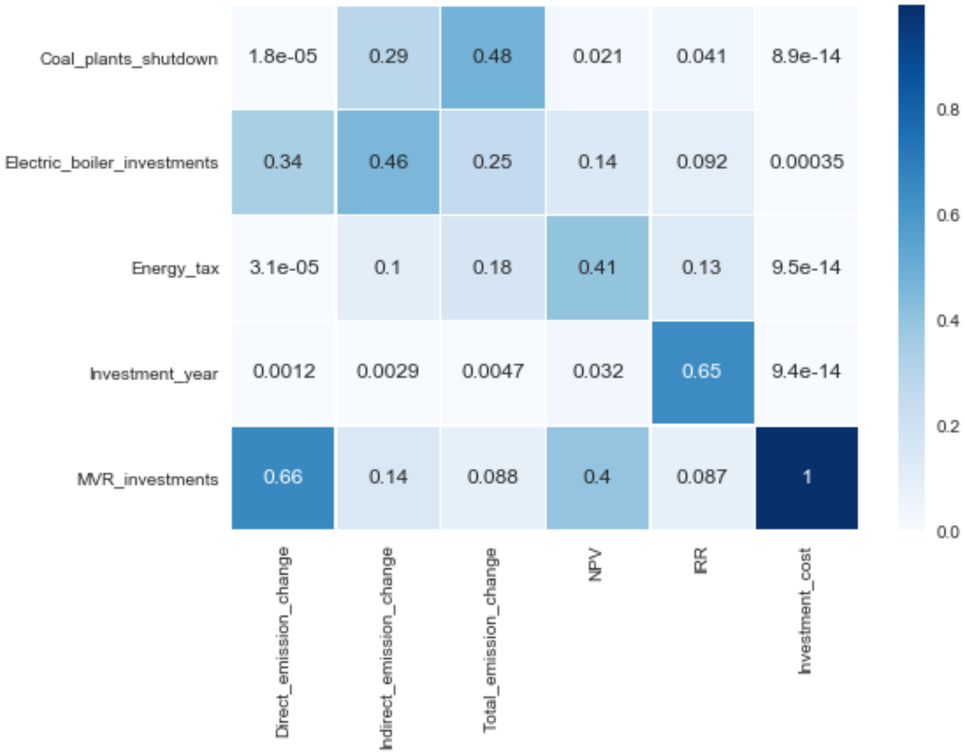
From Figure 17, it is also clear that the costs of investment are mostly affected by investments in mechanic vapor recompressors. This is due to the fact that the costs of investment in electric boilers are very minor, as was seen in Section 4.3.3. This is an important aspect to keep into account as the energy intensive salt industry is unlikely to make substantial capital investments into an industry that makes only marginal profits. Additionally, the feature scores of NPV and IRR and the technology investments also show that small changes in the MVR lever have greater effects in the profitability of the overall investment than small changes in the electric boiler lever do. This too indicates that careful considerations must be made about the extent to which MVR technology is deployed across the salt industry.

As for the feature score maps of the chlor-alkali industry, Figure 18 shows that the largest change in direct emissions is gained by the deployment of electric boilers. The deployment of biomass boilers too has an effect on the change in direct emissions, but much less. Indirect emissions, which, for the chlor-alkali industry are far greater than its direct emissions, are mostly affected by investments in zero-gap technology. This finding is in accordance with statement made by industry stakeholders.

Interestingly, Figure 18 shows that the total emission change by the implementation of electric boilers is approximately the same as the implementation of zero-gap technology. Considering the fact that the projected investment returns into zero-gap electrolyzers is far greater than the investment returns on electric boilers, it is important to investigate how not only indirect but also direct emissions of the chlor-alkali industry can be reduced by 2030. This will further be investigated in the sections below.

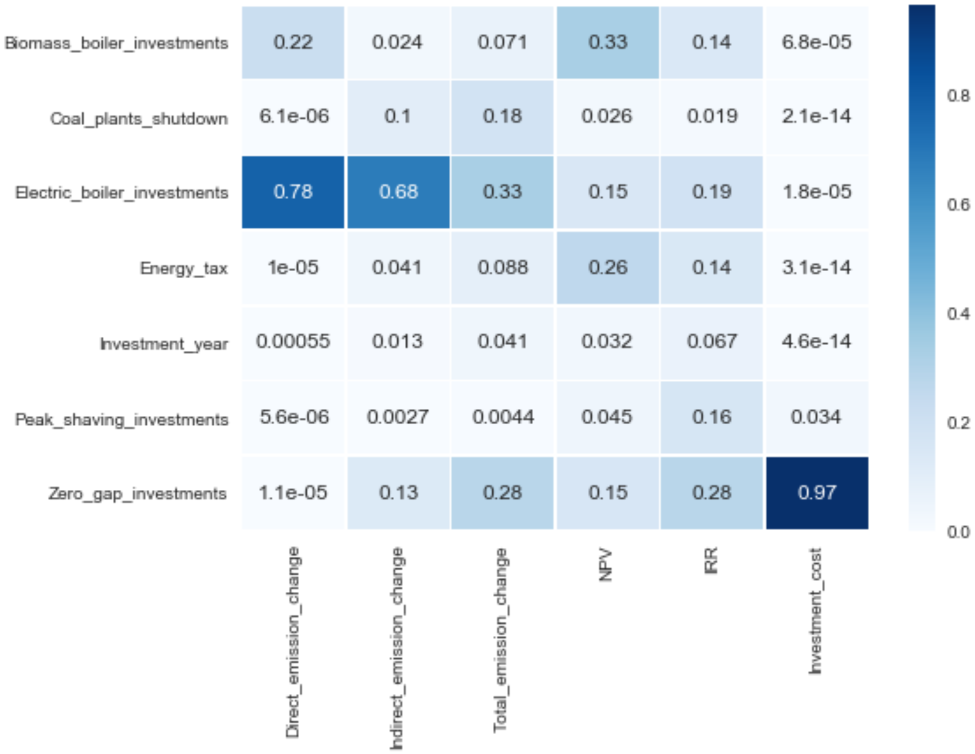
Investments in peak-shaving technology, although they may be profitable to the industry itself, seem to have little effect on the net direct and indirect emissions. Thus, this technology is less interesting for the scope of this investigation.

As a whole, it is clear that a number of technology and policy levers need more careful examination. The effects of shutting down the coal-fired power stations and gas tax and their relations to the attractiveness of investments in alternate technologies can further be investigated by identifying desirable output spaces and examining how the different policy levers are related to each other within this output space. For the salt industry, a further investigation into investments in electric boilers and mechanic vapor recompressors will be conducted, whereas for the chlor-alkali industry the focus will lay on the impact of investments in zero gap technology and electric boilers.



	Direct_emission_change	Indirect_emission_change	Total_emission_change	NPV	IRR	Investment_cost
Coal_plants_shutdown	1.8e-05	0.29	0.48	0.021	0.041	8.9e-14
Electric_boiler_investments	0.34	0.46	0.25	0.14	0.092	0.00035
Energy_tax	3.1e-05	0.1	0.18	0.41	0.13	9.5e-14
Investment_year	0.0012	0.0029	0.0047	0.032	0.65	9.4e-14
MVR_investments	0.66	0.14	0.088	0.4	0.087	1

Figure 17: Feature score of decision space of the salt industry



	Direct_emission_change	Indirect_emission_change	Total_emission_change	NPV	IRR	Investment_cost
Biomass_boiler_investments	0.22	0.024	0.071	0.33	0.14	6.8e-05
Coal_plants_shutdown	6.1e-06	0.1	0.18	0.026	0.019	2.1e-14
Electric_boiler_investments	0.78	0.68	0.33	0.15	0.19	1.8e-05
Energy_tax	1e-05	0.041	0.088	0.26	0.14	3.1e-14
Investment_year	0.00055	0.013	0.041	0.032	0.067	4.6e-14
Peak_shaving_investments	5.6e-06	0.0027	0.0044	0.045	0.16	0.034
Zero_gap_investments	1.1e-05	0.13	0.28	0.15	0.28	0.97

Figure 18: Feature score of decision space of the chlor-alkali industry

Desired output space exploration

The computational experiments of the DPE models of the salt and chlor-alkali industries both span the output space which encompasses direct and indirect emissions and information about the financial attractiveness of a technological investment (NPV, IRR, investment costs).

By isolating the subspace in the output space that contains all desirable combinations of outcomes and studying this subspace, it is possible to identify uncertainty and decision subspaces that map to the desired outcome subspace.

The 'filtered' outcome space contains all cases in which the salt and chlor-alkali industries meet their respective restrictions on direct emissions as stipulated by the Emissions Trading System. According to the ETS, CO_2 emissions must be reduced by 1.74% annually until 2021; whereupon the CO_2 emissions of involved companies must be reduced by 2.2% annually. Thus, the maximum level of direct CO_2 emissions of the salt manufacturing industry in 2030 is 475 kilotons per year, compared to 550 kilotons per year in 2016. Similarly, the chlor-alkali industry must reduce its carbon dioxide emissions from 186 kilotons in 2016 to 167 kilotons in 2030. The ETS also applies to the Dutch power generation companies. As such, their reduced emissions are also accounted for in the projections of the NEOMS and in the CO_2 intensities of the generation of electricity from the grid. This means that when exploring the desired output spaces, the total change from the industries under investigation must also be negative and must decrease at a rate proportional to the overall reduction in direct emissions. Thus, the total emissions change of the salt manufacturing industry is restricted as being a reduction of at least 66 kilotons in 2030; for the chlor-alkali industry, the total emission reduction must be at least 105 kilotons.

Lastly, for the scope of this investigation the desired output spaces to consider also must present positive business cases for the companies involved. Thus, the output space is further partitioned to only include the investments where the internal rate of return and the net present value of investments are greater than zero.

The output spaces spanned by these restrictions are shown in Figure 19 and Figure 20. The restrictions imposed on the output spaces are marked in purple along the axes of the parallel axis plot. Furthermore, the 'base case' scenario, if no policies are implemented and the uncertainties follow baseline conditions (see Table 18) is shown in orange. The visualization of the output space data along a parallel axis plot allows to view the different trade-offs that occur, and can provide useful insights to stakeholders involved in the decision-making process of the research at hands. It also allows the decision makers to see what is likely to happen if no decision is made.

In Figure 19, is interesting to note that almost in all explored output spaces for the salt manufacturing industry, the level of indirect emissions increases substantially. In the partitioned output space, the indirect emissions of the salt industry will have increased by an average of 200 kilotons in 2030 compared to the indirect emissions in 2016. Nonetheless, due to substantial reductions in the direct emission levels, the total emission change remains negative. This poses a clear compromise for policymakers and industry representatives alike; by investing in the electrification of heat (re-)generation processes (MVR and electric boilers), the salt industry's indirect emissions increase. Furthermore, it makes the salt industry far more dependent on electricity price fluctuations. Nonetheless, the partitioned output space covers a relatively large proportion of the total output space; the partitioned space covers 21% of the 48,000 experiment runs, or a total of 9,851 combinations of outputs in the output space.

The partitioned output space for the chlor-alkali industry in Figure 20 covers an even larger proportion; of the 108,000 model runs, 32% (or 34,640 runs) are covered by the partitioned subspace. In this subspace, one can see that the capital investments are relatively high, but that they generate positive internal rates of return. By inspecting this figure, one can see that the dominant trade-off for policy makers and industry stakeholders in decarbonizing this industry is the high investment costs that the industry is likely to face, and whether the involved companies are prepared to make such high capital investments for the returns they will gain from it.

From both Figure 19 and Figure 20, it can also be seen that if no new alternative technology investments are made, and no policies are applied by the government, the salt manufacturing industry as well as the chlor-alkali industry are unlikely to reach the emission levels required by the Emissions Trading System. This observation underscores the necessity for the various stakeholders involved in these industries to reach agreement on their respective approaches to achieving considerable emission reductions.

Having identified partitions output spaces that are more desirable than others, further inspection can be conducted on the distribution of the decision space that maps to this partition. As such, robust strategies to decarbonize these industries can be uncovered.

