Delft University of Technology

Master Thesis

Technology adoption at the PoR chlorine cluster

A study on the effect of market & behavioural barriers on technology adoption at the Port of Rotterdam chlorine cluster.

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Technology adoption at the PoR chlorine cluster

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Summary

Problem situation

In order for the Netherlands to reach CO2 neutrality by 2050, large investments in zero emission technologies are needed. These investments would comprise out of renewable energy generation, higher energy efficiency alternatives and electrification of end uses. Allthough climate mitigation has become an ever growing societal concern since the ratification of "het klimaatakkoord", progress in the industrial sector has been seriously lagging in the Netherlands. In 2021 the reduction of CO_2 emissions in the Netherlands stagnated and the emissions of the industrial sector actually slightly rose. So too in the Port of Rotterdam, where the chlorine cluster is not showing any significant CO_2 reductions. There are several potential explanations why there is a gap between what should be invested and what actually is invested. They define the gap as, 'the apparent reality that some technologies that would pay off for adopters are, nevertheless, not adopted'. So, why do decision makers under invest in zero emission technologies? The explanations of fall into two broad categories:

- Market barriers
- Behavioural barriers

Research question

Following the problem situation, this thesis focused on researching to what extent market & behavioural barriers contribute to the investment gap in the Port of Rotterdam Chlorine cluster, by incorporating both market and behavioural barriers in a quantitative investment model. The incorporation of these barriers in the model result in a range of investment types, some of them non-optimal and varying in perspectives on valuing the future. By simulating technology adoption under the assumption of this range of varying configurations of market and behavioural barriers, it is possible to determine the effect of those two categories of barriers on technology adoption at the PoR chlorine cluster. The obtained insights of this research feed into the larger study of quantitative decision models for the industrial sector. Where the following main research question is answered:

What is the effect of market and behavioural barriers on zero emission technology adoption at the PoR chlorine cluster?

Research approach

To answer the main research question, the model represents the PoR chlorine cluster on a highly detailed level and bases it's technical system's configuration on a thorough plant-process-product & zero-emission technology inventarisation. These two inventarisations give the current and possible future configuration of the PoR chlorine cluster's technical system. Consequently, this makes it possible to explicitly model the technology stock at the chlorine cluster and determine technology adoption on an asset level. The market & behavioural barriers are represented by 8 evaluation types. These evaluation types represent 8 varying configurations of the market & behavioural barriers. Consequently, a scenario analysis was conducted with the model.

Results

The scenario analysis resulted in transition pathways, total CO_2 emissions and total cash flows between 2022-2050. The model results show that the incorporation of market and behavioural barriers lead to postponed adoption of zero emission technology adoption. This is reflected by the lower number of years that these alternatives are installed between 2022 and 2050. The lower adoption lead to an increase of 288% total CO_2 emissions between 2022-2050, compared to the optimal solution. Underneath, the key findings from the model results are presented.

- The market & behavioural barriers lead to less zero emission technology adoption, compared to the normative baseline benchmark. Additionally, the barriers explain the existence of the perceived investment gap.
- Most of the direct CO_2 reduction can be achieved by decarbonising utility assets like steam boilers and cracking facilities.
- The pay-back period of three years, which represents a risk averse investor, leads to postponed zero emission technology investments.
- The build up of barriers is meaningful, because it makes it possible to identify interaction effects between barriers.

First off, the results clearly show that the incorporated barriers lead to a significant deviation from the normative baseline benchmark. This suggests that the incorporation of the theoretically sound barriers lead to very different results compared to the currently used normative optimisation models. The incorporation of the barriers show that the optimisation models overestimate the adoption of zero emission technology and might suggest why there is a perceived investment gap. As stated in the first chapter, according to the investment gap there should be made more investment than there are currently being made. But the results from this thesis suggest that it seems logical that these investments are not being made because of the mostly the perceived uncertainty and risk appetite of the companies at the cluster.

Secondly, the model results show that the quickest gains can be made by decarbonising the utility assets at the chlorine cluster. This is where the most direct CO_2 emissions are produced. In addition, the secondary emissions could be drastically reduced by the consumption of renewable electricity, due to the large consumption of electricity at the chlorine cluster's production processes. The placement of electric and biomass boilers to reduce the industry's direct emissions, as well as zero-gap membrane electrolyzers to tackle the industry's electricity consumption, and thus its indirect emissions.

Third, the used level for the pay-back period strongly influences the adoption for zero emission technology, as depicted by the results from decision evaluation type bounded rationality and split incentives. The companies at the PoR chlorine cluster use a pay-back period of three years in order to select their alternatives. Due to the large CAPEX of the zero emission technologies, the three years pay back period is too short to adopt new technology. So, the risk averseness of the investors leads to the postponement of technology adoption.

Lastly, the build-up used for the model experimentation is meaningful, as it identifies the interaction effects between barriers. This is best seen in decision evaluation types 'access to capital' and 'all market barriers'. Here, the limited access to capital results in lower total emissions as some of the high CAPEX polluting alternatives which have low OPEX are not adopted because it is not possible. There the somewhat lower CAPEX alternatives with high OPEX are adopted earlier. This is also due to the effect imperfect information and hidden costs have on the relative attractiveness of the technology alternatives. In a next study it would be interesting to conduct a full factorial experiment with the barriers to fully study the relative impact and interaction affect of the barriers on technology adoption.

These results suggest that the theoretically sound market & behavioural barriers might explain the investment gap. The model results suggest that the normative optimisation models gravely overestimate the future savings of zero emission technologies, underestimate the upfront & operating costs and fail to account for the subjectivity of investment decision makers.

Recommendations

The insights from this master thesis result in the following key recommendations for investment decision makers:

1. Consider the incorporation of market & behavioural barriers in investment models for the industrial sector.
2. The companies at the chlorine cluster should adjust their currently used decision acceptance criteria to further decarbonize the cluster.

3. Policy should be made to increase the relative attractiveness of sustainable utility assets at the cluster to achieve large CO_2 reductions.
4. Proceed with the Brine recirculation alternative, as it seems to be profitable in all the scenario's.
5. Water Energy Intelligence (WEI) should dedicate to the expansion of the model and create a support base among the Harbour Industrial Complex Rotterdam-Moerdijk.

First off, investment decision makers should become more aware that zero emission technology investment is subjected to various market & behavioural barriers. As the model results show a discrepancies between normative benchmark optimizing and non normative optimisation, in case of the PoR chlorine cluster. This result is juxtaposed from the perceptions of the experts at Nobian and Westlake. They did acknowledge that the considered barriers are theoretically sound, but did not perceive them as thus impactful to consider in their investment models. Therefore, the recommendation to incorporate market & behavioural barriers in investment models to more incorporate more of the possible costs and benefits. This leads to a far more accurate representation of technology adoption and might prove insightful for possible paths of decarbonisation. Also, the industrial sector should alter their decision acceptance criteria to a less risk averse ones. As is clearly seen for some of the alternatives in the model results file, the pay-back period of three years strongly impacts the adoption of zero emission technologies. Eventually, we will probably achieve a situation where the zero emission technology alternatives are within the margin of a three year pay-back period. A situation with a extreme surplus of cheap renewable electricity, more proven technology and higher CO_2 prices. However, the time that we lose with the postponement of adopting zero emission technology might lead to irreversible negative consequences for society.

Secondly, as shown in the results from 6, the pay-back period chosen by the companies strongly influences the postponement for the adoption of zero emission technology. This in turn leads to lower profits for the companies over time and an increase in total CO_2 emissions. Therefore, it is recommended for the companies to use less risk averse decision acceptance criteria.

Thirdly, a recommendation to policy makers. As explained earlier, the large and cost-effective gains regarding (CO2) emission reduction can be made in the utility alternatives for the chlorine cluster. These are mainly the utility technologies responsible for heat and steam production. Financial stimulation of these specific technology alternatives could make quick gains in CO_2 reduction by the subsidisation of these technologies and higher taxation on gas use & CO_2 costs.

Fourthly, the model results show that the brine recirculation alternative between Nobian and Westlake is profitable under almost every circumstance. Therefore, it is suggested to proceed with the alternative and scale the project up from the demonstration site to full scale recirculation. Of course, this recommendation is only based on the financial profitability of the project and the companies should consider the desirability of further interconnection & interdependence.

Lastly, WEI should dedicate to the expansion of the model with more of the PoR industrial cluster and simultaneously create a support base among these companies for the use of the model. This thesis has proven the functionality of Linny-R by being able to present possible transition pathways on an asset level, in combination with CO_2 reduction. Especially the ease of modelling in combination with the graphically appealing representation of technical systems, should be reasons to adopt the Linny-R modelling method. In light of the IMPETUS project the model could be expanded with the rest of the industry in Rotterdam-Moerdijk and result in a model that would give insight to all the relevant parties. At the same time a strong support base for the model should be created among the potential users, in order for the model to be accepted and actually be used in the future. To achieve that, WEI could opt for a more cooperative modelling approach with the potential users and create a easily accessible version of the model in the form of a online decision support system. A lot of inspiration could be drawn from the ETM from Quintel.

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1 Introduction

1.1. Research Introduction

1.1.1. Investments needed to halt climate change

According to the 2022 Global Risks Report, climate change is the largest long-term threat facing humanity [175]. The report states that climate change in the form of extreme weather events and biodiversity loss, could lead to various devastating consequences to global society. Examples of consequences are: the erosion of social cohesion, economic divergence and geopolitical tensions [183]. Although climate change has not yet led to worldwide societal collapse, effects of climate change are already observed. Worldwide temperatures are rising, drought and wild fires are starting to occur more frequently, rainfall patterns are shifting, glaciers and snow are melting and the global mean sea level is rising [53]. Therefore, it is imperative to mitigate climate change by reducing or preventing the emissions linked to human activities.

To limit the negative consequences of climate change, 196 countries pledged to contribute to limit global warming in 2015 at the Paris Convention. The agreement has set out a global framework to avoid dangerous climate change, by limiting global warming well below 2 degrees Celsius before the end of this century [129]. In order to reach that goal, the complete reduction of greenhouse gas emissions is needed and a radical change to the current energy systems [180].

Therefore, the Netherlands has translated the Paris Agreement into national climate action plan called "Het klimaatakkoord" [115]. The klimaatakkoord contains more than 600 arrangements on how to transition the current fossil-based energy systems towards sustainable energy systems. Eventually, this should lead to $co_2{-}eq$ net neutrality by 2050.

In order to reach CO_2 neutrality by 2050, various large investments in zero emission technologies are needed. These investments would comprise out of renewable energy generation, energy conservation, higher production efficiency, electrification of end uses and many more. According to the 'Planbureau voor de Leefomgeving' (PBL), an estimated 350 billion euro investment is needed between 2020 and 2040 in order for the Netherlands to achieve net neutrality by 2050 [132]. This investment will have to be made by both public and private investors, as they will be essential for the financing and acceleration of investments in the energy transition in the Netherlands [131].

1.1.2. The investment gap: to what extent do market failures and behavioural explanations contribute to the investment gap?

Allthough the signing of the Paris Agreement and klimaatakkoord were promising, progress has been seriously lagging in the Netherlands [71]. In 2021 the reduction of total CO_2-eq emissions stagnated and the CO_2 emissions of the industrial sector actually slightly rose [52] [122]. The apparent underachievement of national climate mitigation policies like the klimaatakkoord is unfortunately not uncommon. An example is the collapse of the UK's thermal improvement policy, the 'green deal' or the American congressional bill to cap-and-trade economic incentive schemes [167] [99]. So, what are explanations for the apparent lack of progress regarding CO_2 reduction? Following the report of Mckinsey and Company [120], there should be a yearly global CO_2 reduction of 11Gt per year by investing in cost-effective sustainable technologies. These investments are currently not being made, although there are enough cost-effective alternatives according to Mckinsey and company [120] [77]. According to generally accepted economic theory, a profit-maximising company should invest in energy efficient or zero-emission technologies whenever future savings outweigh the upfront cost [97].

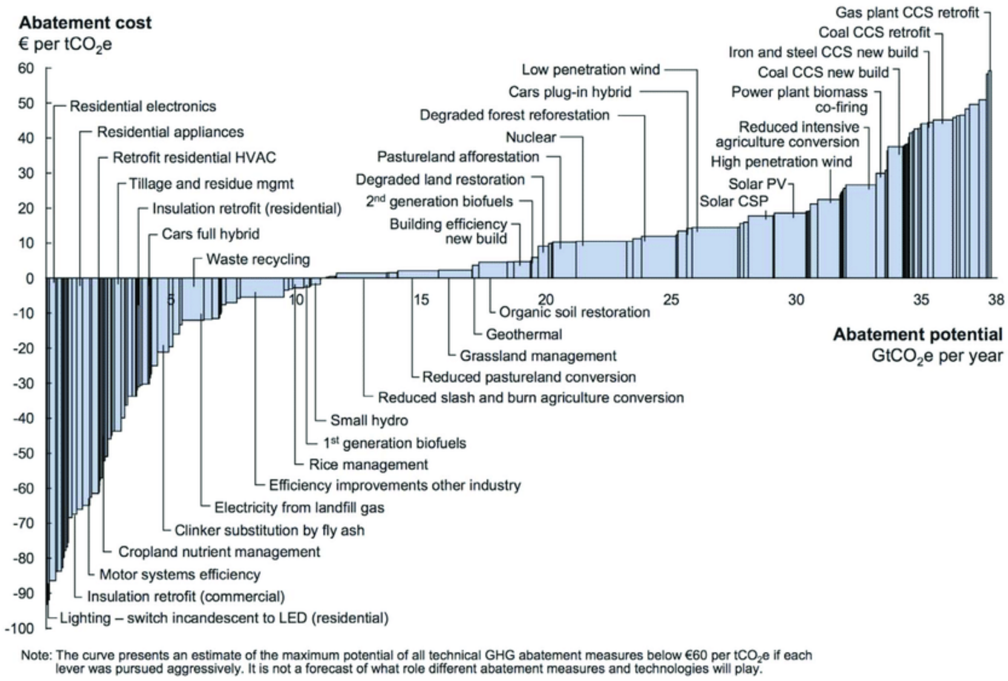

Figure 1.1: Abatement cost curve [120]

According to Gerarden et al.[68] there are several potential explanations why there is a gap between what should be invested and what actually is invested. They define the gap as, 'the apparent reality that some technologies that would pay off for adopters are, nevertheless, not adopted'. Although the authors focus on the specific case of energy efficiency investments, the explanations can also applied to zero emission technology adoption following Knobloch & Mercure [97]. So, why do decision makers under invest in zero emission technologies? The explanations of Gerarden et al. [68] fall into two broad categories:

- Market failures
- Behavioural explanations

Market failures like information problems, capital market failures and energy market failures might be explanations for the apparent existing investment gap. In addition to that, bounded rationality and systematically biased beliefs might be explanations from a behavioural perspective [68]. Allthough they conclude that these two categories of explanations are theoretically sound, they address that there is currently only limited empirical evidence that these two categories might be explanations for the investment gap. The authors therefore state that future research could contribute to the validity of these explanations and the degree to which each category contributes to the investment gap. This in turn could be relevant for a better understanding of the investment gap. Therefore, this thesis aims to further explore the investment gap.

1.1.3. The Port of Rotterdam chlorine cluster as a case

To examine to which degree the market failures and behavioural explanations play a role in the investment gap, this thesis uses the Port of Rotterdam (PoR) chlorine cluster as a case. Hereunder a description of the Dutch industrial sector and the chlorine cluster is given. Followed by three arguments why this specific case is chosen.

As a large producer of industrial products and user of energy, the PoR is responsible for a sizeable amount of Green house gas (GHG) emissions per year. With 18,7 CO_2-eq megatons in 2019, the PoR is responsible for 37,9% of the total Dutch industrial emitted GHG [121]. Especially the chemical and petrochemical industries at the PoR are a driving force behind the high emission levels [122]. The emission intensity of these two sub sectors is almost five times higher than that of the other industrial sub sector, according to the CBS [24]. The PoR has the obligation to reduce 10 megatons by 2030 and reach CO_2 net neutrality in 2050 [114] and thus has a large challenge ahead.

Most of the Dutch industrial sector is concentrated in industrial clusters. Industrial clusters are collections of industries with high levels of co-location in terms of employment and production [41]. In these clusters, separate industries engage in a collaborative approach to gain competitive advantage involving physical exchange of materials, energy and/or other by-products [30]. The physical exchange within the cluster is facilitated by an interconnected infrastructure of pipelines, power-lines and transportation infrastructure. The Netherlands has six industrial clusters spread around the country, of which the harbour industrial cluster Rotterdam-Moerdijk is the largest with over 120 industrial companies. During this thesis the harbour industrial cluster Rotterdam-Moerdijk will be referred to as the Port of Rotterdam (PoR).

The PoR chlorine cluster is highly interconnected part of the PoR where four companies are exchanging chlorine, caustic soda, hydrogen and hydrochloric acid among each other. The four companies within the cluster are called Nobian, Westlake, Shin-Etsu and Huntsman. These companies combined, emit around 270 kton of CO_2 per year [122]. Although there are various zero emission technology alternatives for the chlorine cluster, there have been no large sustainable investments at the chlorine cluster. As is reflected by the yearly figures of the PoR company and which is also reflected in the combined production & emission figures of the CBS that were mentioned above [145]. Think of zero emission technology alternatives that aim to, electrify production processes, gain higher process efficiency and enable the use of carbon capture storage (CCS) [96].

The PoR chlorine cluster as a case is chosen because of the following arguments:

- Investment gap is also noticed at the PoR chlorine cluster
- Following the suggested directions for future research from Scherpbier [151]
- Availability of data for the PoR chlorine cluster

Just as the industrial sector in general, the chemicals sector also has a large CO_2 reduction potential with negative abatement costs [120]. An example of an investment that should have been made is an e-boiler at Westlake Epoxy. The e-boiler uses electricity to produce heat for the epoxy production process. Westlake Epoxy currently uses refinery gas that they receive from Shell, to use in their combustion boiler [17]. Following a simple NPV calculation with a discount rate of 3 percent, an e-boiler that delivers the same heat output would save Westlake around 112 million euros over it's entire economic lifetime. As the CAPEX of an gas boiler is higher and fuel + CO2 costs are higher than using electricity as an energy source [24]. Following, this simple calculation (shown in appendix A) shows there is a viable decarbonisation option for the chlorine cluster. However, there have been no large sustainable investments at the PoR chlorine cluster, as is reflected by the yearly figures of the PoR company [145]. Is this due to market failures or behavioural explanations or the two combined?

The second reason for choosing this case is based on the suggested directions for future research from Scherpbier [151]. Scherpbier performed an analysis of decarbonization pathways in the salt and chlor-alkali industries in the Netherlands. He states that the focus should be taken wider and industries closely related to the salt-chlor-alkali chain, like the Dutch plastics manufacturing industry should be included in one study. As he mentions: "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" [151]. The Dutch chlorine cluster is a good example of a site, where multiple manufacturing chains are located together and closely integrated. So, by choosing the entire chlorine cluster as a case, further insights about the energy transition in the Dutch industrial sector can be gained.

Lastly, the availability of data is favorable for this case. That is due to the openly available data of the MIDDEN-database and the information available via the internship at Water Energy Intelligence (WEI). The MIDDEN-database contains information on the current energy and material use of the manufacturing industry the Netherlands and it's options for decarbonisation of its processes [133]. Secondly, WEI is currently affiliated with the European Water-mining and IMPETUS projects [181] [87]. Both of these projects have sub projects where the PoR chlorine cluster is addressed. Therefore, this internship gives access to expert contacts within the PoR chlorine cluster.

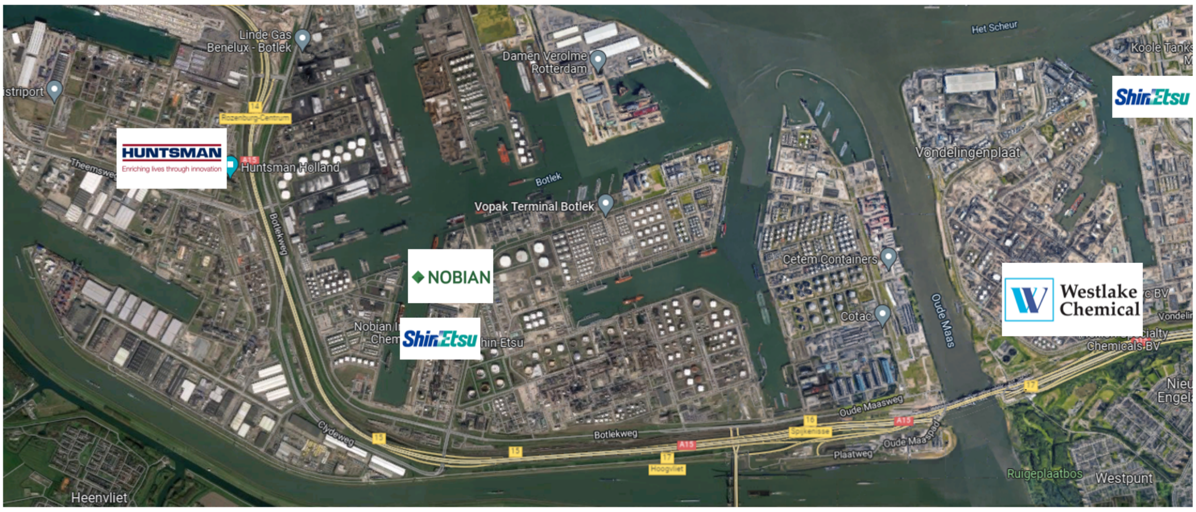

Figure 1.2: The locations of the four PoR chlorine cluster's companies.

1.2. Core concepts to investment

To further elaborate on the previous section, three core concepts are discussed in this section. These concepts are investment decision-making, quantitative decision support methodologies and market & behavioural barriers to investment.