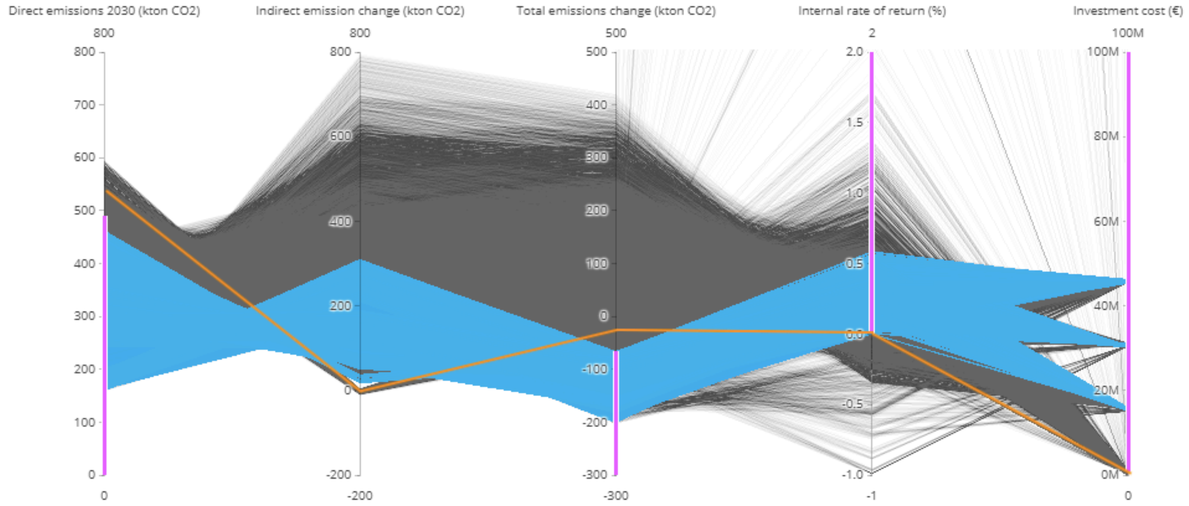


Figure 19: Parallel axis plot showing the desired output space as a partition of the total output space for salt industry (restrictions on axes are marked in purple, base case scenario without policies is shown in orange)

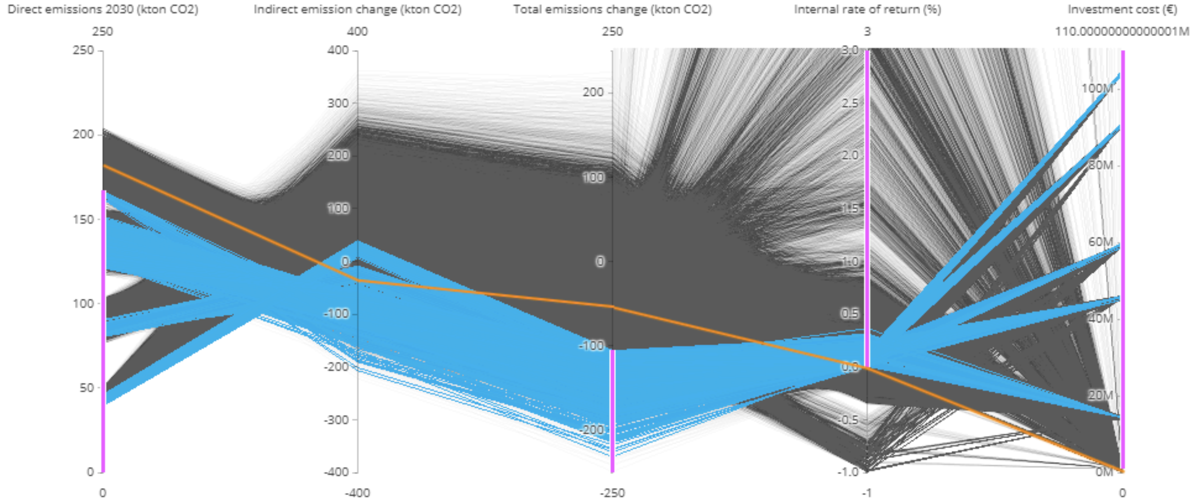


Figure 20: Parallel axis plot showing the desired output space as a partition of the total output space for chlor-alkali industry (restrictions on axes are marked in purple, base case scenario without policies is shown in orange)

Robust policy and investment strategy exploration

Figure 21 and Figure 22 show dimensional stacks of the partitioned subspace. These dimensional stacks allow for the exploration of robust policy and investment strategies when examining how the salt and chlor-alkali industries can be decarbonized.

In Figure 21, it can be observed that the most robust strategies for the decarbonization of the salt industry involve a combination of policies and investments. Shutting down the coal-fired power plants forms an absolute boundary condition, but when combined with a 25% gas tax and investments in predominantly mechanic vapor recompressors, the salt industry is likely to experience reductions in its carbon dioxide emissions. Extra small investments in electric boilers further aid the transition, as the dimensional stack shows that only investing in MVR without investing in electric boilers is generally insufficient.

Similarly, an inspection of Figure 22 that shows how the decision space in the chlor-alkali industry maps to the partitioned desirable output subspace, one sees that the shutdown of the coal-fired power plants considerably aids the decarbonization of the industry. The extent to which a gas tax is necessary for decarbonization is less clear than in Figure 21, but it is clear too that this policy certainly helps. Lastly, it is clear that the investment in electric boilers certainly aids the decarbonization of the chlor-alkali industry. Nonetheless, only investing in boilers will cause a significant increase in indirect emissions, which can be compensated by also investing zero-gap technology. Thus, just as with the salt manufacturing industry, a combination of different technology investments in parallel supplemented by policies to further support decarbonization pathways is the most robust strategy to decarbonize the chlor-alkali industry.

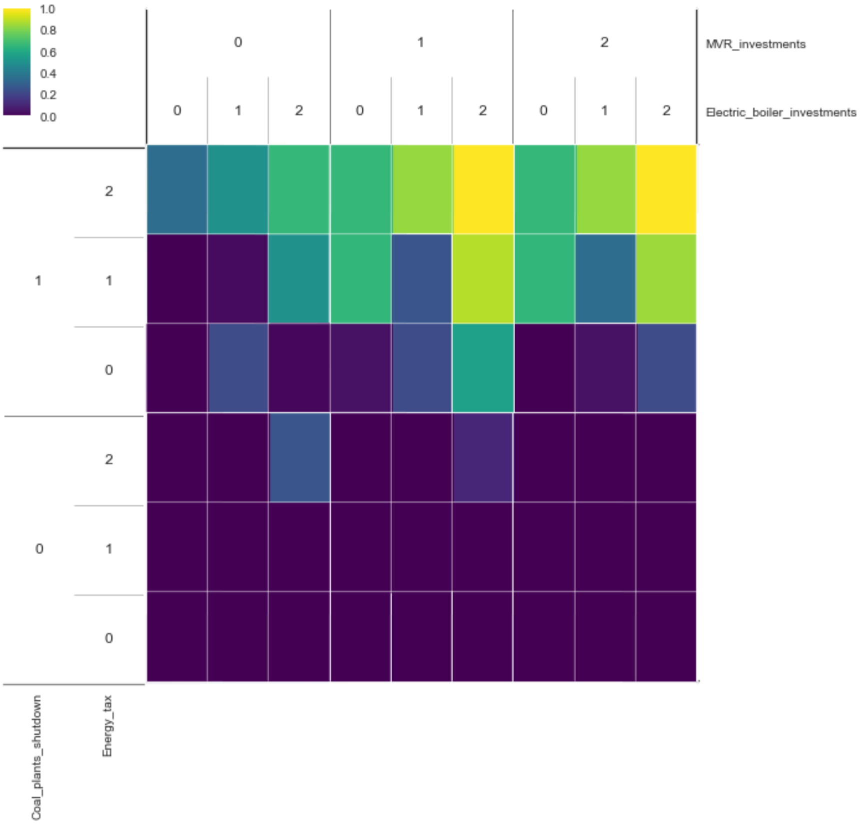


Figure 21: Dimensional stack of decision space on a desirable partition the of outcome space for the salt industry

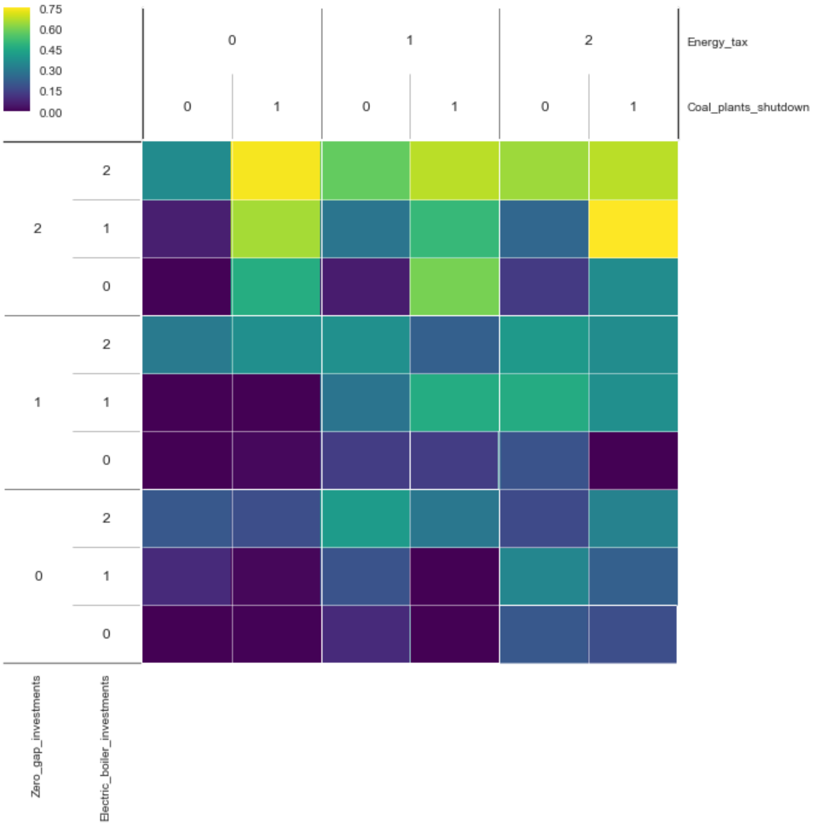


Figure 22: Dimensional stack of decision space on a desirable partition the of outcome space for the chlor-alkali industry

Chapter 8: Discussion

In this chapter, the results of Chapter 7 will be discussed and synthesized with findings from Chapters 3 and 4, whereupon the implications of the research are outlined for the salt and chlor-alkali manufacturing industries. As a result of the way in which the models were conceptualized, and the way in which the model experiments were carried out, there are limitations to the outcomes and to the extent to which they apply. These too will be addressed in this chapter.

8.1 Implications for the salt manufacturing industry

In order to identify robust strategies through which the salt manufacturing industry can be decarbonized, the industry was studied in depth in Chapter 3, conceptualized into a model in Chapter 5 and analyzed in Chapter 7. By means of a thorough analysis of the different processes at play and the various technologies implemented across the four salt production plants in the Netherlands, two alternative technologies were identified that can support decarbonization efforts of the salt manufacturing industry; the implementation of electric boilers to generate steam, and the implementation of mechanic vapor recompressors to vaporize the brine. These two alternative technologies, together with the full scope of the 'current' processes (reference year: 2016) at play in the salt industry, were conceptualized into a model aimed at evaluating and exploring the financial feasibility and extent to which the industry can reduce its CO_2 emissions.

The various salt production plants together need to reduce their emissions by at least 75 kilotons by 2030 in order to meet the emission reductions stipulated by the ETS. Furthermore, this step towards decarbonization is only deemed desirable if it causes net emission reductions when accounting for indirect emissions, as well as if the technology investments form a positive business case for the industries involved. In order to explore opportunities for decarbonization, 48,000 model experiments were run, whereupon approximately 10,000 desired output spaces were identified and analyzed.

The empirical research in Chapter 3, as well as the analysis in Chapter 7 showed that the large-scale implementation of mechanic vapor recompressors across the salt manufacturing industry is both a financially feasible and effective way to reduce direct emissions. The analysis shows that by 2030, the implementation of 2 to 4 mechanic vapor recompressors (see Table 8) across the industry can help to lower CO_2 emissions by more than 75 kilotons by 2030. When taking a closer look at what this means for the individual plants under study, it requires serious investments on behalf of AkzoNobel in its two salt manufacturing plants. The Dutch salt manufacturing industry's two heaviest polluting plants, AkzoNobel Hengelo and AkzoNobel Delfzijl, already have a small pilot MVR facility each, but will require an extra investment of 15 to 30 million euros in this technology by 2030 to reduce their direct emission levels. Despite these relatively high investment costs, the business case for these investments is positive, as the experiment results indicate strongly positive net present values and internal rates of return on these investments.

Furthermore, the research indicates that the investment in MVR technology alone will not suffice. The implementation of mechanic vapor recompressors significantly reduces the steam demand on a plant level. This can cause the deployment of CHP plants for steam generation to become financially unfavorable, and as such the deployment of industrial electric boilers is deemed a preferred parallel investment. The results from Chapter 7 indicate that the investment in electric boilers alone does not create positive business cases for the salt industry, but that the investment in electric boilers together with the implementation of MVR does. The deployment of MVR technology alone without the deployment of electric boilers is technically and financially unrealistic, as large CHP plants need to produce large amounts of steam to remain feasible under the Dutch market conditions of relatively high gas prices and low electricity prices. Thus, the experimental results indicate that the installation of approximately 50 to 100 industrial electric boilers (see Table 7) across the plants where MVR technology is deployed are a necessary extra investment to replace steam generation from closed down CHP facilities.

Although the above results are in accordance with more general findings of larger studies of the Dutch chemical industry (Krebbekx et al., 2015; VNCI, 2018), these salt industry-specific findings have some limitations. The model deployed to investigate the effect of the investments in the two technologies does not formally account for the closing down of a specific CHP facility involved in the salt manufacturing industry. This is due to the fact that plant-specific data was aggregated together to gain an industry-wide perspective (see section 5.1.2). Thus, the model does not make a specific assumption of where the technologies themselves will be implemented. Nonetheless, based on the plant-specific knowledge gained in Chapter 3, it is evident the technological investments in the salt manufacturing industry will need to be done in Hengelo and Delfzijl, as elucidated above. The results of this exploration therefore give an indication of how the salt industry can reduce its CO_2 emissions in a financially feasible manner, but they do not make suggestions for where the specific technologies should be implemented. Thus, these results can be used as a first exploration of robust strategies for decarbonization, but cannot be used as a manual for stakeholders involved in the salt manufacturing industry to decarbonize specific plants.