1.2.1. Investment decision-making: effective allocation of capital

As mentioned in the previous section, large investments in zero emission technologies are needed at the chlorine cluster in order to reach CO_2 net neutrality by 2050. In the context of energy transitions, the main question is how to use investment capital to transition from fossil fuel based technologies towards renewable or less polluting technologies [148]. As effective allocation of investment capital is key to corporate success [7]. Therefore, this subsection introduces the concept of investment decision-making. Investment decision-making is defined as an investor's action to invest funds in several investment options, both in the physical and financial assets [79]. Think of physical investments like machinery or buildings; or of financial investments like stocks or bonds [177]. According to Virlics [177], decision analysis in economic theory states that the decision making is based on the following two points:

1. An objective analysis of the investment's possible outcomes and its calculated payoff.
2. On the subjective perspective of the investor.

Making use of an investment analysis is a common practice to structure the way decision makers handle the risk, uncertainty and expected stream of payoffs [59]. Risk is defined as the chance that the outcome of an investment's actual gains will differ from an expected stream of future payoffs [63]. By conducting an investment analysis, the decision maker can identify the factors that are responsible for the largest risks of a investment project. Uncertainty and risk are always present in an investment, if that has more than one possible outcome [14]. This uncertainty and risk should be identified and analysed.

An investor can decide what to do regarding this uncertainty based on the results of his analysis of risks, he can decide how to manage these risks and whether to invest or not [177]. Secondly, investors perceive risk, uncertainty and future pay offs heterogeneously. According to Virlics [177] the subjectivity is based on the involvement of psychological and emotional factors. This manifests itself by the fact that decision makers also make investments based on his/hers personal knowledge of the investment project or personal risk perception, which are subjective factors [81]. She concludes with the remark that investment risks should be analysed from a behavioural perspective and not solely as an objective component [177].

An example of a investment decision analysis method, that both incorporates the objective analysis and subjective perspective of the investor, is shown in figure 1.3. This method combines objective techniques of operations research and system analysis with professional judgements and values. The combination of the two can be used to quantify likelihoods of various consequences of alternatives.

The first step is dedicated to the structuring of the decision problem and includes the finding of alternatives and the specification of the decision maker's objectives [93]. The second step determines the possible impacts for each alternative. This is presented for example as a set of possible consequences and the probabilities of them occurring. Third, "are the potential benefits of having things go right worth the risks if things go wrong [93]". This step is about the risk attitudes of decision makers and it aims to created a model of values to evaluate the alternatives. This is can be done in a structured discussion between a analyst and a decision maker, to quantify value judgements about the effect of alternatives. The last step is dedicated to the evaluation and comparison of alternatives.

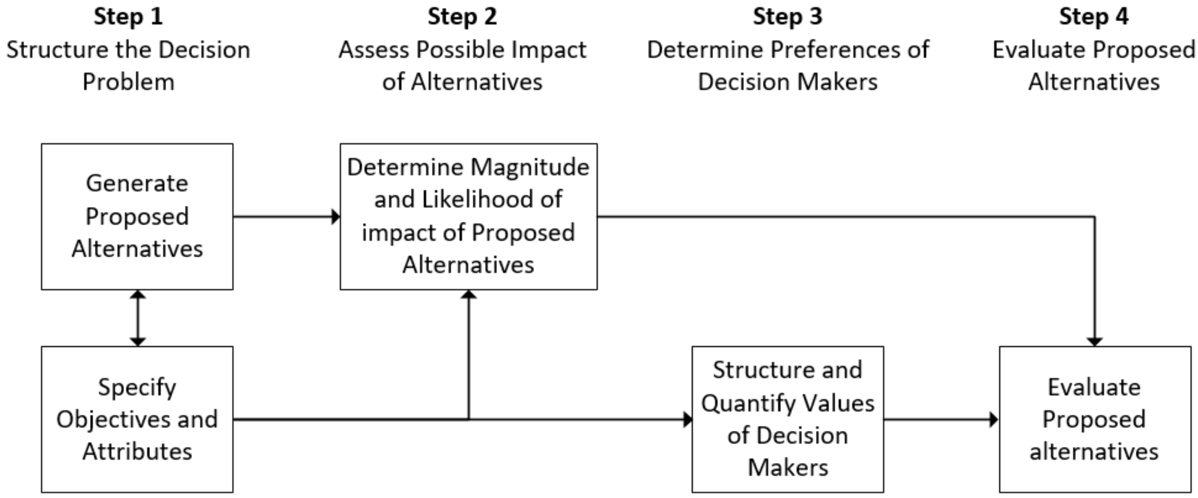

Figure 1.3: Methodology of decision analysis decomposed in four steps [93]

When it comes to the type of investments decision makers make in the industrial sector, mainly two types occur [110]:

1. Expansion investments
2. Replacement investments

The expansion investments are typically characterized by a large upfront investment, followed by a flow of uncertain future pay offs. Think of the expansion of production capacity or the investment in a new production line. The replacement investments on the other hand usually entails determining the optimal moment to replace an aging asset with a new asset that performs minimally as good as the previous asset. Where in the case of the PoR chlorine cluster, Nobian could invest in an electric boiler to replace it's aging combined heat and power (CHP) plant for the production of heat [110].

1.2.2. Quantitative decision support models play an important role in decision making

As of late, there is an increasing awareness of the complexity of investment decision making. Which is reflected in the increased use of quantitative models to enhance the effectiveness of decision-making, see for example [89] [85] [23] [179]. The models offer the decision maker insights to make better decisions, by making predictions of risk and future payoffs [9]. In the light of assessing long term investments, like zero emission technology at the PoR chlorine cluster, precludes the use of quantitative decision support models. Given that the energy transition of the PoR chlorine cluster is subjected to conditions of large risks & uncertainty [102] [94].

Several types of models can be used for decision support. Chappin et al. [26] defines two main conceptually different models used to study energy and climate policy in energy systems like the chlorine cluster. These two main groups of models are techno-energy system models (TES) and agent-based models (ABMs). The TES models are commonly applied for investment assessments, according to Nerini [123] and Moallemi [116]. As, TES models provide a holistic approach towards the configuration and operation of such systems, and facilitate the optimal trade-off between energetic, economic and environmental performances [168]. These models are mostly optimisation models, which find a pathway or final state of the energy system under consideration. This approach leads to finding a least cost solution [26]. Further examples of TES models are, the myopic investment models of Poncelet [138], Sagdur [149] and Nerini [123]. Also, Agent-Based Models (ABM) have shown great potential for modelling energy systems [74]. Instead of determining optimal transition pathways, these models assume a descriptive approach. Where these models don't assume perfect information and optimal behaviour, but rather aim to capture system level behaviour out of the individual behaviour of its economic agents [25]. The agent-based models can provide an understanding of the emergent properties of many interacting elements in complex situation where intuition of decision makers fail [147]. The core of the methodology is the definition of different heterogeneous agents rather than treating all the model agents as a single representative agent.

1.2.3. Market & behavioural behavioural barriers

This subsection explains the introduced categories that explain the investment gap to zero emission technology adoption [68]. Where market failures and behavioural explanations are addressed.

Market failures

First off, the market failures to investment. Many studies attempt to explain the investment gap according to the neoclassical economic theory, where a representative agent adopts cost-minimizing or utility-maximising technology alternatives. Sutherland [163] for example, argues that it is rational for decision makers to reject sustainable technologies, because of risk & uncertainty. The large uncertainty of future energy prices, policy uncertainty and uncertainty about the profitability of investments make the investment appraisal very difficult. Especially when considering that the risks & uncertainties lead to many investments turning out less profitable than they seem to be, according to Mercure [111]. The complexity and uncertainty that go hand in hand with large investments present serious challenges to decision makers charged with their appraisal [42].

Behavioural explanations

The market failures explain a part of the investment gap, but other authors question the realism of investment decision behavior in classic economic theory [39][72]. These authors address the behavioral barriers to zero emission technology adoption [137][102]. Li [102] for example, states that decision makers do not always exhibit cost optimising behaviour. This is for example noticed in the under-achievement in energy efficiency programs [46]. Where rational economic analysis indicates that cost-effective zero-emission technology should be adopted, but is apparently prevented by decision makers acting under behavioural reasoning [102]. Thirdly, the modeling flaws found by Gerarden et al. [68]. The modeling flaws refer to the errors made in models, regarding understated costs of technology adoption, ignoring heterogeneity among decision makers and the incorrect modeling of discount rates.

Taxonomy of six barriers to zero emission technology investment

Sorrel et al. [159] have developed a taxonomy of six barriers to zero emission technology investment, which depict the two above mentioned market failures and behavioural explanations. They define of barriers as follows [159]: barriers comprise all factors that hamper the adoption of cost-effective energy-efficient technologies or slow down their diffusion. This definition for barriers has been widely adopted in scientific literature [97] [65] [171]. These barriers are regarded in contrast to a commonly used investment decision logic that only considers financial costs (investment costs and energy savings) and perfectly rational cost-minimizing agents with perfect foresight and perfect knowledge. The barriers of Sorrel et al. [159], depict four market barriers in the form of risk, imperfect information, hidden costs and access to capital. Besides four market barriers, Sorrel also identifies two behavioural barriers: split incentives and bounded rationality.

Risk is concerned with the short paybacks required for zero emission technology investments may represent a rational response to risk. This could be because such investments represent a higher technical or financial risk than other types of investment, or that business and market uncertainty encourages short time horizons [159].

Imperfect information can occur when a decision maker does not have information regarding a technology alternative or any other information relevant to an investment. Lack of information on sustainable technologies may lead to cost-effective opportunities being missed [159].

The **hidden costs** in engineering-economic analyses may fail to account for either the reduction in required utility associated with energy efficient technologies, or the additional costs associated with them. As a consequence, decision makers may overestimate energy efficiency potential. Examples of hidden costs include overhead costs for management, disruptions to production, staff replacement and training, and the costs associated with gathering, analysing and applying information [159].

When a company has insufficient **access to capital** through internal funds, and has difficulty raising additional funds through external financing, energy efficient investments may be prevented from going ahead. Investment could also be inhibited by internal capital budgeting procedures, investment appraisal rules and the short-term incentives of energy management staff [159].

Decision makers are not rational in reality and behave **bounded rational**. Due to constraints on time, attention, and the ability to process information, decision makers do not make decisions as assumed in common economic models. As a consequence, they may neglect energy efficiency opportunities, even when given good information and appropriate incentives [159].

Energy efficiency opportunities are likely to be foregone if actors cannot appropriate the benefits of the investment. For example, if individual departments within an organization are not accountable for their energy use they will have no incentive to improve energy efficiency. This barrier results in so called **split incentives** [159].