Another reservation on the above findings is that the experiment results do not account for the reliability of the deployed technologies. AkzoNobel has deployed two pilot MVR facilities across its two salt production plants, but has been struggling with malfunctions since its implementation in 2017 (Klein & Ybema, 2018). The model simply assumes that MVR technology will be ready for large-scale deployment in the salt industry as of 2020, and simulates the effects on emission reductions for the year that it is simulated to be implemented in. The reliability of the technology however, is a factor that influences the financial attractiveness of a technology, as well as the resulting emission reductions. When the MVR facility malfunctions, the plant will revert to multiple effect vacuum evaporation, which is dependent on considerably larger amounts of steam. These backward and forward chain effects are kept outside the scope of this research, as the deployed model essentially simulates the integral replacement of one technology by another. The fact that the salt manufacturing industry can only be decarbonized by the implementation of MVR technology however, underscores the urgency of the need for increased technology reliability.

As a whole, the identified technological investments imply a gradual electrification of heat generation processes across the salt manufacturing industry by 2030. Where this electrification can reduce gas consumption by approximately 3.2 to 5.4 PJ per year, electricity consumption can rise by 1.9 to 4.0 PJ per year. This electrification also causes the involved salt production plants to become increasingly dependent on electricity as an energy carrier, while reducing their dependence on natural gas. The exploratory results from Chapter 7 indicate that, under the current national predictions of the Dutch electricity system, the indirect emissions of the salt manufacturing industry are likely to increase considerably as a result of this electrification. Depending on the extent of MVR and electric boiler deployment, and the different scenarios of the CO_2 intensity of the Dutch power system, the indirect emissions are projected to increase by approximately 50 to 300 kilotons per year. This broad bandwidth of projected indirect emissions is a reminder of the high uncertainty the system faces in undergoing decarbonization efforts, but is also a reminder of the limitations of the methods used to conceptualize this transition.

Since this research is focused on identifying strategies to reduce the salt industry's direct emissions, the projected indirect emissions provide relatively rough indications. Thus, in considering strategies for the decarbonization of the salt manufacturing industry, it is important to keep in mind that the electrification of heat generation processes can also inhibit net total emission reductions. Increased certainty on the future of the Dutch electricity supply can strongly influence the extent to which it is attractive to electrify heat generation processes. This, however, is beyond the scope of this research. The results from this investigation simply indicate that the reduction of the CO_2 intensity of power supply is a boundary condition for the decarbonization of the salt industry. The way in which this reduced CO_2 intensity can be achieved is up to electricity generation companies, net operators and government regulators.

For the salt manufacturing industry as a whole, the challenge ahead is complex and difficult to tackle. By gaining insight into the different processes at play in the industry, along with obtaining a more thorough understanding of technological developments and the impact they can have on the industry as a whole, the mechanisms to tackle this challenge become apparent for policymakers and industry stakeholders alike. This research is aimed at providing a contribution to the identification of these mechanisms.

8.2 Implications for the chlor-alkali manufacturing industry

Robust decarbonization strategies of the chlor-alkali industry were identified in this research by studying the industry in Chapter 4, conceptualizing it into a model in Chapter 5, and by performing experiments and analysis with the conceptual model of the industry in Chapter 7. The extensive study of the different processes deployed in the three chlor-alkali plants across the Netherlands, as well as the evaluation of the various technologies implemented across these processes with industry stakeholders, resulted in a series of promising alternative technologies that can support decarbonization efforts in the chlor-alkali industry. The placement of electric and biomass boilers to reduce the industry's direct emissions, and peak-shaving technology as well as zero-gap membrane electrolyzers to tackle the industry's electricity consumption, and thus its indirect emissions. A model was conceptualized that allowed for the exploration of the effects of the implementation of these four alternative technologies on financial and emission-related performance indicators.

Under the conceptualized model, the Dutch chlor-alkali industry 'base case' (in 2016) consumes 2.8 PJ of gas resulting in approximately 180 kilotons of CO_2 emissions, while using almost 7 PJ of electricity resulting in roughly 1,500 kilotons of indirect CO_2 emissions. From this conceptualization, it becomes apparent that the real challenge in decarbonizing the chlor-alkali industry does not lay in its reduction of direct emissions, but more in lowering its indirect emissions. The three chlor-alkali plants in the Netherlands together must reduce their direct emissions by approximately 15 to 20 kilotons by 2030 according to the ETS, while no explicit regulations exist for their indirect emissions. Based on expert elicitation, this research defined a minimum net emission reduction (direct and indirect together) of approximately 110 kilotons of CO_2 per year in 2030. Furthermore, the feasibility of investments in alternative technologies was investigated. In this research, feasible and consistent strategies for the reduction of direct as well as indirect emissions are explored based on these indicators, by identifying approximately 35,000 desirable output spaces in a total of 108,000 model experiment runs.

Based on the empirical research in Chapter 4, as well as the model experimentation and analysis in Chapter 7, the large-scale implementation of zero-gap membrane electrolyzers is a pivotal technology that can aid to reduce the net emissions of the chlor-alkali industry. Across the current chlor-alkali industry, only 10 zero-gap membrane electrolyzers are installed in AkzoNobel's plant in Botlek. Based on estimates from this research, the implementation of approximately 30 more zero-gap membrane electrolyzers across AkzoNobel's plants in Botlek and Delfzijl, as well as Sabic's plant in Bergen-op-Zoom, can aid to reduce the chlor-alkali's electricity consumption by 0.7 to 1.2 PJ per year by 2030. This measure will require a considerable investment of approximately 85 to 100 million euros before 2030, which is only financially feasible when electricity prices are considerably reduced. Moreover, it will require the replacement of finite-gap membrane electrolyzers, which have been installed across the Dutch chlor-alkali industry in the early 2000s, which may require the premature writing off of previous capital expenditures for the chlor-alkali producers. However, this significant reduction in electricity demand does not only support decarbonization efforts of the industry, it makes the Dutch chlor-alkali industry more competitive in the European landscape, and can lead to greater future profits. The total reduced yearly indirect emissions based on this technological investment is estimated between 85 and 120 kilotons of CO_2.

Nonetheless, investments in zero-gap technology do not contribute to lowering the direct emissions of the industry. Based on this research, the small-scale implementation of biomass boilers as well as electric boilers can support Sabic and AkzoNobel meet the thresholds for direct emission reductions stipulated by the ETS. Nevertheless, this research shows that if significant improvements are made in the internal efficiency of the chlor-alkali production chain, the necessary investments in electrifying steam generation are relatively minor; an investment of €150,000 in electric boilers can already reduce the direct emissions by more than 20 kilotons of CO_2 per year by 2030.

Despite the concrete indications for the decarbonization of the chlor-alkali industry, there are a series of limitations to these findings that are important to consider. As was addressed in Sections 6.3.4 and 8.1, the focus of this investigation lay in the reduction of the salt-chlor-alkali production chain's direct emissions. However, as this research has shown, the key to decarbonizing the chlor-alkali chain lies in efficiency improvements in its power consumption. As a consequence, the effect of power consumption reduction measures on indirect CO_2 emissions in a chlor-alkali plant is subject to large uncertainty in this investigation. Chlor-alkali industry stakeholders play a minor role in the way in which power is generated in the Netherlands, and therefore they have little control over how the CO_2 intensity of power consumption evolves over time. Since the effectiveness of the decarbonization of the chlor-alkali industry largely depends on the implementation of zero-gap electrolyzers, by extent it depends on the future of the CO_2 intensity of power generation in the Netherlands. Thus, this research underscores the necessity for clear country-wide arrangements and agreements about the future of the Dutch electricity market. The research therefore cannot make concrete conclusions about whether or not the implementation of zero-gap electrolyzers will indeed lead to a net reduction of CO_2 emissions, it can only indicate that the implementation of these electrolyzers can considerably reduce the electricity consumption of the chlor-alkali industry.

Furthermore, the empirical research of the chlor-alkali industry showed that industry stakeholders of AkzoNobel are already investing in the increase of their production capacity in order to deploy peak-shaving technology. By late 2021, the construction of a second chlor-alkali plant in Botlek will be finalized which makes use of this technology. This is an investment that is primarily aimed at reducing the costs of production of chlorine, caustic soda and hydrogen as the technology makes use of the imbalance energy market by increasing production levels when electricity prices are low and decreasing production levels when electricity prices are high. From this research, it is unclear how this can affect the indirect emissions of the chlor-alkali industry. Further research is needed to adequately conceptualize how this development will affect the future of the Ducth chlor-alkali industry.

Another limitation of this research is the fact it does not account for the marginal reduction in technology investment costs over time. Although the results give upper and lower bounds for the investment costs in different technologies, the model assumes an integral replacement of current technologies by alternative technologies, and therefore cannot account for lower investment costs over time. It may prove valuable to critically compare the results of this investigation to other studies of investments in the Dutch chemical industry, where S-shaped curves are used to model technology adoption and costs (VNCI, 2018; Den Ouden et al., 2017).

Despite the attractiveness of investments in zero-gap electrolyzers, a side effect of the implementation of this technology is that less residual heat is produced during the electrolysis process. With the finite-gap electrolyzers, the residual heat is used to heat the brine and caustic soda to desired levels. Lowering the residual heat generated by electrolysis may lead to an increase in steam demand on a plant level, which can cause an increase in direct emissions when the on-site CHP is utilized to meet this demand. Although this shift in heat demand is quantified and studied within the boundaries of this investigation, this is subject to high uncertainty and more plant specific information is required to adequately model these chain effects. Since this research focusses on the effects of the industry as a whole, the precise plant-level implications cannot be determined.

The direct emissions of the chlor-alkali industry are almost all attributed to the steam generation process needed for vaporization of caustic soda. Based on findings in the empirical research, this study has focused on the implementation of sustainable alternatives for heat generation. Nonetheless, based on the expert elicitation conducted in this research, these sustainable alternatives may be less desirable in a transition to zero net emissions beyond 2030. Beyond 2030, the salt-chlor-alkali production chain is likely to become more dependent on hydrogen-based steam generation and geothermal steam generation. Therefore, industry stakeholders must be wary of the lock-in risks involved with implementing electric boilers to meet short-term emission goals while undermining longer term full decarbonization strategies. This aspect, however, is beyond the scope of this research but is a strong limitation on the findings of strategies to reduce the chlor-alkali industry’s direct emissions.

Additionally, as was discussed in Section 4.2.2, another aspect that could considerably reduce the direct emissions of caustic soda production is if the demand for high concentration caustic soda were to change to lower concentration caustic soda. However, this can only be achieved by developments in other industries, and therefore is not studied within the scope of this research. Nonetheless, in the light of MIDDEN and the study of chain effects of material flows across the entire Dutch industrial sector, this is an important aspect to monitor in future research.

By thoroughly studying the chlor-alkali industry on a process level, and through the discussions of technological developments with a large range of industry stakeholders, the key technologies that can aid to enable an energy transition in the chlor-alkali industry were identified. Despite the future of Dutch chlor-alkali industry facing a complex palette of opportunities and risks for decarbonization, this investigation has shown that the most robust way forward is to focus on the large-scale implementation of zero-gap electrolyzers. The small-scale implementation of sustainable heat generation facilities can allow the chlor-alkali plants to fulfill emission demands stipulated by the ETS, but may prove to be a disadvantageous investment in the run-up to full decarbonization by 2050. The extent to which the indirect emissions of the chlor-alkali can be reduced by 2030 is predominantly dependent on the carbon intensity of power generation in the Netherlands, and not in the hands of the chlor-alkali industry stakeholders.

8.3 An energy transition under deep uncertainty in the salt-chlor-alkali chain

This research has shown that although the salt and chlor-alkali manufacturing industries have very different carbon intensities, their transition to a more sustainable future is subject to similar uncertainties. Due to the interwovenness of the two industries, it was possible to identify key uncertainties and policies that affect the decarbonization of the salt-chlor-alkali production chain as a whole.

The research has shown that for both industries, the key uncertainty from the perspective of industry stakeholders is the way in which energy carrier prices develop. As was discussed in Chapter 7, the attractiveness of investments in alternative technologies is predominantly defined by the price scenarios. Thus, for policy makers and industry stakeholders alike, increased transparency on planned investments and envisaged energy policy can ensure that the involved stakeholders support each other's efforts to decarbonizing this production chain. The Dutch economy which is stooled upon the principle of consensus-based decision-making, gives room for such an approach. The data gathered and analyzed in light of MIDDEN is aimed at increasing this transparency, and allows for a quantitative technical discussion between industry stakeholders, researchers and decision-makers from government about the future of the salt-chlor-alkali production chain.

In Chapter 7, it was also shown that of all the uncertainties faced by the two industries under investigation, their respective production levels themselves have a strong impact on emission levels. A projected increase in chlorine capacity caused by the construction of a second chlor-alkali plant in Botlek in 2021 (Verbraeken, 2018b), may therefore lead to an increase in salt production upstream, which subsequently causes a further increase in emission levels. As this research shows, it is therefore of high importance that policy makers and industry stakeholders together are aware of such chain effects, in order to account for these changes in planning strategies to decarbonize the industry.

This chain effect is also reflected in this research's observation that the abolishing of chlorine transport in the Netherlands has caused the carbon intensity of the salt industry to increase. Prior to 2000, chlor-alkali production occurred on the same location as where salt was solution-mined (in Hengelo and Delfzijl), but due to changes in regulations and due to the locations at which chlorine is further used in the industrial sector, the solution-mined brine nowadays is vaporized to salt, whereupon it is transported, only to be remixed with diluted water to form brine again for electrolysis. This example of unwanted effects of path-dependency stresses the importance of open and thorough discussions between the industrial sector and the Dutch government to formulate tailored solutions for the decarbonization of the respective manufacturing chains.