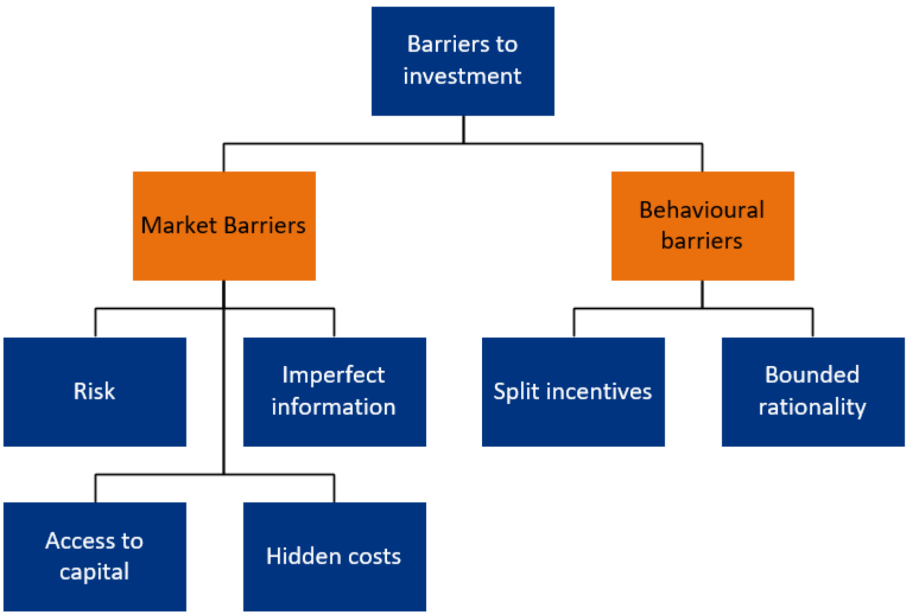

Figure 1.4: Taxonomy of investment barriers [159]

1.3. Research gap

The conducted literature research has given a better understanding on currently used quantitative decision support models that can be used to support the investment decision making process. The used research strategy for this literature research is shown in table 1.1. The literature was retrieved from Google Scholar and Scopus. Moreover, the snowballing and citation search method were used, mainly in the literature review papers.

Table 1.1: Search terms used for the research gap

Keywords	Industrial sector	Sustainable	Market barriers	Quantitative decision support
Synonym	Industry	Renewable	Behavioural barriers	Models
	Port of Rotterdam	Energy transition	Investment gap	Study
				Investment decision making

This conducted literature research led to the following research gap:

Research gap: Current quantitative decision support models for energy systems fall short in representing market & behavioural barriers.

The research gap is explained by an explanation of currently used models and followed by the shortcomings of currently used models. Lastly, by the suggestion of a optimisation model that both incorporates market behavioural barriers and includes investment behaviour.

Currently used Quantitative Decision Support models
Decision makers at the chlorine cluster can use various types of quantitative investment models to support the investment decision-making process [67]. The models represent certain characteristics or behaviors to show the eventual real effects of alternative conditions and courses of action [168]. The currently used models for quantitative decision support methodologies (See table 1.2) prove to be mostly techno-economic energy system models, in the form of bottom-up optimisation models & myopic optimisation models or Agent-Based models. The optimisation models are appropriate to use for normative exploration and identification of desirable future configurations of systems [111]. The models are set-up to either maximize or minimize an objective function under various case-specific constraints. Given that they are very detailed and tested, they have proved as effective and useful tools for problem solving in the power and supply sector [13]. As mentioned in the core concepts, it is imperative for decision makers at the PoR chlorine cluster to effectively allocate their capital. Therefore, the normative characteristic of optimisation models is suitable for the PoR chlorine cluster's decision makers. The agent-based models on the other hand focus on the simulation of actions and interactions of agents in order to understand the behavior of a system. Where the agents can represent unique actors or decision makers that are behaving under a set of rules and recognizes differences among the modeled agents [126]. In contrast to an economic model where all the agents are assumed to be identical is called a representative agent model. The agent based models are suitable for the exploration of long-term investment planning under other assumptions than the optimisation models. The agent-based models can for example explore the heterogeneity of actors, consequences of imperfect expectations and investment behaviour outside of ideal conditions [26].

Shortcomings currently used models
In table 1.3, the barriers and models that have been introduced in sections 1.2.3 & 1.3 have been compared. The table shows which barriers per model have been incorporated. Models that focus on the energy transition should pay attention to different forms of investment behaviours and characteristics of the key stakeholders involved in the transition according to Mercure [111]. Mercure states that paying attention to the behaviours and characteristics is needed to understand the barriers that such aspects could pose to reaching a sustainable transition. However, table 1.2 shows that almost none of the models include the barriers to investment. 12 of the 16 models are optimisation models, of which none include all of the barriers. The ABM models are able to incorporate all the barriers, but ABM models are less suitable in determining under which conditions the most effective allocation of capital can be realised. Therefore the shortcomings of the currently used models come down to the following three points:

1. Most of the optimisation models do not incorporate all market & behavioural barriers.
2. Optimization models neglect the inclusion of investment behavior.

3. Agent-based models are not suitable to determine how to optimally allocate investment capital.

Table 1.2: Currently used quantitative models

Model	Reference	Sectors modeled	Approach
DNE21+	[124]	Iron and steel + energy supply	Optimisation model
MARKAL	[69]	Industry + energy supply	Optimisation model
AIM	[91]	Iron and steel	Optimisation model
TIMES	[104]	Energy systems	Optimisation model
ETEM	[48]	Energy systems	Optimisation model
OSeMOSYS	[86]	Electricity	Optimisation model
EnergyPLAN	[106]	Energy systems	Optimisation model
EINSTEIN	[153]	Industry	Optimisation model
OSMOSE	[127]	Industry	Optimisation model
BRAIN-Energy	[10]	Energy systems	Simulation model
PowerACE	[155]	Electricity	Simulation model
BLUE	[102]	UK Energy system	Simulation model
GPM	[97]	Mobility sector	Simulation model
LUSYM	[138]	Electricity	Linear partial equilibrium model
MIDO	[149]	Electricity	Myopic optimisation model
MY-UK TIMES	[123]	UK Energy system	Myopic optimisation model

While these optimisation models are very useful for providing the optimal solution via their normative approach, they are unable to characterise and explain regularities in the choices that people are supposed to make. As, the normative approach of optimisation models provide an account of the choices that should be made. Secondly, the current optimisation models do not fully consider the investment behavior of real-life decision makers and the possibility that these decision makers may not be fully rational. [172]. These models assume perfect foresight and rational investment behavior by neoclassical behavioral assumption [31]. They neglect attention to the actors' bounded-rationality [88]. In reality, decision makers do not have access to perfect foresight at the time of the decision making and are not able to completely analyse all the available information, thus cannot behave as rational actors [66][138][88][116]. In addition, a decision maker at the chlorine cluster does not have insight in future energy prices, future climate policy regulations or profitability of an investment, especially over a long time-horizon [111]. Thirdly, these models do not account for actor heterogeneity. The optimisation models assume homogeneous and rational economic actors [8]. This leads to the fact that the models do not include differences among actors. Li [102] argues that, because of the influence of actors on decarbonisation pathways, actors' heterogeneous and non-optimal behaviours should gain a central role in energy system models. Therefore, despite their high degree of technological detail and mathematical precision, these models had to compromise on defining and aggregating decision-makers. For this reason Bale et al. [8] argue that optimisation models are not be suitable to study real systems made of heterogeneous decision makers.

The chlorine cluster in fact consists out a many type of actors, with varying actor-specific characteristics. The Simulation models can capture (see table 1.2), especially the BRAIN-Energy [10] and GPM models [97]. These agent based simulation models are able to capture the behavioural barriers mentioned in the previous section, unlike the optimisation models. These behavioural barriers all have actor specific origins and therefore a model that takes into account heterogeneity can incorporate these barriers. Even though, these models show the modeling of barriers, they have not modeled industrial systems. The BRAIN-Energy model was used to model energy systems in general and the GPM model used a mobility study as a case. Allthough the ABM models are able to incorporate market and behavioural barriers, they do not fit the purpose that decision makers at the PoR chlorine cluster would need. The decision makers at the PoR chlorine cluster must allocate their investment capital most effectively in order to achieve corporate success [7]. Because of the descriptive approach of ABM models, they are less suitable for finding that normative result.

Table 1.3: Currently used models and incorporated barriers (OM = optimisation model, SM = Simulation model, LPEM = Linear partial equilibrium model)

Model	Approach	Reference	Risk	Imperfect information	Hidden costs	Access to capital	Split incentives	Bounded rationality
DNE21+	OM	[124]						
MARKAL	OM	[69]	X					
AIM	OM	[91]						
TIMES	OM	[105]	X					
ETEM	OM	[48]	X					
OSeMOSYS	OM	[86]	X					
EnergyPlan	OM	[106]	X					
EINSTEIN	OM	[153]	X	X				
OSMOSE	OM	[127]	X	X				
BRAIN-Energy	SM	[10]	X	X	X	X	X	X
PowerACE	SM	[155]	X	X				X
BLUE	SM	[102]	X	X	X		X	X
GPM	SM	[97]	X	X	X	X	X	X
LUSYM	LPEM	[138]	X	X				X
MIDO	Myopic OM	[149]	X	X				X
MY-UK TIMES	Myopic OM	[123]	X	X				X

Suggested approach

So in short, the current optimisation models do not incorporate various market & behavioural barriers or types of investment behaviour. Even though it's claimed importance by multiple authors [68] [159]. However, the optimisation models are very suitable for finding the optimal allocation of capital, which is required by users of decision support models in the industrial sector. Next, Although the ABM models do incorporate these the two categories of barriers, they are not very suitable in determining the most effective allocation of capital due to their descriptive characteristics. So, the currently used models lack the required functionalities to be useful as decision support methodologies in the industrial sector. Therefore, we argue for a model that does have the ability to incorporate the barriers & investment behaviours and at the same time is suitable for finding the optimal solution for the allocation of capital.

An approach that could overcome the shortcomings is suggested by Mier and Azarova [113]. In their paper 'Investor type heterogeneity in Bottom-Up Optimization models', they argue for the expansion of current optimization models with the inclusion of various investment types. They introduce three investor types that are heterogeneous in their investment cost specifications, financing costs and discounting. According to the results of their model, the pace and rate for technology adoption is substantially different [113]. They have made the three types of investment behaviours, by representing them in parameters. The same could argued for representing market and behavioural barriers, where several levels of investment decision making can represent various configurations of barriers. This makes it able to research to what extent market and behavioural barriers contribute to the investment gap at the PoR chlorine cluster.

1.4. Research scope

1.4.1. Research objective

This thesis focuses on researching to what extent market & behavioural barriers contribute to the investment gap, by incorporating both market and behavioural barriers in a quantitative investment model. The incorporation of these barriers in the model result in a range of investment types, some of them non-optimal and varying in perspectives on valuing the future. By simulating technology adoption under the assumption of this range of varying configurations of market and behavioural barriers, we can determine the effect of those two categories of barriers on technology adoption at the PoR chlorine cluster. The obtained insights of this research feed into the larger study of quantitative decision models for the industrial sector.

1.4.2. Research questions

The identified research gap and research objective, lead to the following main research question:

What is the influence of market & behavioural barriers on investment decisions, at the PoR chlorine cluster?

The main research question is to be answered by the sub-questions depicted beneath:

1. What are possible zero-emission technologies that can be implemented at the PoR chlorine cluster?
2. How can we represent market & behavioural barriers in an investment model at the PoR chlorine cluster?
3. What is the effect of market and behavioural barriers on zero emission technology adoption at the PoR chlorine cluster?