In order to study how policymakers can facilitate the transition to a more carbon-neutral salt-chlor-alkali production chain, this research looked at how stronger taxation of gas prices and the reduction of carbon intensity of the electricity sector can aid to achieve these goals. In Chapter 7, the experimentation and analysis of the two conceptual models of the salt and chlor-alkali industries showed that decarbonization of the industries can only be attained if the carbon intensity of electricity generation is considerably reduced. Furthermore, it showed that a gas tax mostly supported the electrification of heat generation processes in the salt manufacturing industry. The decision space analysis shows that, in order to attain desired output spaces of feasible decarbonization strategies, the carbon intensity of power generation in the Netherlands should reduce from 120 tons of CO_2 per terajoule to approximately 30 to 60 tons per terajoule between 2016 and 2030. This carbon intensity bandwidth lies within the most optimistic projections of the used scenarios of the National Energy Outlook (see Section 5.2.1 and Appendix D), which are based on the closing down of all Dutch coal-fired power stations, the growth of gas-fired electricity imports, and the rapid deployment of sustainable electricity generation technologies (Schoots et al., 2017).

These more general research observations come with strong reservations. In Chapter 6, the extent to which these scenarios of the carbon intensity of power generation can be applied to the industries was evaluated and analyzed. Especially when considering the fact that the chlor-alkali manufacturing industry is gearing up to increased flexibilization – the effects of which are not studied in this research – it is difficult to project what the future of indirect emissions in the salt-chlor-alkali chain entails. A larger and more thorough approach which incorporates the way in which the electricity system evolves is necessary to make concrete policy recommendations about the reduction of indirect emissions in the energy intensive chemical sector.

Moreover, every model is by definition a simplified version of reality. Although the central production processes and technologies at play in the seven salt and chlor-alkali manufacturing plants were conceptualized, verified and tested, the way in which the salt-chlor-alkali production chain works in reality is subject to far more uncertainties than those that could be captured within the scope of this investigation. Manufacturing plants are run, managed and improved over time by a complex network of industry stakeholders, factory workers, researchers, corporate managers, shareholders and even private equity funds, and the decisions of each affect the way in which the industry as a whole evolves over time. This investigation captures only a glimpse of the direction in which the salt-chlor-alkali chain is evolving over time. Nevertheless, the deployed model shines light on the way in which the implementation of the investigated alternative technologies can be steered by policymakers, as well as the effects this can have on the production chain's emission levels.

Exploring the opportunities and threats to an energy transition in the salt-chlor-alkali production chain with the use of the EMA workbench (Kwakkel, 2017) proved to be both a complex as well as fruitful research strategy. By running large amounts of model experiments, the range of plausible futures could be explored in an unbiased manner, allowing to uncover the key dynamics of the modeled system. Nonetheless, due to the complexity of a manufacturing plant's internal production chain, the explorative nature of this investigation is at times difficult to rhyme with the industry-level observations this research makes. The modeling technique however is very suitable for the identification of robust strategies to decarbonize an industry, and further deployment of exploratory modeling and analysis in the field of energy transition planning can help to uncover the key aspects to focus on for the stakeholders involved.

Deep uncertainty is a notion that has only been discussed in scientific literature since the early 21st century (Lempert et al., 2003; Agusdinata, 2008; Hamarat et al., 2013), yet it is an aspect central in the long and ongoing energy and climate debate. By conceptualizing and studying the key relations, uncertainties and decision levers at play in a system, exploratory modeling and analysis can support decision making over a deeply uncertain future. The key deep uncertainty in the scope of this investigation is the structure of the future energy supply. By analyzing the relations between the decision space and the range of possible futures in this investigation, policy- and technology-related strategies were uncovered that provide a robust pathway to decarbonizing the salt-chlor-alkali production chain.

8.4 Directions for future research

Research is often said to lead to more questions than answers. Although the findings of this research lead to new insights on the energy transition for the Dutch salt-chlor-alkali production chain, it is valuable to reflect on its limitations and on the new directions the findings lead to.

The clear frame of this research implies that it sheds the light on only one of many pieces of the puzzle of the energy transition in the Dutch industrial sector. To obtain a complete understanding of the necessary decarbonization measures in a specific industry, one must also gain a complete understanding of the Dutch industrial sector as a whole. Research similar to this research on other specific chains in industry may provide further and complementary insights to how the energy transition can be shaped.

Furthermore, by focusing on industries closely related to the salt-chlor-alkali chain, other chain effects can be investigated. For example, a study of the Dutch plastics manufacturing industry can prove to be beneficial to understanding the effect of environmental policies aimed at reducing the production of PVC on the Dutch chlor-alkali industry. Furthermore, in the light of AkzoNobel's ambitions to become a leader in hydrogen production, the integration of that industry with the salt-chlor-alkali chain can prove interesting and fruitful to further analyze in the light of an energy transition in industry.

Another aspect important to further analyze in the light of this research is the technologies that lie on the horizon for the salt and chlor-alkali industries. A series of these technologies were identified and discussed in Sections 3.2.2 and 4.2.2. Nonetheless, these technologies were not further conceptualized for the MIDDEN database, as they were deemed out of scope for this research. These technologies will, however, become of vital importance for an energy transition to a fully carbon-neutral industry in 2050. Thus, further research into these technologies and the extent to which they can support full decarbonization ambitions is of high interest.

This investigation sheds light on the key uncertainties and decision levers that affect the decarbonization of the salt and chlor-alkali industries. However, this investigation does not investigate the interaction between the decision levers and uncertainties. A more elaborate investigation which also looks at this interaction may prove valuable to further uncover robust strategies for decarbonization of the salt-chlor-alkali production chain.

Lastly, this research deployed exploratory modeling and analysis techniques for a specific industry and for the implementation of specific processes. Although the EMA workbench proved to be valuable for the purpose of this research, it may be of even higher value when a system is studied on a higher level of aggregation. Since the workbench offers decision-support under deep uncertainty, studies that conceptualize the Dutch energy system and the Dutch industrial sector as a whole could possibly benefit even more from the use of the EMA workbench.

Chapter 9: Conclusion

Throughout this research, an inventory was made of the processes, products and plants involved in the salt and chlor-alkali manufacturing industries. Furthermore, an analysis is conducted of the landscape of the salt-chlor-alkali production chain and key driving forces are identified. The inventory was subsequently processed into a modular database that enabled the conceptualization of the industries into a model. A series of computational experiments were conducted with these models in order to explore the way in which the identified uncertainty and decision spaces influence the way in which the salt and chlor-alkali industries can be decarbonized. Having analyzed and discussed the results, this research returns to the research question:

What are robust strategies to decarbonize the Dutch salt and chlor-alkali manufacturing industries in light of a deeply uncertain energy transition, analyzed until 2030?

The inventorization, conceptualization, experimentation and analysis of the salt and chlor-alkali industries helped to understand the opportunities and threats to decarbonizing the production chain and uncovered insights for key stakeholders. The findings of this investigation further underscore the multi-actor nature of the research problem; robust strategies for decarbonization of the salt-chlor-alkali production chain only exist when industry actors and policymakers both act and cooperate.

In the salt manufacturing industry, the key opportunity lies in the electrification of its heat processes by means of the implementation of mechanic vapor recompression technology, in combination with the adoption of electric boilers. For the chlor-alkali industry, the key opportunity before 2030 is the large-scale implementation of zero-gap membrane electrolyzers to reduce electricity consumption. Where the measures in the first industry can significantly contribute to direct emission reductions, the measures in the second can only aid to reduce indirect emissions. Under these conditions, the total abated yearly emissions in the salt-chlor-alkali chain as a whole can range between 150 and 400 kilotons of carbon dioxide and will require chain-wide investments ranging between 100 million and 150 million euros. Although the industries themselves are in control of the technologies they invest in to meet the thresholds stipulated by the ETS, a considerable part of the speed at which the salt-chlor-alkali chain can be decarbonized is affected by external factors.

This research shows that robust strategies for the decarbonization of the salt-chlor-alkali production chain cannot be formulated by the industry alone. Without the support of the government, the involved industry stakeholders from AkzoNobel, Sabic, Frisia Zout and NedMag often will not be able to formulate positive business cases to invest in the necessary technologies. Furthermore, even if business cases are positive, they may actually result in net increases of CO_2 emissions under certain scenarios. As such, the research reveals that policymakers are instrumental in decarbonizing the this production chain. Policymakers have significant power to influence the financial attractiveness of these alternative technologies through the taxation of gas prices. Furthermore, since the alternative technologies generally imply a higher electricity demand, the question of whether or not the two industries can be decarbonized at all directly depends on the carbon intensity of the Dutch power grid. Although the way in which the Dutch power supply can be decarbonized is not studied in this investigation, the research shows that the carbon intensity should be reduced from approximately 120 tons of CO_2 per terajoule to approximately 30 to 60 tons per terajoule between 2016 and 2030. This research thus emphasizes the importance of lowering the carbon intensity of the Dutch power grid, but further research is necessary in order to provide policymakers with concrete advice on how they can attain this.

To conclude, in identifying robust strategies to decarbonize the salt-chlor-alkali production chain, it is important to keep an overview of the entire energy system, while incorporating the necessary specific plant- and technology-level knowledge about the manufacturing processes involved to account for effects within the chain. The development of the Dutch energy system as a whole, and most notably the electricity sector, strongly defines the way in which the electrification of heat processes in the salt industry, and the implementation of zero-gap technology in the chlor-alkali industry can benefit decarbonization efforts. This research can therefore be used as an explorative inventory of the challenges and opportunities faced by both industry stakeholders as well as policymakers involved in the planning of this energy transition. Only through open, sustained and coordinated efforts by both policymakers and industry stakeholders, can a coherent vision be formulated on how to decarbonize the industrial sector.

Chapter 10: Reflection

10.1 Scientific relevance

While conducting this research, scientific knowledge and pragmatic expertise were synthesized and combined to conceptualize the salt-chlor-alkali production chain. This was achieved through a series of scientific structures, calculation frameworks, open-ended interviews with stakeholders and iterative modeling techniques. Together, these approaches resulted in a clear and concise methodology to conceptualize and analyze an industry from the bottom up as well as from the top down. The value of the approaches adopted in this research will be reflected upon in the following paragraphs.

This investigation's conceptual framework (see Figure 3), which combined the scientific frameworks of Bartel et al. (2007) and Bradfield et al. (2005) into the technological transition paradigm of Geels and Kemp (2002) proved useful for the purpose of this research. The plant-process-product analysis by Bartel et al. (2007) allowed the author to structure the precise industrial engineering aspects of this research. In doing so, the author was able to gain specific knowledge about thermodynamical and chemical processes, to obtain an understanding of how the salt and chlor-alkali industries work from the bottom up. The more qualitative STEEP framework (Bradfield et al., 2005; Szigeti et al., 2011) allowed the author to identify the key driving forces at play in the salt-chlor-alkali production chain as a whole, and analyze the industry from the top down. The combination of these bottom-up and top-down approaches enabled not only to gain a multi-actor perspective of the research problem, it helped to uncover the key uncertainties and decision levers relevant to the system under study. The synthesis of findings allowed for a clear and thorough overview of the salt-chlor-alkali chain, and for the conceptualization and analysis of decarbonization strategies on the meso-level.

This conceptual framework can be of value to researchers conducting an industry analysis. When used together, the plant-process-product framework and the STEEP framework, lend themselves for the analysis of technological transitions across any industry. As such, this conceptual framework may not only prove valuable to the research client and MIDDEN, but also to other researchers conducting industry analyses. In the current scientific literature, no standardized methodology for conceptualizing an industry exists. This research contributes to existing scientific literature in that it proposes a more standardized approach through the conceptual framework deployed. The framework used in this research has already been adopted by other researchers currently involved with other industry researches the MIDDEN knowledge network. Since this investigation served as a pilot project to MIDDEN, and this framework has proved useful for the purpose of this investigation, new MIDDEN studies may further expand on this conceptual framework.

Furthermore, this research may also prove relevant to other scientific studies of the salt-chlor-alkali production chain. The institutions in the Netherlands are similar within other European countries, and as such this research may be of interest to similar studies elsewhere. The normalized process overviews (Figure 8 and Figure 11) give a clear and standardized overview of how the salt manufacturing process and the chlor-alkali manufacturing process can be conceptualized as a whole. Furthermore, the aggregation techniques used to define a more simplified overview for the MIDDEN dataset can be of use to other researchers involved in the analysis of specific industries.

To identify robust strategies for decarbonization, the conceptualized industries were analyzed under a relatively new decision-support paradigm, known as ‘decision-making under deep uncertainty’ (Agusdinata, 2008; Kwakkel et al., 2016). The key idea deployed within this paradigm was that of exploratory modeling. The use of the Exploratory Modeling workbench (Kwakkel, 2017) and the use of an open exploration approach proved to be of great value to identify robust strategies for decarbonization, as the search and sample over the uncertainty and decision space allowed the author to uncover the key mechanisms that lead to desired output spaces. Thus, the EMA workbench was of great value for the purpose of this research and may prove to be of use to other exploratory studies aimed at identifying robust decarbonization strategies.

10.2 Societal relevance

This research is conducted while the national discussion about climate policy and the sustainability of Dutch energy system is at a new high. With the development of the Dutch Climate Agreement of 2018, where stakeholders involved in different sectors are collaborating and discussing how emission reductions can best be achieved on a national level, the societal relevance of this investigation is clearly apparent. The parties involved at the Dutch ‘Industry Table’ are to publish the first main lines of the Climate Agreement in July of 2018. Next, it is up to the government and the House of Representatives to appoint directional choices based on research findings and political interests. Subsequently, the involved parties can collaborate and negotiate to formulate concrete and binding agreements. This research aims to enlighten stakeholders about strategies to decarbonize the salt-chlor-alkali industry and enable a constructive discussion about the Dutch energy transition as a whole. Although the scope of this research is too specific for discussions about an energy transition in the Dutch industrial sector as a whole, it can provide useful insights to others studying the system at a higher level of aggregation.

This research is the first complete industry investigation in the light of the MIDDEN knowledge network and was conducted as a pilot project to help structure and give shape to the MIDDEN database that is to be built in the years to come. Together with energy specialists from PBL and ECN, the way in which the MIDDEN database is constructed for the salt and chlor-alkali industries was evaluated, and the value of the collected data was assessed in the light of further model-based analysis. Thus, this research forms a preliminary attempt to show what can be done with the data collected for the MIDDEN knowledge network.

On a broader level, this research touches upon the key challenges faced in planning an energy transition as a whole. What are the consequences for society if a transition in energy usage is too slow? What are the consequences for society if the Dutch industry is no longer internationally competitive as a result of stringent emission reduction policies? Who is to carry the (financial) burden of an energy transition in the industrial sector? How can the future of energy usage be shaped with ever-growing populations and ever-increasing demands from society? The societal interest in answers to these ostensibly rhetorical questions has been increasing rapidly over the past few years as the effects of anthropogenic environmental impact are unmistakable.

10.3 Research process evaluation

Independently conducting scientific research, writing two extensive reports on industries unfamiliar to me, collaborating with a large range of industry stakeholders, while interning full-time at the national government’s energy advice agency proved to be a great but inspiring challenge to me personally. I especially enjoyed learning about how complex and seemingly insurmountable trade-offs faced by decision-makers involved in the planning of an energy transition can be tackled and challenged. Furthermore, I enjoyed working at PBL at a time where the climate discussions were at an all-time high. It was truly energizing to see the Dutch so-called “polder model” – a consultative economy with consensus-based decision-making – in progress in the months on the PBL work floor. I was inspired to see how people with different insights, motives and objectives all collaborate and work together to try to achieve a higher-order common goal.

Throughout the course of my Masters, it had always been my ambition to write a thesis about a concrete, socially relevant problem. I sincerely and humbly hope that this research, as well as my involvement in the set-up of the MIDDEN knowledge exchange network, can contribute to the planning and shaping of an energy transition in the Dutch industry.

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Appendices

Appendix A: Explanation salt manufacturing sub-processes

A.1: Solution mining

Salt solution mining is defined as the mining of various salts by dissolving them in freshwater and pumping the resulting brine to the surface. The saturated raw brine that results from the salt solution mining process has a salinity of approximately 310 g/L, which corresponds to about ten times the salinity of seawater. In the solution mining industry, a general rule is that between 7 and 8 m^3 of freshwater pumped into a cavity dissolves approximately 1 m^3 of halite.

In order to reach the underground salt layers, one or several boreholes are created at the surface. A single access hole is drilled, whereby water is pumped down at high pressure (approximately 1.7 MPa) (Strucker, 1994) to form a small cylindrical cavity underground filled with brine. The access to this cavity (also named cavern) may subsequently be increased by multiple drillings from the ground hole. Along these drillings, three concentric tubes allow for the freshwater to be pumped in, a liquid blanket to be pumped in and out, and for the brine to be pumped out.

Two types of solution mining techniques can be distinguished; ‘direct circulation’ (by bottom injection) and ‘reverse circulation’ (by top injection). In general, cavern development is initiated with direct circulation, whereupon after the cavern has the adequate shape, the circulation is switched to indirect circulation. With both methods, insoluble rocks gradually collect at the bottom of the cavern.

In both cases, the outermost casing of the tubing allows for a ‘blanket fluid’ to be pumped in and out of the cavern. This fluid blanket is less dense than the freshwater (1000 g/L) and brine (1200 g/L), and as such ‘floats’ on top of the other solutions. The halite cannot dissolve in this blanket fluid, and thus this layer protects the top of the cavern from dissolving. It is possible to control the shape of the cavity that is being formed by increasing and decreasing the volume of blanket fluid in the cavern. In the Netherlands, diesel (800 g/L) is often used as blanket fluid.

In the Netherlands, the solution mining process occurs at a large range of depths, depending on the salt production plant. Table 24 gives an overview of depth ranges of the different concessions active in 2018.

Table 24: Depth ranges of salt solution mining for currently active concessions

Rock salt extraction licenses:		***Depth range (m)***	***Salt layer name***
P1	*Adolf van Nassau II*	*700-1600*	*Strassfurt formation (Z2)*
P2	*Uitbreiding Adolf van Nassau II*	*700-1600*	*Strassfurt formation (Z2)*
P5	*Barradeel*	*2250-3000*	*Strassfurt formation (Z2)*
P6	*Barradeel II*	*2250-3000*	*Strassfurt formation (Z2)*
P10	*Twenthe-Rijn*	*350-500*	*Röt formation*
P11	*Uitbreiding Twenthe-Rijn*	*350-500*	*Röt formation*
P12	*Twenthe-Rijn Helmerzijde*	*350-500*	*Röt formation*
P14	*Veendam*	*1300-1800*	*Leine formation (Z3)*

The processes at play at these different depths are outlined below.

Shallow rock salt extraction (350-500m)

At the Hengelo drilling site under the Twenthe-Rijn extraction license, brine is extracted from two types of caverns. In the older type of the two, the cavern is developed through three boreholes, each 40 meters apart. In the other cavern, the brine is extracted from one single central tubing system.

The Röt formation in which this process occurs is subdivided into four salt types; from top to bottom salt A, B, C and D. Between each layer lay thin dolomitic clay bricks. The raw brine production process takes place mainly in salt A and B, and occasionally in salt C. As can be seen from this, the development of all salt extraction was started at the bottom or the salt formation. As soon as the initial cavity has been developed, production of raw brine is conducted by means of solution mining, by leaching the cavity in both horizontal and vertical direction.

The caverns that are created under the Twenthe-Rijn extraction area form small cylinders of diameter 100-120 m and a height of approximately 25-30 m. Above each cavern, a 'safety roof' of rock salt of sufficient thickness remains. This safety roof prevents the cavern from collapsing under its own weight, and thus prevents sinkhole formation at ground level. Future salt extraction will continue higher up above this safety roof.

Since the start of production in 1936 at the Hengelo concession more than 450 drillings have been made in the area and more than 75 million tons of salt have been produced, which amounts to about successfully excavated 130 caverns.

Medium depth rock salt extraction (600-1600m)

The Winschoten and Zuidwending drilling sites, that fall under the extraction licenses of Adolf van Nassau and Uitbreiding van Adolf van Nassau respectively have salt caverns that fall under the medium depth salt extraction category. All twelve caverns at Winschoten and nine caverns in Zuidwending were created with a single borehole.

For the Winschoten concession the cavern roofs are at depths of 700-750 m and have a height of approximately 550-630 m. For the Zuidwending concession, these depths and heights are 450-500 m and 800-850 m respectively. The caverns have a diameter of up to 125 m and are 250 m apart in a hexagonal grid. The total production since the start of production in 1954 (Winschoten) and 1967 (Zuidwending) more of 90 million tons. This amounts to about 10 successfully excavated caverns.

The soil subsidence at the ground level due to volume convergence - the resulting decrease in the volume of a cavern due to the creep of the salt - amounts to 1 to 2 mm per year. The total, cumulative subsidence since the start of the extraction, for example in Zuidwending, is approx. 4 cm in the center of the soil subsidence basin.

Deep rock salt extraction (2250-3000m)

The deepest solution mine in the world are supervised under the extraction licenses of Barradeel and Barradeel II. Concessions built under these licenses deliver raw brine to the salt factory in Harlingen. Two caverns have been developed under Barradeel, and two more have been developed under Barradeel II. Salt extraction at Barradeel is slowly coming to an end.

The top 30 m of the Strassfurt formation (Z2) contains carnallite deposits, which are soluble in water. To prevent the contamination of the brine, an oil blanket is used. The rock temperature in the vicinity of these caverns is approximately 105°C. As a result, 'salt creep' occurs at a high rate. This is a process where the raw brine crystallizes on the edge of the tubing and top of the cavity, which may clog the system. This effect is further enhanced by a pressure difference of 28 MPa between brine pressure in the cavern (hydrostatic pressure 34 MPa) and the locally prevailing lithostatic pressure (rock pressure

62 MPa). The high temperature does not affect the solubility of the rock salt but has a high effect on its dissolution rate.

In the rock salt layers that are located closer to the Earth's surface, it usually takes one to two years before a sufficiently large cavity has developed to produce saturated brine. At this depth, the saturated brine can be extracted from the deep caverns within a few months. For deep extraction, the high pressure from the rock layers above, cause the rock caverns to stop increasing beyond a certain equilibrium (at a volume of approximately 400,000 m^3); the volume increase of the cavern from dissolving salt is compensated by the volume decrease due to volume convergence of the cavern . This can directly be observed at ground level; an extraction of 230,000 m^3 of halite leads to a sinkhole of approximately 4-5 cm per year at ground level. Since the total permissible soil subsidence is limited to 35 cm, there is a limit to the amount of salt that can be extracted from a cavern. This is why the production of caverns is coming to a halt in Barradeel.

The NedMag solution mining facility near Veendam in the Netherlands produces magnesium from magnesium chloride brine by solution mining a Zechstein salt dome, targeting beds that are a mixture of carnallite ($KCl\cdot MgCl_2\cdot 6H_2O$), bischofite ($MgCl_2\cdot 6H_2O$) and halite ($NaCl$), with some sylvite ($KCl$) and kieserite ($MgSO_4\cdot H_2O$). Target intervals at Veendam average 100 m (combined) thickness at depths, dipping around 20°, at depths between 1,400 and 1,800 m. About a 100 m of halite lies above the target magnesium salts and more than 1,400 m occur below. In 2010, NedMag excavated one of the deepest solution mining cavities in the world at 2,890 m. Each year the NedMag plant produces in excess of 200,000 tonnes of high purity synthetic dead-burned magnesia and more than 70,000 tonnes of magnesium chloride in liquid or solid form. The four wells producing MgCl-brine from "squeeze caverns" at Veendam are almost saturated with respect to bischofite, rendering a high-quality brine product with less than 1 % by weight of non-magnesium chloride salts. In 2012, NedMag has started using a patented process to produce brines that are also saturated with respect to carnallite from carnallitic beds previously considered sub-economic.

A.2 Brine purification

At the salt production facilities, large pumps suck the brine out of the underground caverns, through pipelines over the ground to the brine purification facility.

Impurities from salt dissolved in brine are precipitated with chemicals and removed by various processes. The raw brine that was formed underground generally contains very few impurities. Table 25 shows the weight percentages of all solvents in raw brine that was produced from solution mining.

Table 25: Weight percentages of solvents in raw brine

Percentage of solvent	Solution-mined salt
NaCl %	25.0
Ca^{2+} %	0.118
Mg^{2+}%	0.011
SO_4^{2-} %	0.284
Insoluble %	-

Calcium is removed using soda, obtained by the carbonation of the diaphragm base with carbon dioxide from the gases escaping from a combined heat and power (CHP) plant. Magnesium is removed with a diaphragm base – a diluted lye solution (sodium hydroxide $NaOH$) in kitchen salt. Sulphates can be removed with barium carbonate, barium chloride or calcium sulphate. The different precipitation processes are explained below:

The precipitation of calcium, magnesium and sulfate from brine is described by the following chemical reactions:

Calcium precipitation $Ca^{2+} + Na_2CO_3 = CaCO_3 + 2\ Na^+$
Molar mass 40 108 100

This chemical reaction shows that each 40 kg of calcium impurity entering the chlor-alkali process with salt requires 108 kg of soda ash for precipitation and formation of 100 kg of calcium carbonate.

Magnesium precipitation $Mg^{2+} + 2\ NaOH = Mg(OH)_2 + 2\ Na^+$
Molar mass 24 82 58

This chemical reaction shows that each 24 kg of magnesium impurity entering the chlor-alkali process with salt requires 82 kg of sodium hydroxide for precipitation and formation of 58 kg of magnesium hydroxide.

Sulphate precipitation with BaCO3 $SO_4^{2-} + BaCO_3 = BaSO_4 + CO_3^{2-}$
Molar mass 96 197 233

Sulphate precipitation with BaCl2 $SO_4^{2-} + BaCl_2 = BaSO_4 + 2\ Cl^-$
Molar mass 96 208 233

Sulphate precipitation with CaCl2 $SO_4^{2-} + CaCl_2 = Ca\ SO_4 + 2\ Cl^-$
Molar mass 96 111 136

These chemical reactions show that each 96 kg of sulfate impurity entering the chlor-alkali process with salt requires either 197 kg of barium carbonate or 208 kg of barium chloride or 111 kg of calcium chloride for precipitation and formation of either 233 kg of barium sulfate or 136 kg of calcium sulfate. Upon purification, the brine is pumped through to the vacuum evaporation facility.

The cost associated with brine purification is the cost of chemical reagents and the investment and operating cost of the brine treatment plants. The cost of contaminated sludge disposal, purge decontamination and the loss of salt in purge also represent substantial costs.