1.4.3. Addressing the CoSEM perspective and relevance for WEI

This research is conducted to complete the curriculum of the master degree Complex Systems Engineering and Management (CoSEM). Additionally, this thesis is carried out during an internship at WEI. For both CoSEM and WEI this thesis is relevant. The CoSEM programme focuses on the design in and of complex socio-technical systems. Following the description of the PoR chlorine cluster, the case for this thesis can be seen as such a system. Furthermore, a typical CoSEM thesis has a clear technological component, uses a system engineering approach, complex engineering issues are dealt with, CoSEM methods are assessed to determine the impact of technical solutions an the subject covers values from both the public and private domain. As this thesis considers a highly complex technical system and determines the effect of complex barriers on the technological development of the PoR chlorine cluster, this thesis would fit in the category of a typical CoSEM thesis. Next, for WEI this research is relevant because of the insights that are gained for this specific case and the possible use of this modelling approach in regards to the Water-mining and IMPETUS project. Additionally, the model results give insights for possible decarbonisation pathways at the PoR chlorine cluster.

1.4.4. Structure

Chapter 2 builds forth on the first chapter and it's introduced topics. The second chapter identifies methods to answer the research questions mentioned above. Next, chapter 3 analyzes the PoR chlorine cluster and answers sub-question one. Followed by chapter 4, where we further dive into how we can represent the barriers in an investment model and conceptualise several decision evaluation types which are used in this thesis. In addition, chapter 5 explains how sub-questions one and two are used to conceptualise the investment model and where a detailed explanation is given about how the specifications of the model configuration for this thesis. Next, chapter 6 is dedicated to the application of the model and use & analysis to answer sub-question three. Chapter 7, concludes the thesis with a conclusion, discussion and recommendation.

2
Methodological framework

In this chapter, literature is reviewed in order to find methodologies to answer the sub questions formulated in the previous chapter. First, in section 2.1 the plant-process-product analysis and zero emission technology inventarisation are introduced to answer sub question one. They give an overview of the entire PoR chlorine cluster's technical system and propose a list of alternatives. Secondly, literature on market & behavioural barriers, and how they are incorporated in current models, is reviewed to answer the second sub-question. This method is used to represent market & behavioural barriers in the form of decision evaluation types. Methods for the third sub-question, were also determined by reviewing existing models in section 2.3. Also, this section explains why a modelling approach is chosen. The section also elaborates on the scenario analysis method as a way to use the model. The fourth section combines all the methods in a proposed approach in section 2.3. Lastly, section 2.4 gives a schematic representation of the research activities and research questions that are conducted in this thesis, in a research flow diagram.

2.1. Analysing the case: the PoR chlorine cluster

Two methods have been identified to answer the first sub-question. The first method is the Plant-product-process analysis method. This method gives us a comprehensive overview of the current state of the chlorine cluster. The second method aims to generate a set of alternatives by performing a zero-emission technologies inventarisation. Zero-emission technologies are the technologies that could be employed to achieve zero green house gas emissions. The three main zero emission technology classes that are generally applicable across multiple industrial sub sectors are energy efficiency measures, fuel switching, and carbon capture storage (CCS) [57]. This analysis eventually gives us a set of alternatives for possible future configurations of the PoR chlorine cluster. Both of these methods are used in the industrial sector for energy system related studies according to Scherpbier [151]. In the end, the results of this analysis are used to construct a quantitative investment model.

1. *What are possible zero-emission technologies that can be implemented in the PoR chlorine cluster*

2.1.1. Rationale for choosing plant-process-product & zero-emission technology inventarisation as methods

Sub-question one aims to attain the current state of the PoR chlorine cluster's technical system and technology alternatives that can be implemented at the cluster. Obtaining this information is important, as the goal is to determine the effects of market & behavioural barriers on the adoption of technology alternatives in the chlorine cluster. So, we conceptualize both the current and technology alternatives applicable specifically to the PoR chlorine cluster, in order to explore possible future configurations. There are several methods for analysing the current state of manufacturing processes like the ones at the chlorine cluster. Most of these methods are based on the following two principles:

- System definition
- Process balance

The system definition determines the level of detail of that is chosen to fit the purpose of the study. As we want to know what the possible future configurations are on a asset level, the inventarisation of the technical system should minimally on the same level. Next, the process balance aims to quantify all the elements of the system. These are product flows, energy flows, emissions, waste, etc. A method to analyse systems according to these two principles, is by a material flow analysis (MFA). The MFA identifies a set of inputs and outputs of a manufacturing process and then relates these two to provide information to a mathematical model that can be used to explore opportunities for technology adoption. Therefore, this thesis conducts a MFA on the plant, process and product level in order to attain the current state of the manufacturing systems of the chlorine cluster. Next, an inventarisation of zero emission technologies makes it possible to explore future configurations of the cluster.

2.1.2. Plant-process-product inventarisation

In his master thesis [151], Scherpbier analysed both the chlor-alkali manufacturing industry and the Dutch salt manufacturing industry. He states that the plant-process-product method can be used to adequately analyse industrial manufacturing systems. This method is also used in energy efficiency studies of the industrial sector by Wees and van Arkel [182]. The analysis considers three layers of an industrial plant, the plant level, process and product level.

The data requirements are fulfilled by the MIDDEN database and additional desk research performed where the MIDDEN database does not suffice. The MIDDEN database, short for Manufacturing Industry Decarbonisation Data Exchange Network, contains information on current energy and material consumption of the manufacturing industry in the Netherlands and options for decarbonisation of its processes [134]. The database is structured in four data types GPD, PCD, TC and CD. The General Plant Data (GPD) data set contains basic information about the industrial plants and includes high-level estimates based on public information. Plant Configuration Data (PCD) links plants to the applied technologies. It provides insights on which technologies are or can be applied, on annual production capacities, load factor/utilisation rates, and may include the total annual consumption of certain energy carriers. Third, Technology Characteristics (TC) specifies information on the technologies applied in the plant configurations and information about the inputs and outputs of the processes. Additionally, the data set elaborates on decarbonisation options by giving type of technology, the expected year of introduction, upfront investment and operation & maintenance costs. Lastly, Commodity Data (CD) contains a list of all the raw material, energy and product inputs and outputs represented in the database. Any omissions in the MIDDEN-database are complemented with further desk research.

Plant level

The plant level collects general data about the company, its location, the years of construction, the greenhouse gas emissions. This data level gives insight into how valuable and feasible certain zero-emission technology investments are from the perspective of the company. The plant level inventarisation makes use of the MIDDEN and GPD, PCD and TC dataset tabs. These tabs contain information about about the information of Nobian, Westlake, Huntsman and Shin-etsu on plant level, see 2.1. The product of this part of the analysis are the values of the variables shown in the table below for the four companies.

Table 2.1: Plant level variables and units

Variable	Unit
Plant description	[Description]
Total CO2 emissions per year	[kt/year]
Plant production	[kt/year

Process level

The second level, is the process level. The process level gives a thorough description of the individual process steps that are necessary to produce a certain product. This allows for the identification of possible processes that are viable for alternative zero emission technologies. Moreover, within the considered companies a range of data is gathered to create a detailed technical overview. Where process flow schemes, physical and energetic inputs and outputs, chemical formulas and emissions are given. This gives insight in how the entire value chain is build up and how a change within the an individual process might affect the manufacturing chain [151]. Information on a process level can be found in the TC database tab. The inputs and outputs of specific processes are given, as seen in table 2.2. The product of this part of the analysis is to construct a process overview per company and the corresponding process values.

Table 2.2: Process level variables and units

Variable	Unit
Process description	[Description]
Input per process	[kt/year]
Output per process	[kt/year]

Product level

Last, the product level gives an overview of the outputs sold by the considered companies. The analysis of this level aims to gain a detailed description of the products, production volume, their applications and trade prices. This is helpful in order to asses potential zero emission technologies investments. The product level analysis is conducted by analysing the process overview maps made in the process level analysis and information from the MIDDEN-database. Lastly, all of the variables of table 2.3 are considered and their respective values collected.

Table 2.3: Product level variables and units

Variable	Unit
Product description	[Description]
Market value	[kt/year], [PJ/year]
Main applications	[kt/year], [PJ/year]

2.1.3. Zero-emission technologies inventarisation

After the plant-product-process analysis has made clear how the industrial plants are configured, it becomes possible to identify possible zero emission technology alternatives to the base configuration. Zero-emission technologies are defined as follows:

Zero emission technology refers to any form of technology that releases no greenhouse gasses to the atmosphere [1].

The generally applicable technologies for the industrial that are considered for this thesis are energy efficiency measures, fuel switching and carbon capture storage (CCS) [57]. The data that results from the zero-emission technologies inventarisation should be the type of technology, the renewed process configuration, economic life time, capacity, investment costs, operation & maintenance (O&M) costs. This list of technology alternatives is later on used in the quantitative modelling part of this thesis.

Lastly, this part of the analysis collects all the zero-emission technologies from the MIDDEN database. Both the PCD and TC database tabs are used for this part of the analysis. The PCD tab depicts an alternative technology for the base technology, which leads to a zero-emission configuration. Secondly, the TC tab gives the investment costs and estimated technical lifetime of the installation. The information that is retrieved from these tabs is shown in the table 2.4. These technologies are later on used in the quantitative model, as investment options for the PoR chlorine cluster.

Table 2.4: Zero-emission technologies variables and units

Variable	Unit	Datatab
Technology description	[Description]	PCD
Section within production process	[Section]	PCD
Capacity required	[MWth, kton per year]	PCD
Cost per capacity	[EUR/Unit]	PCD
CAPEX	[EUR]	TC
OPEX	[EUR per year]	TC
Economic lifetime	[year]	TC

2.1.4. Expert elicitation sub-question 1

Three experts have been consulted to obtain information about the PoR chlorine cluster's technical system. Specifically for sub-question one, experts were asked about plant-process-product and zero-emission technology inventarisation. Contact with these experts was set up through the internship at Water Energy Intelligence (WEI). Attention was paid, to specifically contact experts who were involved with the production processes at the respective companies. The personal communication with the three experts are summarized in Appendix C.

2.2. Representing market & behavioural barriers

This section dives deeper into relevant literature regarding market & behavioural barriers. First, several perspectives on the barriers are given and how they lead to the taxonomy of six barriers. Followed by section 2.2.3 that further explains the market & behavioural barriers of Sorrell [159] . Then, existing models from section 1.3 have been reviewed and new literature was added (see search strategy 2.5). This resulted in finding a method of representing market & behavioural barriers in the form of a decision protocol, decision evaluation types and decision acceptance criteria, which are discussed in the last subsection.

2. *How can we represent market & behavioural barriers in an investment model at the PoR chlorine cluster?*

2.2.1. Perspectives on barriers to zero emission technology adoption

According to Sorrell, there are multiple perspectives that give their view on the barriers to the adoption of zero emission technologies. He discusses these perspectives according to, the nature of human rationality, the role of markets and the usefulness of several schools of economic thought [159]. In line with his reasoning, this section gives an overview of four economic perspectives and their views on barriers to zero emission technology adoption. The four perspectives are orthodox economics, agency theory and economics of information, transaction cost economics and behavioural economics (see figure 2.1).