Table 26: Overview of impurity, reactant, precipitate and products involved in brine purification

Impurity				Reactant			Precipitate			Product
Formula	**Percentage in brine**	**Molar mass (g/mol)**	**Mass/1L brine (g)**	**Formula**	**Molar mass (g/mol)**	**Mass/1000L brine (g)**	**Formula**	**Molar mass (g/mol)**	**Mass/1000L brine (g)**	**Formula**
CaCl2	0.00118	40	1.416	Na2CO3	108	3823.2	CaCO3	100	3540	NaCl
MgCl2	0.00011	24	0.132	2NaOH	82	902	Mg(OH)2	58	319	2NaCl
Na2SO4	0.00284	96	3.408	BaCO3	197	6993.5	BaSO4	233	8271.5	Na2CO3
Na2SO4	0.00284	96	3.408	BaCl2	208	7384	BaSO4	233	8271.5	2NaCl
Na2SO4	0.00284	96	3.408	CaCl2	111	3940.5	CaSO4	136	4828	2NaCl

A.3 Vaporization of water

The brine is pumped into large vacuum pans. These pans are closed metal cylinders with conical bottoms. They are often arranged in a series of three, with each one in line under a greater vacuum than the preceding pan. The vacuum pans operate on a simple principle: the boiling temperature of water decreases when the pressure is lowered. Furthermore, the resulting steam in the first pan is used to heat the second pan, and so on. Vacuum pans may operate as low as 35°C.

In the vacuum evaporation process, steam is fed to the first pan, causing the brine in the pan to boil the steam from the boiling brine is used to heat the second pan. Since the pressure in the second pan is lower, the steam made by boiling the brine first pan allows the brine in the second to boil too. The pressure is lowered in each subsequent pan. This allows the steam made by boiling the brine in the previous pan to boil the brine in the next. More pans in a row allow for greater energy efficiency as less steam needs to be produced in the first place to cause the brine in the first pan to boil.

Steam from a power plant at a pressure of 3.3 bar and temperature of 150°C heats the brine to its boiling point via a heat exchanger (2 bar, 120°C), such that the dissolved salt crystallizes. As the brine boils, salt crystals begin to form and sink to the bottom of the evaporator. This produces a thick mixture of salt crystals and salt solution, called a slurry, which is fed into another evaporator to repeat the process and concentrate the salt further. In subsequent steps, lower pressure and temperature are deployed; 0.9 bar and 95°C, 0.3 bar and 70°C, 0.1 bar and 50°C.

Optionally, a concentrator is located between the last evaporator and the condenser. This extra evaporator will evaporate the brine that is not completely saturated to the point of saturation. The evaporator uses the vapor originating from the last evaporator of the vacuum evaporation facility (temperature approximately 50°C). The resulting slurry that formed in the evaporators is pumped to the centrifuges where the remaining water is removed. At the installation in Hengelo there are two evaporation installations consisting of four evaporators. An overview of the vacuum evaporation process is shown in Figure 23.

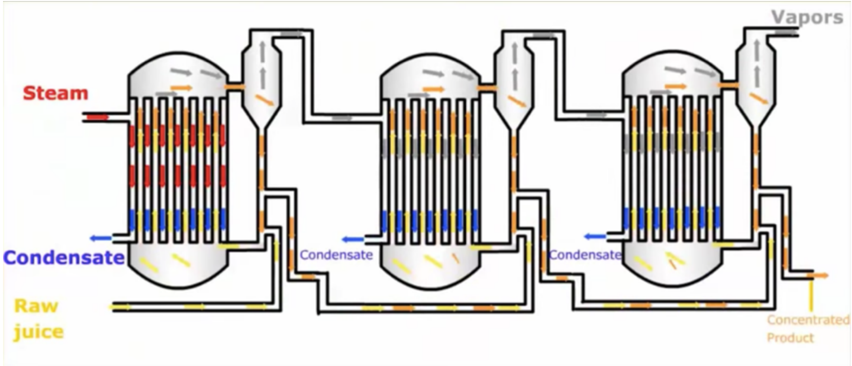

Figure 23: Triple effect vacuum evaporator

A.4 Brine centrifugation

The slurry that leaves the vacuum evaporation facility is transported on to large salt centrifuges. In these centrifuges, the salt is finally separated and stored in a large storage shed. The separated fluid, known as the mother liquor, is transported back to the brine purification facility. In the centrifuges, the salt slurry is stripped of the last moisture that is still in the salt. The salt that remains, contains about 2% moisture and is ready for industrial use.

It is possible that a certain amount of salt does not meet the production and environmental requirements. In the case of production errors earlier in the production chain, the salt will no longer meet the quality requirements, in which case this salt is considered unsuitable for further processing. This salt still meets the environmental requirements for road salt and can be used as a road salt.

A.5 Drying and sifting process

A separate compartment ensures the drying of salt beyond the moisture level of 2% after which it is suitable for packaging in special products for consumers and industry. The remaining amount is stripped of residual water to a humidity level of about 0.1–0.15%.

Appendix B: Explanation chlor-alkali manufacturing sub-processes

B.1: Brine preparation

The brine preparation process contains two separate salt sources, each of which are prepared in a different way. The membrane electrolysis process allows for the recirculation of depleted brine from the electrolysis cells, and thus a central aspect of the brine preparation is the treatment of depleted brine. Secondly, newly supplied salt must also be dissolved to re-saturate the brine that is fed back into the electrolytic cell. This second aspect includes the supply and dissolution of salt, and treatment of the brine.

Brine saturation

The salt that is supplied to the chlorine production plants in the Netherlands originates from solution-mined, vacuum evaporated dry salt, which contains small traces of water (2 wt%).

For the different chlorine production facilities, the salt is delivered in different ways. For the chlor-alkali production facility at Botlek, and the vacuum salt is transported by ship from Hengelo. Similarly for the Sabic chlorine plant in Bergen-op-Zoom, the salt is produced off-site and is transported to the production facility. Lastly, the chlor-alkali production plant in Delfzijl uses salt that was solution mined by AkzoNobel in an on-site production plant. The dry salt is subsequently diluted with dilution water and with depleted brine that is returned after electrolysis and dechlorination.

Brine treatment

The salt that is supplied to the chlorine production plants in the Netherlands originates from solution-mined, vacuum evaporated salt and has extremely high purity; the dry basis of the vacuum salt contains 99.95% NaCl. An overview of the vacuum salt quality is given in Table 27.

Table 27: Vacuum salt quality

Contents	Mass fraction (ppm)	Weight percentage (wt%)
Dry basis		***98%***
NaCl		97.951%
Sulphates	400.00	0.0392%
Calcium	12.00	0.00118%
Magnesium	1.00	0.000098%
Iron	1.00	0.000098%
Copper	0.04	0.00000392%
Insolubles	50.00	0.00490%
Wet basis		***2%***
Water		2%

For the membrane cells that are used in the electrolysis, water hardness (the amount of magnesium and calcium dissolved in the brine) must be below 20 parts per billion (ppb). Specially designed resins enable ion exchange to reduce the water hardness. These resins require periodic regeneration with caustic soda (NaOH) and hydrochloric acid (HCl), which, in turn produces wastes.

This resin technology enables the membranes in the electrolytic cells to have a useful life of 4 years (Brinkmann et al., 2014). Over that period, the calcium and magnesium will be precipitating on the membranes, but this occurs very gradually and results in a gradual decline in the efficiency of the cell as well as an increase in the power consumed by the cell. The required purity level will depend on the operating current density of the electrolytic cell. The ion exchange resin is periodically regenerated with HCl and NaOH. The pH going into the ion exchange is typically measured to avoid damaging the resins.

Brine heating
After the ion exchangers, the brine is transferred to storage tanks to be pumped into the cell room. The pure brine is heated to the necessary temperature of approximately 90°C (temperatures vary per production plant between 80°C and 90°C).

Brine dechlorination
Brine exiting the cell room must be treated to remove residual chlorine and control pH levels before being returned to the saturation stage. This can be accomplished via dechlorination towers with acid and sodium bisulfite addition. Failure to remove chlorine can result in damage to the ion exchange units (see 3.2.2). Brine should be monitored for accumulation of both chlorate anions and sulfate anions, and either have a treatment system in place, or purging of the brine loop to maintain safe levels, since chlorate anions can diffuse through the membranes and contaminate the caustic, while sulfate anions can damage the anode surface coating.

For the membrane cell technique, complete dechlorination is achieved by passing the brine by using chemical reducing agents such as sulfite. Residual levels were reported to be < 0.5 mg/l or below the detection limit (Euro Chlor, 2011) and < 0.1 mg/l (Dibble and White, 1988).

Chemical reducing agents such as sulfur dioxide (SO_2), sodium sulfide (Na_2S), sodium sulfite (Na_2SO_3), sodium thiosulphate ($Na_2S_2O_3$) or hydrogen peroxide (H_2O_2) are used to destroy the free chlorine in the brine. The chlorine or hypochlorite is reduced to chloride (Cl^-). The choice of the chemical reducing agent is influenced by cost, availability, and ease of handling. Depending on the reducing agent, the following reactions take place (BREF, 2014).

Sulfur dioxide:	$SO_2 + NaOCl + 2\ NaOH \rightarrow Na_2SO_4 + NaCl + H_2O$
Sodium sulphide:	$Na_2S + NaOCl + H_2O \rightarrow S + NaCl + 2\ NaOH$
Sodium sulphite:	$Na_2SO_3 + NaOCl \rightarrow Na_2SO_4 + NaCl$
Sodium thiosulphate:	$2\ Na_2S_2O_3 + NaOCl + H_2O \rightarrow Na_2S_4O_6 + NaCl + 2\ NaOH$
Hydrogen peroxide:	$H_2O_2 + NaOCl \rightarrow O_2 + NaCl + H_2O$

Chemical reducing agents have the advantage of also reacting with chloramines and bromamines. Sufficient residence time and an excess of reducing agents are required to ensure the complete destruction of free chlorine (Dutch Ministry 1998). In order to control the heat of the exothermic reaction, diluted solutions are used to limit the temperature to about 50 °C. For example, to reduce 1 kg of chlorine absorbed, 4.45 kg of reactive agent $Na_2S_2O_3$ or 89 kg of diluted 5 wt-% solution are required (Le Chlore 2002).

B.2: Membrane electrolysis

General description
Chlorine, hydrogen and caustic soda are obtained by the electrolysis of brine. All three products are highly reactive, and the membrane electrolysis technology has been developed to separate these different products and keep them apart.

This technology has several key advantages as opposed to mercury and diaphragm electrolysis methods deployed in other European countries: the process costs less energy per unit of product than mercury and diaphragm electrolysis; the caustic soda produced is very pure; no environmentally harmful substances such as mercury and asbestos are used (Struker, 1995).

The electrolytic cell consists of two chambers – a cathode chamber and an anode chamber – separated by a cation-exchange membrane. This membrane is permeable to positive ions such as H^+ and Na^+, but not to the negative ions such as Cl^- and OH^-. The membrane is impermeable to water, which is why saturated brine (23wt%) is continuously fed into the membrane anode cell while the depleted brine after electrolysis (17wt%) is drained. Conversely, at the cathode cell, lower concentration aqueous sodium hydroxide (30wt%) is fed into the system than is drained back out (33wt%).

In the two electrolytic cells, different reactions occur, which each have an influence on the production process.

At the anode, chloride ions are oxidized, losing electrons and becoming chlorine gas:

$$2\,Cl^- \rightarrow Cl_{2(g)} + 2\,e^-$$

At the cathode, positive hydrogen ions pulled from water molecules are reduced by the electrons provided by the electrolytic current, to hydrogen gas, releasing hydroxide ions into the solution:

$$2\,H_2O + 2\,e^- \rightarrow H_2 + 2\,OH^-$$

The ion-permeable ion exchange membrane at the center of the cell allows the sodium ions (Na+) to pass to the second chamber where they react with the hydroxide ions to produce caustic soda (NaOH). The overall reaction of the membrane electrolysis process, depicted in Figure 2, can thus be described with the following equation:

$$2\,NaCl + 2\,H_2O \rightarrow 2\,NaOH_{(aq)} + H_{2(g)} + Cl_{2(g)}$$

Aside from the above reactions, some side reactions occur during electrolysis, which lead to efficiency losses. At the anode, water is oxidized to oxygen and hypochlorous acid is oxidized to chlorate.

$$2\,H_2O \rightarrow O_2 + 4\,H^+ + 4\,e^- \qquad \text{and/or} \qquad 4\,OH^- \rightarrow O_2 + 2\,H_2O + 4\,e^-$$

$$12\,HClO + 6\,H_2O \rightarrow 4\,ClO_3^- + 8\,Cl^- + 24\,H^+ + 3\,O_2 + 12\,e^-$$

Hypochlorous acid is formed by disproportionation (dismutation) of chlorine in water:

$$Cl_2 + H_2O \rightleftharpoons HClO + H^+ + Cl^-$$

Chlorate is also produced by chemical reactions in the anolyte:

$$2\,HClO + ClO^- \rightarrow ClO_3^- + 2\,Cl^- + 2\,H^+$$

These four major side reactions are repressed by lowering the pH value. The pH value is usually lowered by acidifying the brine with hydrochloric acid to pH < 6. This does not only reduce the formation of oxygen, hypochlorite and chlorate, but also increases the lifetime of the anode coating.

Because of the corrosive nature of chlorine production, the anode must be made from a non-reactive metal such as titanium (commonly RuO_2, IrO_2 and TiO_2 coating on a Ti substrate), whereas the cathode can be made from a more easily oxidized metal such as nickel (commonly nickel coated with noble metal-based coatings).