According to Sorrell, the orthodox economic perspective is based on formalised mathematical models and unrealistic assumptions about human decision-making. This is in contrast to transaction cost economics, where decision makers do not make optimal solutions, but rather rely on routines and rules of thumb [158]. Behavioural economic takes it a step further and argues that decision-making is not only bounded rational, but also systematically biased and erroneous [90]. Sorrell [159] states that all of these perspectives are relevant and therefore bases his taxonomy of barriers on the combination of these perspectives, see figure 2.1.

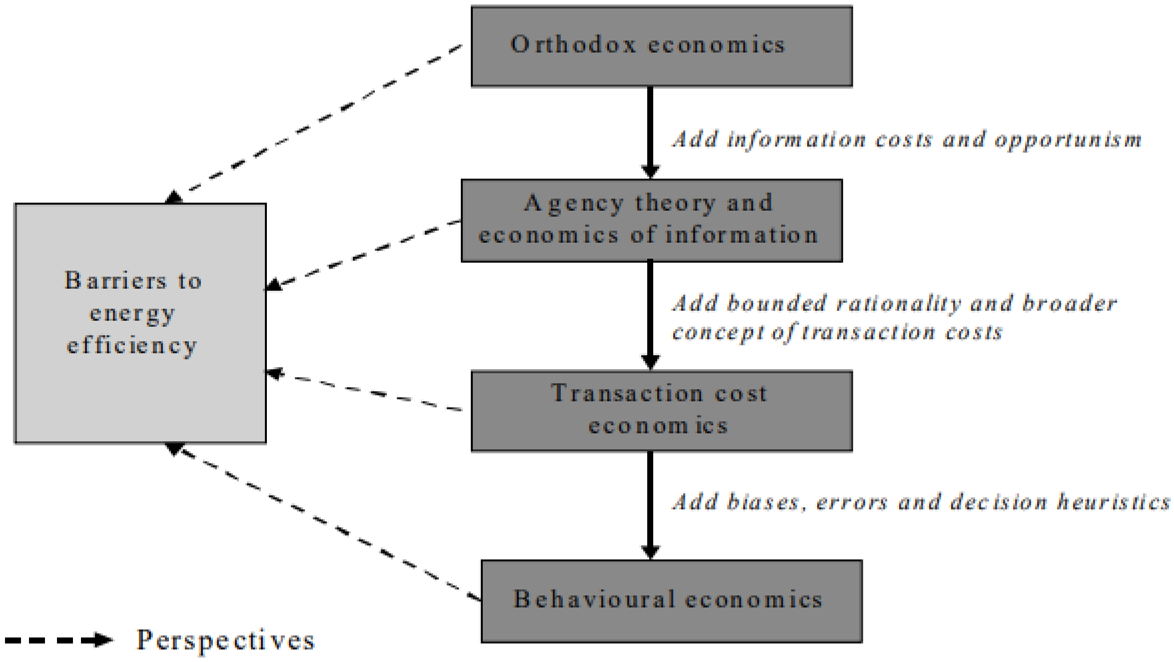

Figure 2.1: Perspectives on barriers [159]

2.2.2. Market barriers

Risk

The decision-making at the chlorine cluster, largely depends on anticipating change in a highly uncertain environment [109]. These uncertainties are caused by the imperfect foresight of the future as, it is impossible for decision makers to determine the outcome of a investment project with absolute certainty. Such a situation characterises itself where there exists a many plausible futures without knowledge about the relative likelihood of these futures [98]. Uncertainty caused by imperfect foresight leads to risk for the investor, as unexpected variations in determining factors could seriously impact the outcome of an investment. The sources of risk ranges from, the macro economic trend, government policy, uncertainty in fuel and electricity prices, financing risks and technical risks. [150] [47].

Imperfect information

The second barrier of the barriers debate regards the importance and implication of imperfect information. The importance of imperfect information as a barrier has often been empirically shown. The term comprises the knowledge about the availability of an energy-efficient technique, but also about its characteristics like costs and saving potentials as well as the actual energy consumption of the equipment in place [66]. De Groot et al. [37] conducted a survey among Dutch firms and found that 30% of the companies interviewed were not, or only to a minor extent, aware of new existing energy-efficient technologies or practices. Next, the actually realized savings of an alternative might turn out to be lower than expected. Comparable to the brochure about the fuel efficiency of a car. The brochure said that the car should run at 20 km/l on average. However, in reality it turns out to be 17 km/l. As many case specific factors play a role in the performance of technical systems like, the driving style of driver, the weather, the alterations of the car all have an impact on the mileage.

Hidden costs

Hidden costs refer to the costs which are generally not included within commonly used quantitative models[159]. There are roughly three main possible sources of hidden costs: the general overhead costs of energy management, the costs which are specific to an individual investment or the choice of a technology and it's potential loss of utility [159]. The general overhead costs might occur due to the costs of employing specialist employees or due to the cost of energy auditing. Followed by costs involved in individual technology decisions, that leads to additional staff costs for maintenance or the cost of formal investment appraisal. Lastly, the loss of utility associated with energy efficiency choice. All of these costs have effect on the eventual OPEX of an technology alternative. Where before hand the costs were expected to be X, but after installation the costs turn out to be 1.1*X.

Access to capital
Access to capital is a commonly used barrier in literature [82]. The access to capital barrier has two parts: no access to internal capital and issues in raising capital through external sources [119]. The restricted access to internal sources of capital are mainly due to the organizational culture towards energy investments. These investments are most of the time classified as business maintenance projects, which are given lower priority than either essential business maintenance projects, such as replacing a failed pump, or strategic business development investments, such as a new manufacturing plant [159]. Second, such projects tend to be evaluated using payback rates rather than discounted cash flow analysis, with the required rates of return exceeding those for business development projects [170]. The issues in raising capital through external sources, is often based on a negative corporate bias to raising external funds. According to Sorrell firms appear to be reluctant to borrow money to finance energy investments due to the perceived risk of taking loans.

2.2.3. Behavioural barriers

Behavioural economics is an economic school which studies the effects of psychological, cognitive, and social factors on economic decision-making and how those decision may vary from classical economic theory [103]. According to the school, realistic decision behaviour is less rational and stable than assumed in classic economic theory. The reduced rationality and stability result in the bounded rationality and split incentives barriers [159].

Bounded rationality
The theory on bounded rationality was first coined in 1957 by Herbert Simon. Simon suggested that bounded rationality takes into account the cognitive limitations of the decision-maker of both knowledge and computational capacity [173]. This leads to the decision maker not knowing all the investment alternatives, consequences and preferences. These limitations lead to the decision maker making sub-optimal decisions. But this does not mean that the decision maker makes decisions out of thin air. The decision making is taken to be procedurally rational which implies that individuals are rational in the sense that their decisions are goal directed [184]. The neoclassical economic perspective states that individuals and organizations can be conceived as perfectly rational and utility maximizing [36]. The available information is complete and the decision maker has complete access to it, with which he makes optimal rational choices. However, the reality shows that the assumption of profit-maximisation may be a oversimplification of real-life investment behavior[111] [32]. Since most of the decisions are made by decision makers display behaviour characteristics [157] [77]. This is due to the bounded rationality of decision makers.

Split incentives
Split incentives result from asymmetric information and transaction costs. The barrier used a lot in relation to rental housing, but is also wider applicable [159] In the rental housing sector, split incentives follow from the landlord-tenant problem. The landlord and tenant have varying incentives when it for example comes to energy-efficiency. Most of the rented out housing is owned by large investors who treat the property purely as an asset, while management is outsourced to for example, property consultants who pay little attention to energy efficiency. The tenants in turn may have little to no motivation to increase the energy efficiency of an asset they do not own [159]. The landlords are happy to pass on the energy costs to their tenants. In many cases, tenants will simply pay a fixed share of the building's energy bill, which means the savings generated by investment or behavioural changes by one tenant would flow to all the other tenants as well, thereby weakening the incentive. This example of the landlord-tenant problem can also be used to the PoR cluster's case. Within organizations, the bias towards projects with short term paybacks may also result from split incentives. It is often the case that managers remain in their post for relatively short periods of time [38]. In large companies, there may even be a policy of job rotation. But a manager who is in a post for only two or three years has no incentive to initiate investments that have a longer payback period. This may result in the decision to invest in assets that have large returns on the short-term. Although these investment may prove inferior to other investments in the long term. As with landlords and tenants, problems of asymmetric information and transaction costs may prevent the incentive structure from being modified. Even if the short rotation period is not present, Statman and Sepe [160] mention that decision makers remain biased towards investments with short-term payback periods.

2.2.4. Review of models that include market & behavioural barriers

This section elaborates on how models incorporate the explained barriers from the previous section. The found models are depicted in table 2.6. For the used research strategy, the terms shown in table 2.5 were used. The literature was retrieved from Google Scholar and Scopus. Moreover, the snowballing and citation search method were used.

Table 2.5: Search strategy literature study

Keyword	Decision behavior	Models	Energy systems
Synonym	Investment decision-making	Quantitative modeling	Energy transition
	Market & behavioural barriers	Investment modeling	Industrial sector

Table 2.6: Models that include market & behavioural barriers

Model	Reference	Method	Decision metric	Parametrisation
BRAIN-Energy	[10]	Decision heuristics	Single objective: NPV	Discount rates
BLUE	[102]	decision evaluation types	N.A.	hurdle rates
GPM	[97]	decision evaluation types	Single objective: NPV/NPB	Discount rates
SAVE	[34]	decision evaluation types	Single objective: NPV	Discount rates
ISIndustry	[55]	decision evaluation types	Single objective: NPV	Discount rates
LIEF	[143]	decision evaluation types	N.A.	N.A.

Barazza [10] introduces an agent based electricity model (BRAIN-Energy) that assumes a great diversity of types of market players and their characteristics. With that model, Barrazza shows the effect actors' heterogeneous characters barriers pose to effective decarbonisation efforts. Economists mostly use the term "heterogeneity" to refer to the multiple dimensions according to which economic agents could differ [141]. As, the results of the article show a significant difference between scenarios that have ran with and without heterogeneous characteristics. In the end, article concludes with the importance of incorporating barriers like bounded rationality and split incentives to better represent real life decision making.

Barrazza models heterogeneous decisions makers in the model by using investment protocols to represent different types of market players. The protocols represent 'rules of thumb' that are used to select alternatives. The modeled approach employs a practical method that is not guaranteed to be optimal, perfect or rational, but is sufficient for reaching an approximation. The variation between market players is represented by the level of rationality. Market players have different strategies, which define their behaviour and actions through time. For example via profit maximisation. Followed by the availability of information, which is modelled with limited foresight and the selection of alternatives with the technology preference characteristic. To conclude, the investment protocols are reflected by combining all the different market player characteristics and strategies.