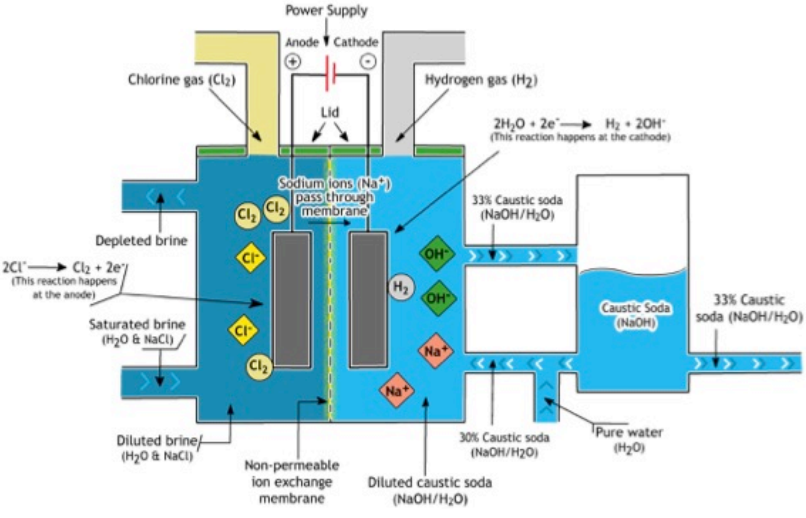

Figure 24: Overview of membrane electrolysis sub-process

The membrane electrolysis generally operates at high temperature to keep its electrical conductivity high and with the right electrolyte concentrations to achieve a desirable rate of osmotic water transport and maintain the right equilibrium water content in the polymer. Table 2 gives typical operating conditions according to O'Brien et al. (2007) and Brinkmann et al. (2014).

The temperatures of the feed caustic and brine are monitored and controlled throughout the electrolysis process. Pressure control valves control the pressures in the chlorine and hydrogen headers. The production rate is controlled by changing the voltage of each cell throughout the process.

Table 28: Membrane electrolysis operating conditions

Parameter	Allowable range	Typical value
Feed brine concentration	270–305 gpl	300gpl
Exit brine concentration	190–230 gpl	200gpl
Feed brine pH	< 11.6 at 23°C	
Exit brine pH	>2	2–4
Feed NaOH concentration	28–32% (w/w)	30%
Exit NaOH concentration	30–33% (w/w)	32%
Exit caustic temperature	80–90°C	87°C
Exit brine temperature	80–90°C	87°C
Differential pressure	5–30mbar	20mbar
Current density	1.5–6.0 kA m^{-2}	
Cell voltage	2.35–4.00 V	

B.3: Chlorine processing

Full processing of chlorine gas takes a hot, wet vapor at approximately atmospheric pressure and converts it to a cold, dry liquid under significant positive pressure. The common processing steps therefore are cooling, drying, compression, and liquefaction. The severity of the two latter processes depends on the desired degree of recovery of chlorine as the liquid and on the composition of the gas produced in the cells.

From chlorine processing, 200 kg of condensed water per tonne of chlorine cooled from 90 °C to 25 °C are typically recycled (EuroChlor, 2011). The output chlorine has approximately the following impurities: oxygen (0.5–2.0 vol-%), hydrogen (0.03–0.3 vol-%).
Cooling is accomplished in either one stage with chilled water or in two stages with chilled water only in the second stage. The chlorine can be cooled indirectly, directly or through a combination of both. The indirect method causes less chlorine to be condensed or absorbed and generates less chlorine-saturated water for disposal. For the direct cooling method, water is sprayed into the top and flows countercurrent to the chlorine. This treatment thoroughly washes the chlorine; however, dechlorination of the wastewater consumes a large amount of energy. This direct method has the advantage of better mass transfer characteristics and higher thermal efficiencies (BREF, 2014). In closed-circuit cooling, the advantages of both methods are combined. To avoid solid chlorine hydrate formation, the gas is not cooled below 10°C. Maintaining temperatures above 15 °C prevents blockages in the process equipment (Ullmann, 2006).

Chlorine after cooling is still too wet for processing in ferrous-metal equipment. Chlorine from the cooling system is more or less saturated with water vapour. There still is 1–3 vol-% of water in the chlorine, which must be reduced to avoid corrosion and to minimize the formation of hydrates. The chlorine drying is conducted with concentrated sulfuric acid (96 – 98 wt %), and the moisture level is reduced to less than 20 mg/m^3.

The dried chlorine gas is usually compressed before use. The level of compression depends on the application. A large fraction of the world's output of chlorine is consumed on site. The production of ethylene dichloride (EDC) is the single largest-volume use. The dry gas supply pressure then is determined by the needs of the EDC process.

Some of the compressed gas is also liquefied with an electric compressor. An increase in liquefaction pressure equates with an increase in energy costs of chlorine compression. Nonetheless, this results in an overall reduction in energy requirement. To achieve a liquefaction pressure of 0.8 MPa, at room temperature conditions, the electrical energy requirement for the liquefaction of 1 ton of chlorine gas is 42 kWh/t (Ullman, 2015).

B.4: Caustic soda processing

Upon the electrolysis process, the caustic soda (32 wt%) needs to be concentrated to a 50wt% to meet market demands. Concentration is normally achieved in two or three stages using multiple effect evaporators. The number of stages depends on factors such as plant size and the cost of steam. The caustic soda from membrane cells is of high quality, although the caustic soda produced (Ullman, 2015). Caustic solutions require steam or electrical heating where temperatures can fall below the freezing point. Depending on the concentration, the freezing point can be higher than 0 °C; for example it is 5°C for 32 wt-% NaOH and 12°C for 50 wt-% NaOH.

B.5: Hydrogen processing

Hydrogen leaving the cells is highly concentrated (> 99.9 vol-%) and normally cooled to remove water vapor, sodium hydroxide and salt. The solution of condensed salt water and sodium hydroxide is recycled to produce caustic, as brine make-up or is treated with other waste water streams (EuroChlor, 2011). From hydrogen processing, 50–100 kg of condensed water per ton of chlorine produced are typically recycled, depending on the cooling intensity (EuroChlor, 2011). The cooling is usually carried out by one or more large heat exchangers. Some uses of hydrogen require additional removal of traces of oxygen, which may be achieved by reacting the oxygen with some of the hydrogen over a platinum catalyst.

The hydrogen sold to distributors is usually compressed at pressures higher than 100 bar and is injected into a pipeline network. Otherwise, the hydrogen is transported in dedicated tank lorries or in steel bottles at pressures of up to 300 bar. For these high pressures, the gas is further dried and traces of oxygen are usually removed (EuroChlor, 2010). The main utilizations of the co-produced hydrogen are combustion to produce steam (and some electricity) and chemical reactions such as the production of ammonia, hydrogen peroxide, hydrochloric acid and methanol (EuroChlor, 2010). The cooling of hydrogen is usually carried out by one or more large heat exchangers. Electrolytic hydrogen is quite pure and is acceptable for most applications. Hydrogen frequently is cooled by direct contact with brine. This is a simple matter of heat economization.

The extent of hydrogen compression depends on the application. Much of the hydrogen is used as fuel or as raw material for the production of HCl. For this, only modest pressures are required, within the capability of simple rotary blowers. In the membrane-cell process, it is sometimes possible to operate the cells under positive pressure and eliminate the need for a blower. Other applications require higher pressure and the installation of compressors. The synthesis of ammonia is an example. Operating pressures range up to 30,000 kPa. Less frequently, hydrogen is compressed to high pressure and packaged in cylinders. For high-grade chemical applications, oxygen and traces of chlorine may also be removed.

Appendix C: Data inputs for MIDDEN database

The data inputs for the MIDDEN database are too large to show here. These can be found on https://github.com/edzardscherpbier/Thesis-Edzard/tree/master/MIDDEN-modeling/Data inputs

An overview of the necessary inputs for the different datasets is given below.

MIDDEN data inputs for the Plant dataset	
Plant name	Postal code
Year	Town/locality
Subsector (SBI 2008)	Permit number (NEa)
Corporate group	Name of production site (NEa)
Number of employees	Verification
Number of employees; UNIT	ETS emissions 2015 [ton]
Street address	ETS emissions 2016 [ton]

MIDDEN data inputs for the Technology characteristics dataset	
Process name	Other input 2 (per unit of main output)
Year	Other input 2 (per unit of main output); COMMODITY
Process description	Other input 2 (per unit of main output); UNIT
Process type	Other input 3 (per unit of main output)
Main output	Other input 3 (per unit of main output); COMMODITY
Unit of main output	Other input 3 (per unit of main output); UNIT
Unit of capacity	Other input 4 (per unit of main output)
Investment per unit of capacity (new)	Other input 4 (per unit of main output); COMMODITY
Investment per unit of capacity (new); UNIT	Other input 4 (per unit of main output); UNIT
Investment per unit of capacity (refurbishment)	Output Steam (GJ per unit of main output)
Investment per unit of capacity (refurbishment); UNIT	Output Electricity (GJ per unit of main output)
Operating and maintenance costs (per unit of main output)	Output Waste heat (<50 C) (GJ per unit of main output)
Operating and maintenance costs (per unit of main output); UNIT	Other output 1 (per unit of main output)
Operating and maintenance costs (per unit of capacity)	Other output 1 (per unit of main output); COMMODITY
Operating and maintenance costs (per unit of capacity); UNIT	Other output 1 (per unit of main output); UNIT
Balance of other costs and benefits (per unit of main output)	Other output 2 (per unit of main output)
Balance of other costs and benefits (per unit of main output); UNIT	Other output 2 (per unit of main output); COMMODITY
Balance of other costs and benefits (per unit of capacity)	Other output 2 (per unit of main output); UNIT
Balance of other costs and benefits (per unit of capacity); UNIT	Other output 3 (per unit of main output)
Refurbishment interval in years	Other output 3 (per unit of main output); COMMODITY
Input Natural gas (GJ per unit of main output)	Other output 3 (per unit of main output); UNIT
Input Biofuel (GJ per unit of main output)	Other output 4 (per unit of main output)
Input Steam (GJ per unit of main output)	Other output 4 (per unit of main output); COMMODITY
Input Electricity (GJ per unit of main output)	Other output 4 (per unit of main output);
Input H2 (GJ per unit of main output)	Requirements
Other input 1 (per unit of main output)	Demand/production profile
Other input 1 (per unit of main output); COMMODITY	Feasibility
Other input 1 (per unit of main output); UNIT	Verification

MIDDEN data inputs for the Commodity data dataset	
Commodity name	Market price; UPPER LIMIT
Year	Market price; UNIT
Market price	Verification
Market price; LOWER LIMIT	

Appendix D: National Energy Outlook pricing scenarios

Figure 25: Used scenarios from the National Energy Outlook

Appendix E: Python code

Full documentation can be found on GitHub:
https://github.com/edzardscherpbier/Thesis-Edzard/tree/master/MIDDEN-modeling