Next, Li's BLUE model [102] uses market heterogeneity and hurdle rate parameters to explore non-optimal actor behaviour. The market heterogeneity, in the form of 4 different levels of decision behaviour, illustrates ranges of rationality and selection of alternatives. The hurdle rate settings affect the actor sensitivity to up-front investment to reflect the availability of information. Furthermore, the hurdle rates can be used to indicate the extent to which different actors value the present compared to the future and their resulting attitudes towards investments with high up front capital costs [102].

Third, Knobloch & Mercure also make use of several levels of decision-making. They argue that three key areas from behavioural economics are relevant for energy policy, namely bounded rationality, heuristic decision-making and prospect theory. First, bounded rationality replaces unbounded maximisation with satisficing behaviour [97]. The bounded rational investment behavior manifests in the form of critical thresholds. This may explain why companies use simplified pay back thresholds as a key decision criterion instead of net-present-value (NPV) calculations [97]. The last key area, prospect theory helps to explain various behavioural biases that might be relevant for investment in zero-emission technology. An example is an empirical study performed by Greene [76]. The study shows that that losses are weighed almost twice as much as gain. Where for a rational investor a change in loss should have the same effect on a decision as a change in expected future pay offs [5]. This example of a behavioural bias is termed as loss aversion. The investment protocols of Knobloch & Mercure are based on the barriers by Sorrel [159], where they are used to determine parameters for the decision protocols.

The SAVE Production model considers risk, psychological effects of energy price changes and energy efficiency policies and bounded rationality, next tot the cost-effectiveness of the investment as decision factors [66]. The risk and psychological effects in the model, are considered as a discount rate.

The same counts for the ISIndustry simulation model. Both market and behavioural barriers are modeled with discount rates. Where all the barriers are aggregated into a single rate [66].

Lastly, the LIEF model is able to determine main variables based on their historical trend and account for the bounded rationality within firms, while at the same time considering for potential new technologies. In this model the market and behavioural barriers are implicitly considered in that historic trend but not explicitly modeled.

To conclude, various models show that discount rates are used to approach or mimic market and behavioural barriers. Specific causes of implicit discount rates include a lack of information about cost and benefits of efficiency improvements, a lack of knowledge on how to use available information, uncertainties about the technical performance of investments, a lack of sufficient capital to purchase efficient products, high transaction costs for obtaining reliable information, risks associated with investments [118]. Only the BLUE model of Li [102] hurdle rates.

2.2.5. Representing market & behavioural barriers in the form of decision evaluation types

As remarked at the end of the previous subsection, the reviewed models generally use evaluation types and discount rates to incorporate market & behavioural barriers. Where most of the models use discount rates in NPV calculations to aggregate the effect of market & behavioural barriers. Also, the heterogeneity of decision makers within the models is accounted for. Where the perception of risk, level of imperfect information, hidden costs, the access to capital, bounded rationality and split incentives can vary among the decision makers. Below, a further elaboration of decision protocols, decision evaluation types and heterogeneity is given. Afterwards, an approach for the representation of market & behavioural barriers is given to answer sub question 2.

Decision protocols in reviewed models

In this thesis decision protocols refer to procedures used to represent decision making. This subsection examines six different models regarding their incorporated protocols. The six models shown in tab 2.7 are analysed according to two main topics: How technology is modeled and how technology replacement is modeled. First as shown in the first two columns, 4 out of the 6 models explicitly model technology adoption on a detailed technical level. The other two model technology change as a mostly exogenous phenomenon. They did not model technological change, because that level of detail was not necessary for the scope of these models, as these represent systems on national levels and not on an asset level. The last column specifies two ways of modeling technology replacement in the reviewed models. All of the models that explicitly model technology use the replacement after life time rule to model technology replacement. Only the BRAIN and GPM model also use the early replacement allowed rule. So, in that case the investment decision can also be made before the end of lifetime of installed assets.

Table 2.7: Decision protocols in reviewed models

	Technology not explicitly considered	Explicity technology stock model	Technology replacement rules	
	Technology change is mostly exogeneous	*Technology adoption depends on lifetime and the age of current technologies*	*Replacement after lifetime*	*Early replacement allowed*
BRAIN		X	X	X
BLUE		X	X	
GPM		X	X	X
SAVE		X	X	
ISIndustry	X			
LIEF	X			

Decision evaluation types

The methodology of Knobloch & Mercure [97] uses the same market & behavioural barriers, as the ones represented in section 1.2 [159]. Therefore, this method is chosen to conceptualise for this thesis. Their methodology aims at representing the barriers in the form of decision evaluation types. The decision evaluation types are a form of quantitative assessment used for assessing and comparing technology alternatives [185]. The decision evaluation types are build up on four different variables, shown in table 2.8. The eventual metrics result in formulas and are represented in the form of Net Present Value formula's and pay-back periods.

Knobloch & Mercure use a methodology based on three building blocks: perceptions, heterogeneity and risk. They argue that perceptions may differ between individuals. As the interpretation of the same set of data may be interpreted differently by different companies or modellers. Secondly they argue for the incorporation of heterogeneity in their methodology. diversity of economic fundamentals and decision-making perception imply heterogeneous decision makers according to Knobloch & Mercure. Lastly, they state that risk affects the decisions of companies. As risk is not per se an objective value, but can vary between companies depending on the respective perception. This results in their modelling of decision evaluation types by four different building blocks. The level of rationality and it's respective assumptions, barriers and parameters, see table 2.8.

Table 2.8: Decision evaluation metric variables following Knobloch & Mercure [97]

Variables	Description
Levels of decision-making	The levels of decision-making vary in their level of rationality. The modeled rationality goes from assuming a single representative company that decides according to a perfectly rational decision maker, to a totally behavioural decision maker.
Assumptions	The assumptions that are included per decision-making level. Ranging from assumed homogeneous agents with perfect information and unbounded rationality to heterogeneous agents with bounded rationality.
Barriers	The barriers described in section 1.2.3 are linked to the respective assumptions per level. From no barriers to all.
Parameters	The parameters that are used to quantify the assumptions and barriers per decision-making level.

2.2.6. Heterogeneity

The last subsection is dedicated to explaining heterogeneity shown in the the models from table 2.7. Optimization models usually model decision makers as a representative agent. In these models the individual agents are represented by a single decision maker. In the case of the chlorine cluster, this would mean that there would be modeled four different decision makers instead of one. Knobloch & Mercure state that perceptions differ between individuals. The same set of information regarding an investment can be interpreted differently by different companies. Where an investment could be viable for Nobian but not for Shin-Etsu. Secondly, they elaborate on the heterogeneity of economic fundamentals and that decision-making perception imply heterogeneous decision-making. The investment of a homogeneous technology may be viable for the average company, but not for all companies, due to the various contexts and diverse characteristics of the respective companies. Lastly, risk affects the decisions made by companies. There are various aspects that make an investment risky, for example the uncertainty about future profitability or future demand.

2.2.7. Expert elicitation sub question-2

For this sub question, the personal communication with the two of the three experts gives information regarding the company specific decision evaluation types and their decision acceptance criteria. This assignment in turn could be used in one of the scenario's used in chapter 6. The contact with these experts is summarized in Appendix C.

2.3. PoR chlorine cluster investment model

This section is dedicated to sub question 3. The first subsection 2.3.2 explains the rationale behind choosing a modelling approach. Followed by the second section that dives deeper into the theory behind the modeling approach. The last subsection explains how a scenario analysis can be used, to use the model and answer sub-question 3. As, the scenario analysis aims to find what the influence of the behavioural barriers on investment decisions are at the PoR chlorine cluster.

What is the effect of market and behavioural barriers on zero emission technology adoption at the PoR chlorine cluster?

2.3.1. Rationale for choosing a modelling approach

This subsection explains why a modelling approach is chosen to answer this sub question 3. Sub question 3 flows forth from the lack of research regarding the effect of behavioural barriers on the investment gap. So, this question aims to understand how these barriers interact in a socio technical system and to compare the effect that market barriers have on investment decisions. The rationale for choosing the simulation modelling approach is explained by comparing various methods used within the CoSEM programme. A complete list of commonly used methods within the CoSEM programme is shown below. The characteristics of every approach is explained and in the end concluded why the modelling approach is most suitable for this thesis.

- Design approach
- Case study approach
- Quantitative research approach
- Exploratory approach
- Modelling approach
- Mixed methods approach

First, the design approach can be used to fill a void in the functioning of a socio-technical system, by making a design. The TIP-approach is a commonly used design approach at TPM. TIP, short for Technological, Institutional and Process, gives a holistic approach to design from a multi disciplinary perspective. Thinks of design that result in interventions within socio-technical systems or systems as a whole. Second, the case study approach is used to understand phenomena for a very specific situation. The approach can explain for example social phenomena or difficult identifiable mechanisms, where case specific characteristics are significant. Third, the quantitative research approach is for example used to quantify the relation between A and B. A common approach is to formulate hypotheses that are based on a theory or framework to test the relation between A and B. Next, the exploratory approach can be considered to develop theories based on qualitative analysis. Fourth, as mentioned earlier in chapter 1, the modelling approach might be useful to account for shortcomings of currently used models. The modelling approach is commonly used to replicate real-world systems. By replicating the real-world, it becomes possible to identify how the system works under varying conditions and determine the impact of system interventions. Lastly, the mixed methods approach is based on the combination of multiple approaches, like the ones described above. Following the description of the approaches above, the modelling approach fits this sub-question the best. As this thesis focuses specifically on the PoR chlorine cluster and how to replicate that system in a model. Followed, by the determination if market & behavioural barriers affect investment decisions and to what degree. By incorporating these barriers in a model it becomes possible to explore how technology adoption at the chlorine cluster works under varying configurations of these two categories of barriers. To sum up the three reasons:

- Suitable method to replicate a real world system, in this case the PoR chlorine cluster.
- Allows to determine the influence of barriers on investment decisions and thus, gaining a better understanding of the investment gap.
- Follows from the research gap to address the shortcomings of the currently used models.

2.3.2. The modeling approach

In order to determine the influence of market & behavioural barriers on investment decisions at the PoR chlorine cluster, a modeling approach is chosen. According to the theory on modelling approaches, it is important to consider the following three main concepts [94]:

1. What is the purpose of the model?
2. What types of data are available to develop and specify the model?
3. How should the model treat space, time, uncertainty, structure and resolve?

Model purpose

According to Kelly, et al. [94], models can have five different purposes. The models can be used for prediction, forecasting, management & decision-making under uncertainty, social learning and developing system understanding. When a model is used for prediction, it involves estimating the value of a system variable during a specified time period, given knowledge of other system variables during the same time period. They are generally developed to predict the effect of a change in system inputs on system outputs or performance [94]. As a second purpose of models, forecasting can predict the value of a system variable in future time periods, without knowledge of the values of other system variables during the same periods. Examples of such models are weather forecast models or price forecast models. Third, management and decision-making under uncertainty can benefit from models that are used for decision support systems. When models are used for this purpose, they may be simulation-based and answer the 'what if' question. They can also be optimisation-based and search for the best option given the specific circumstances. These two ways of modeling are in line with the models that have been analysed so far. Next, social learning refers to the ability of a network to communicate, learn from past behaviour and perform collective action [78]. Where models can learn users by experimentation to further understand how the modeled system works [94]. Lastly, a model purpose can be used to develop system understanding. Developing system understanding/experimentation is the purpose of many models developed to summarise and integrate available knowledge on system components in order to improve understanding of the entire system and the way it may react to changes in system drivers [94].