D.1: Code used for open exploration of salt manufacturing industry DPE model

```
# coding: utf-8

# # MIDDEN Salt Model - Open Exploration
#
# ## Model initialization

# In[1]:

from __future__ import (division, print_function, absolute_import, unicode_literals)
from ema_workbench import (RealParameter, IntegerParameter, TimeSeriesOutcome, ScalarOutcome,
                           ema_logging, perform_experiments, save_results, load_results)
from ema_workbench.connectors.excel import ExcelModel
from ema_workbench.em_framework import (salib_samplers, samplers, util,
                                        MultiprocessingEvaluator, SequentialEvaluator)
from ema_workbench.analysis import prim
from ema_workbench import ema_logging
ema_logging.log_to_stderr(ema_logging.INFO)

import numpy.lib.recfunctions as rf
import numpy as np
import matplotlib.pyplot as plt
import mpld3
import pandas as pd


# In[2]:

ema_logging.log_to_stderr(level=ema_logging.INFO)

model = ExcelModel("excelmodel", wd="./Models", model_file='MIDDEN Decarbonization options salt
final.xlsx')

#name of the sheet
model.sheet = "Experiment"

# Specification of the uncertainties
model.uncertainties = [IntegerParameter("Price_scenario", 1, 3),
                       RealParameter("Discount_rate", 0.0075, 0.05),
                       RealParameter("Production_uncertainty", 0.85, 1.15),
                       RealParameter("Efficiency_gain", 0.0015, 0.0075)
                      ]


# Specification of the policies
model.levers = [IntegerParameter('Electric_boiler_investments', 0, 3),
                IntegerParameter('MVR_investments', 0, 3),
                IntegerParameter('Energy_tax', 0, 2),
                IntegerParameter('Coal_plants_shutdown', 0, 1),
                IntegerParameter("Investment_year", 2020, 2025)
               ]

# Specification of the outcomes
model.outcomes = [ScalarOutcome("Direct_emissions_2030", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("Direct_emission_change", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("Indirect_emissions_2030", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("Indirect_emission_change", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("Total_emissions_2030", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("Total_emission_change", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("IRR", kind=ScalarOutcome.MAXIMIZE),
                  ScalarOutcome("NPV", kind=ScalarOutcome.MAXIMIZE),
                  ScalarOutcome("Investment_cost", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("Yearly_production", kind=ScalarOutcome.MAXIMIZE)
                 ]


#  ### Running experiment with policies
#

# In[3]:

#Running with policies
```

```
n_scenarios = 100
n_policies = 96
results_bckp  =  './Data/Results  salt  -  {}  scenarios  {}  policies.tar.gz'.format(n_scenarios,
n_policies)

counter = util.Counter()
policies = samplers.sample_levers(model, n_policies)

try:
    # Load results if experiment has already been conducted
    results = load_results(results_bckp)

except IOError:
    # Running in parallel
    with MultiprocessingEvaluator(model) as evaluator:
        results = evaluator.perform_experiments(n_scenarios, policies)

    #Running in series
    #results = perform_experiments(model, n_scenarios)

    save_results(results, results_bckp)

experiments, outcomes = results


# In[4]:

# Creating experiment DataFrame
experiment_data=pd.DataFrame(experiments)
outcome_data = pd.DataFrame(outcomes)
results_df=pd.concat([experiment_data, outcome_data], axis=1)


# ## Feature scoring

# In[5]:

import seaborn as sns
import numpy.lib.recfunctions as rf
from ema_workbench.analysis import feature_scoring
from ema_workbench.analysis.feature_scoring import get_feature_scores_all

experiments, outcomes = results


# ### Feature scoring uncertainties to performance metrics

# In[6]:

# Defining the x space for feature scoring
x = experiments
x        =        rf.drop_fields(x,        ['Electric_boiler_investments',        'MVR_investments',
'Energy_tax','Coal_plants_shutdown', 'Investment_year',
                        'policy','model'],
                   asrecarray=True)


# In[7]:

# Defining the y-space for the feature scoring
y_df = pd.DataFrame(outcomes)
y_df=y_df[['Direct_emission_change','Indirect_emission_change','Total_emission_change','NPV','IRR'
, 'Investment_cost']]

y_dict = y_df.to_dict('list')
for key in y_dict.keys():
    y_dict[key] = np.array(y_dict[key])

y = y_dict


# In[8]:

fs_all = get_feature_scores_all(x, y)
fs_all


# In[9]:

sns.heatmap(fs_all, annot=True, cmap='Blues', linewidths=0.5)
plt.show()


# ### Feature scoring for policy levers
```

```
# In[10]:

# Defining the x space for feature scoring
x = experiments
x = rf.drop_fields(x,
['Discount_rate','Efficiency_gain','Price_scenario','Production_uncertainty',
                       'policy', 'model'],
                   asrecarray=True)
fs_all = get_feature_scores_all(x, y)


# In[11]:

sns.heatmap(fs_all, annot=True, cmap='Blues', linewidths=0.5)
plt.show()


# In[ ]:




# ## Filtering output space to explore desired outcomes

# In[12]:

import copy
data = copy.copy(outcomes)
data = pd.DataFrame(data)


# In[13]:

# Filtering scenarios
data['NPV_pos']=data.NPV>0
data['Direct_emissions_ETS'] = data.Direct_emissions_2030<490
data['Total_emission_change_neg'] = data.Total_emission_change<-65.88
results_df['Filter']=
data['NPV_pos']&data['Direct_emissions_ETS']&data['Total_emission_change_neg']


# In[14]:

filtered_results=results_df.loc[results_df['Filter']]


# In[15]:

# Selecting relevant frames from filters

# Policies
x_df =
filtered_results[['Electric_boiler_investments','MVR_investments','Coal_plants_shutdown','Energy_t
ax']]
x = x_df.to_records(index=False)

# Outcomes
y_df =
filtered_results[['Direct_emission_change','Indirect_emission_change','Total_emission_change','NPV
','IRR']]
y_dict = y_df.to_dict('list')
for key in y_dict.keys():
    y_dict[key] = np.array(y_dict[key])

y = y_dict

fs_all = get_feature_scores_all(x, y)
sns.heatmap(fs_all, annot=True, cmap='YlGnBu', linewidths=0.5)
plt.show()


# In[16]:

filtered_results[['Electric_boiler_investments','MVR_investments','Coal_plants_shutdown','Energy_t
ax']].std()


# In[17]:

filtered_results[['Electric_boiler_investments','MVR_investments','Coal_plants_shutdown','Energy_t
ax']].mean()
```

```
# ## Dimensional stack

# In[18]:

from ema_workbench.analysis import dimensional_stacking

# Selecting successful policies
x_df = results_df[['Electric_boiler_investments','MVR_investments',
                         'Energy_tax','Coal_plants_shutdown' ]]
x = x_df.to_records(index=False)

# Filtering output space
y = np.array(results_df['Filter'])

dimensional_stacking.create_pivot_plot(x,y, 5, nbins=4)
plt.show()


# ## Visualizing filtered output space

# In[19]:

import plotly.plotly as py
import plotly.graph_objs as go

parallel_plot_data = [
    go.Parcoords(
        line = dict(color = 'rgb(0, 176, 240)'
                   ),

        dimensions = list([
            dict(range = [0,800],
                 constraintrange = [0,490],
                 label = 'Direct emissions 2030 (kton CO2)',
                 values = list(results_df['Direct_emissions_2030'])),
            dict(range = [0,800],
                 label = 'Indirect emissions 2030 (kton CO2)',
                 values = list(results_df['Indirect_emissions_2030'])),
            dict(range = [-300,500],
                 constraintrange = [-300,-65.88],
                 label = 'Total emissions change (kton CO2)',
                 values = list(results_df['Total_emission_change'])),
            dict(range = [-1,2],
                 constraintrange = [0,2],
                 label = 'Internal rate of return (%)',
                 values = list(results_df['IRR'])),
            dict(range = [0,(10**8)],
                 constraintrange = [(10**6),(10**8)],
                 label = 'Investment cost (€)',
                 values = list(results_df['Investment_cost'])),
        ])
    )
]

py.iplot(parallel_plot_data, filename = 'parcoord-dimensions')
```

D.2: Code used for open exploration of chlor-alkali manufacturing industry DPE model

```
# # MIDDEN Chlor-alkali Model - Open Exploration
#
# ## Model initialization

# In[1]:

from __future__ import (division, print_function, absolute_import, unicode_literals)
from ema_workbench import (RealParameter, IntegerParameter, TimeSeriesOutcome, ScalarOutcome,
                           ema_logging, perform_experiments, save_results, load_results)
from ema_workbench.connectors.excel import ExcelModel
from ema_workbench.em_framework import (salib_samplers, samplers, util,
                                        MultiprocessingEvaluator, SequentialEvaluator)
from ema_workbench.analysis import prim
from ema_workbench import ema_logging
ema_logging.log_to_stderr(ema_logging.INFO)

import numpy.lib.recfunctions as rf
import numpy as np
import matplotlib.pyplot as plt
import mpld3
import pandas as pd
```

```
# In[2]:

ema_logging.log_to_stderr(level=ema_logging.INFO)

model = ExcelModel("excelmodel", wd="./Models", model_file='MIDDEN Decarbonization options chlor-
alkali final.xlsx')

#name of the sheet
model.sheet = "Experiment"

# Specification of the uncertainties
model.uncertainties = [IntegerParameter("Price_scenario", 1, 3),
                       RealParameter("Discount_rate", 0.0075, 0.05),
                       RealParameter("Production_uncertainty", 0.85, 1.15),
                       RealParameter("Efficiency_gain", 0.0015, 0.0075),
                       IntegerParameter("Investment_year", 2020, 2025)
                      ]


# Specification of the policies
model.levers = [IntegerParameter('Electric_boiler_investments', 0, 2),
                IntegerParameter('Biomass_boiler_investments', 0, 1),
                IntegerParameter('Zero_gap_investments', 0, 2),
                IntegerParameter('Peak_shaving_investments', 0, 1),
                IntegerParameter('Energy_tax', 0, 2),
                IntegerParameter('Coal_plants_shutdown', 0, 1),
                IntegerParameter("Investment_year", 2020, 2025)
               ]

# Specification of the outcomes
model.outcomes = [ScalarOutcome("Direct_emissions_2030", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("Direct_emission_change", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("Indirect_emissions_2030", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("Indirect_emission_change", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("Total_emissions_2030", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("Total_emission_change", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("IRR", kind=ScalarOutcome.MAXIMIZE),
                  ScalarOutcome("NPV", kind=ScalarOutcome.MAXIMIZE),
                  ScalarOutcome("Investment_cost", kind=ScalarOutcome.MINIMIZE),
                  ScalarOutcome("Yearly_production", kind=ScalarOutcome.MAXIMIZE)
                 ]


#  ### Running experiment with policies
#

# In[3]:

#Running with policies
n_scenarios = 50
n_policies = 216 #*5
results_bckp = './Data/Results chlor-alkali - {} scenarios {} policies.tar.gz'.format(n_scenarios,
n_policies)

counter = util.Counter()
policies = samplers.sample_levers(model, n_policies)

try:
    # Load results if experiment has already been conducted
    results = load_results(results_bckp)

except IOError:
    # Running in parallel
    with MultiprocessingEvaluator(model) as evaluator:
        results = evaluator.perform_experiments(n_scenarios, policies)

    #Running in series
    #results = perform_experiments(model, n_scenarios)

    save_results(results, results_bckp)

experiments, outcomes = results


# In[4]:

# Creating experiment DataFrame
experiment_data=pd.DataFrame(experiments)
outcome_data = pd.DataFrame(outcomes)
results_df=pd.concat([experiment_data, outcome_data], axis=1)


# In[5]:
```

```
import seaborn as sns


# ## Feature scoring

# In[6]:

import seaborn as sns
import numpy.lib.recfunctions as rf
from ema_workbench.analysis import feature_scoring
from ema_workbench.analysis.feature_scoring import get_feature_scores_all

experiments, outcomes = results


# ### Feature scoring uncertainties to performance metrics

# In[7]:

# Defining the x space for feature scoring
x = experiments
x = rf.drop_fields(x, ['Electric_boiler_investments', 'Biomass_boiler_investments',
                       'Zero_gap_investments', 'Peak_shaving_investments',
                       'Energy_tax','Coal_plants_shutdown', 'Investment_year',
                       'policy','model'],
                   asrecarray=True)


# In[8]:

# Defining the y-space for the feature scoring
y_df = pd.DataFrame(outcomes)
y_df=y_df[['Direct_emission_change','Indirect_emission_change','Total_emission_change','NPV','IRR'
, 'Investment_cost']]

y_dict = y_df.to_dict('list')
for key in y_dict.keys():
    y_dict[key] = np.array(y_dict[key])
y = y_dict


# In[9]:

fs_all = get_feature_scores_all(x, y)
fs_all


# In[10]:

sns.heatmap(fs_all, annot=True, cmap='Blues', linewidths=0.5)
plt.show()


# ### Feature scoring for policy levers

# In[11]:

# Defining the x space for feature scoring
x = experiments
x                                       =                                        rf.drop_fields(x,
['Discount_rate','Efficiency_gain','Price_scenario','Production_uncertainty',
                       'policy', 'model'],
                   asrecarray=True)
fs_all = get_feature_scores_all(x, y)


# In[12]:

sns.heatmap(fs_all, annot=True, cmap='Blues', linewidths=0.5)
plt.show()


# ## Filtering output space to explore desired outcomes

# In[13]:

import copy
data = copy.copy(outcomes)
data = pd.DataFrame(data)


# In[14]:

# Filtering scenarios
```

```
data['NPV_pos']=data.NPV>0
data['Direct_emissions_ETS'] = data.Direct_emissions_2030<167
data['Total_emission_change_neg'] = data.Total_emission_change<0
results_df['Filter']=
data['NPV_pos']&data['Direct_emissions_ETS']&data['Total_emission_change_neg']


# In[15]:

filtered_results=results_df.loc[results_df['Filter']]


# In[16]:

filtered_results.tail()


# In[17]:

# Selecting relevant frames from filters

# Policies
x_df = filtered_results[['Electric_boiler_investments', 'Biomass_boiler_investments',
                         'Zero_gap_investments', 'Peak_shaving_investments',
                         'Energy_tax','Coal_plants_shutdown' ]]
x = x_df.to_records(index=False)


# Outcomes
y_df                                                                                    =
filtered_results[['Direct_emission_change','Indirect_emission_change','Total_emission_change','NPV
','IRR']]
y_dict = y_df.to_dict('list')
for key in y_dict.keys():
    y_dict[key] = np.array(y_dict[key])

y = y_dict

fs_all = get_feature_scores_all(x, y)
sns.heatmap(fs_all, annot=True, cmap='YlGnBu', linewidths=0.5)
plt.show()


# ## Dimensional stack of filtered space

# In[18]:

from ema_workbench.analysis import dimensional_stacking

# Selecting successful policies
x_df = results_df[['Electric_boiler_investments','Coal_plants_shutdown',
                         'Energy_tax','Zero_gap_investments' ]]
x = x_df.to_records(index=False)

# Filtering output space
y = np.array(results_df['Filter'])

dimensional_stacking.create_pivot_plot(x,y, 5, nbins=4)
plt.show()


# ## Visualizing filtered output space

# In[19]:

import plotly.plotly as py
import plotly.graph_objs as go

parallel_plot_data = [
    go.Parcoords(
        line = dict(color = 'rgb(0, 176, 240)'
                   ),

        dimensions = list([
            dict(range = [0,250],
                 constraintrange = [0,167],
                 label = 'Direct emissions 2030 (kton CO2)',
                 values = list(results_df['Direct_emissions_2030'])),
            dict(range = [-400,400],
                 label = 'Indirect emission change (kton CO2)',
                 values = list(results_df['Indirect_emission_change'])),
            dict(range = [-250,250],
                 constraintrange = [-250,-105.13],
                 label = 'Total emissions change (kton CO2)',
```

```
                 values = list(results_df['Total_emission_change'])),
            dict(range = [-1,3],
                 constraintrange = [0,3],
                 label = 'Internal rate of return (%)',
                 values = list(results_df['IRR'])),
            #dict(range = [-3*(10**8),3*(10**8)],
            #     constraintrange = [0,3*(10**8)],
            #     label = 'Net present value (€)',
            #     values = list(results_df['NPV'])),
            dict(range = [0,1.1*10**8],
                 constraintrange = [10**6,1.1*(10**8)],
                 label = 'Investment cost (€)',
                 values = list(results_df['Investment_cost'])),
        ])
    )
]

py.iplot(parallel_plot_data, filename = 'parcoord-dimensions')
```