Types of data available

Data that is used in models can either be quantitative or qualitative. Quantitative data is information that is numerically measurable. Qualitative data is information that can be observed and can generally not be measured in a numerical way [94]. The model purpose and model conceptualisation is strongly dependent on which data is needed and what is accessible for the researcher.

System conceptualisation

When describing the system that is to be modeled, generally five dimensions can be specified: space, time, uncertainty, structure and resolvement. Underneath the five dimensions are explained.

Treatment of space
According to Kelly [94], there are four different approaches to treating space in a model: non-spatial models, lumped spatial models, compartmental spatial models, grid, cell or element-based spatial models and continuous space models. The non-spatial models do not make a reference to space. These models are used in circumstances where the confinement to space is not relevant to the modeled system. Next, lumped spatial models calculate internal states and provide outputs for the selected area that is modeled. Where in the case of this thesis, that would be the PoR chlorine cluster. Third, compartmental spatial models provide the same information as the lumped spatial models but make more distinction within the systems by making 'compartments'. Kelly [94], uses the example of a lake to explain the compartmental spatial models. A lake can be split up into areas within a short distance from the shoreline, the creek leading into the lake and the deeper lake systems. All the interactions between these three compartments are then considered in the model. In the end, the model is able to calculate internal states and outputs for these specific compartments. Next, the grid, cell or element-based spatial models provide calculations over a uniform or non-uniform grid representation [94]. This type of treatment of space has a lot of overlap with the compartmental spatial models. But in these kind of models, all though

there are homogeneous characteristics between elements, they are still modelled separately. Lastly, the continuous space models take into account every detail of a chosen modelled area.

Treatment of time
Models can treat time via a multiple approaches, these are the common ones [94]: Non-temporal, lumped, discrete temporal, and continuous. Non-temporal models do not make a reference of time and are considered as steady state models. The lumped models give outputs over a single time period, such as the average of a value over the modeled time period. The dynamic models provide output per time step over a specific period. For example over a run time of 30 years with a time step of 1 year, there will be 30 outputs. Lastly, the continuous models model time as infinitely small.

Uncertainty
The uncertainty that is taken in to account can be derived from multiple sources. It might be originating from uncertainties in system understanding, from uncertainties in the interpretation of data or from uncertainty from the inputs/conditions used for model runs [94].

Treatment of entities or structure
Models can treat entities in various ways. Some models are designed to calculate averages for a population or phenomena. These are called aggregated models. On the other hand, agent-based models are designed to simulate individuals as agents and their interactions with each other and their environment [94] These models are referred to as multi-agent systems or individual-based models.

Resolving the model
According to Kelly [94] there are three general approaches for generating output: scenario-based, analytical, optimisation. The scenario-based approach can incorporate impacts of for example management interventions or decision options. This approach is mainly used to allow the model user to explore the effects of these independent variables or the conceptualised dependent variable. Secondly, the analytical approach is used to solve the model equations analytically [94]. This approach gives a very detailed understanding of a selected system. Lastly, the optimisation approach is used to determine the best state of a system given a certain objective function and constraints [94].

2.3.3. The CCI model: A heterogeneous investment level bottom-up optimization model

There are various types of models that fit in the description of modelling approaches shown above. This thesis therefore presents the Chlorine Cluster Investment (CCI) model. Underneath the model is explained by elaborating on the model's purpose, types of data needed and a system conceptualisation.

Model description and purpose
Following the investment gap of chapter 1, we argue that there is a need to better understand the role of market & behavioural barriers on zero emission technology adoption. Moreover, from the research gap followed that the current optimization models fall short in representing market & behavioural barriers, even though importance of it's representation is broadly acclaimed [95]. Even though the ABM models are capable of representing these barriers, they are not suitable in finding the optimal allocation of capital where the decision makers at the PoR chlorine cluster aim for. In order to better understand the role of market & behavioural barriers on technology adoption and filling the research gap, we aim to present a heterogeneous investment level bottom-up optimization model called the CCI (Port of Rotterdam Chlorine Cluster investment) model. This model should be able incorporate the representation of heterogeneous decision makers investment types. Followed by an exploration of the impact of those aspects on the zero emission technology adoption at the chlorine cluster. This makes it possible to possible to gain insights regarding the influence of barriers on investment decisions at the PoR chlorine cluster. The objective for the model would be to minimise the cost of technology adoption under the condition of various configurations of barriers and exogenous market conditions. Think of uncertain exogenous factors like electricity prices, gas prices and commodity prices.

The model is represents the PoR chlorine cluster on a highly detailed level and bases it's technical system's configuration on the plant-process-product & zero-emission technology inventarisations of the first sub question. This makes it possible to explicitly model the technology stock at the chlorine cluster and determine technology adoption on an asset level. The incorporation of the various market & behavioural barriers and investment behaviour is conducted by the methodology described for sub question two. The investment behaviour is represented by the decision protocol and decision acceptance criteria. Where the decision protocol to aims to capture technology replacement behaviour, following the reviewed models in section 2.2.5. Next, the decision acceptance criteria explain under which conditions investments are made in the model. The market & behavioural barriers are represented by different levels of investment decision making. These levels of decision making follow the methodology of Knobloch and Mercure [97].

The eventual model is relevant for both the decision makers and future researchers. This model will enable decision makers at the PoR chlorine cluster to determine the effective allocation of capital for technology investment, given certain configurations of barriers and exogenous factors. Secondly, the model enables future researchers to further research the relationship between market & behavioural barriers and the investment gap. The proposed methodology can be applied to other technical systems and it's representation of the market & behavioural barriers can be varied using the above mentioned methodology. To conclude, the CCI model should lead to a clarification of current understanding of investment decision-making in the industrial sector and aims to improve quantitative analysis.

Types of data used
The model is calibrated using the MIDDEN-database for proposed investments and plant specific data about the chlorine cluster. Next, literature is reviewed to conceptualise the decision protocol, decision evaluation types and decision acceptance criteria. That conceptualisation is shown in chapter 4. Third, quantitative data is collected to conduct the scenario analysis. In order to explore actor behaviour, transition pathways in the energy system that deviate from strict economic rationality are modelled in the context of other key uncertainties such as fuel prices and technology costs. Eventually, cost-optimal investment behaviour is compared against cases where actors make a range of investment choices, some of them non-optimal, and have different perspectives on valuing the future. In order to determine the effect of behavioural in comparison to market barriers on zero emissions technology adoption.

System conceptualisation
The model simulates the chlorine cluster's operations with a yearly time step between 2022 and 2050 and simulates investment decisions under varying decision evaluation types. Both the physical flows and financial flows are modeled between the companies shown in figure 3.3. The investment part of the model is represented by a decision protocol, various investment decision evaluation types and decision acceptance criteria. The investment decisions comprise of either replacement investments or expansion investments, as introduced in chapter 1. Where for example a CHP at Nobian is replaced by a sustainable alternative like an electric boiler. Or the production process is expanded by the installation of pipeline between Nobian and Westlake to transport commodities. Lastly, the model uses a yearly time step and simulate between the period of 2022 and 2050.

All of the above is represented in a simplified manner in figure 2.2. On the left side, the inputs for the CCI model are given. Which is a combination of the technical system, the investment decision making part and the key inputs that come from the exogeneous environment. Think of inputs like energy prices, CO_2 prices and so forth. The model transforms these inputs into three key outputs, the transition pathways, total CO_2 emissions and total cash flows. Where the transition pathways show the technology adoption between 2022 and 2050 on an asset level. The two remaining outputs function as performance indicators for the system.

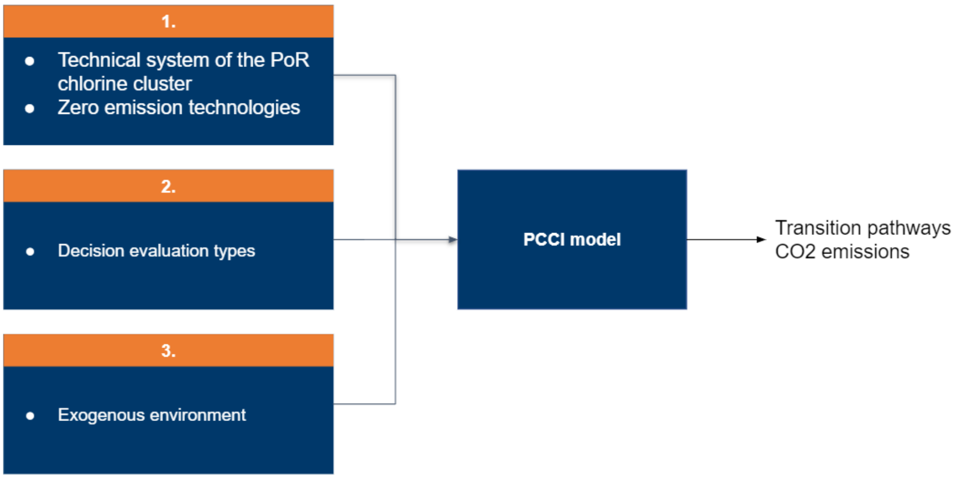

Figure 2.2: Overview of the CCI model

2.3.4. Using the model with a scenario analysis

To use the model and determine the influence of market & behavioural barriers on investment decisions at the PoR cluster, a scenario analysis is conducted. According to Duinker and Greig, scenario analysis has become a popular approach in the field of sustainable development [49]. Scenario analyses can be used as a tool to explore and/or describe future alternatives. Where these futures might be possible, probable or preferable futures. The what may happen, what is most likely to happen and what would we prefer to happen questions are answered. During this thesis the scenario analysis aims to answer the possible futures question. As we aim to explore what a technological system outcome might be in the future given certain model calibrations.

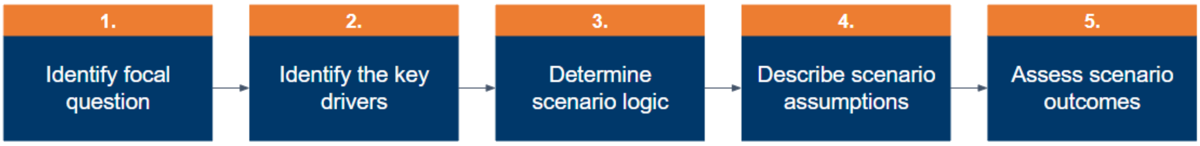

Figure 2.3: Fives steps for scenario analysis [112]

The scenario analysis follows the five steps described in figure 2.3. The identification of the focal question is defined in chapter one, where the main aim of the scenario analysis is to determine the effect of market & behavioural barriers on zero emission technology adoption at the PoR chlorine cluster.The second stage is dedicated to the identification of key drivers that affect the focal question. The analysis for this step is conducted with a STEEP analysis. STEEP stands short for Societal, Technological, Economic, Environmental and Political. The analysis method is used in business studies and policy literature to identify external factors that affect an industry or organization [164]. The analysis is performed with desk research. Szigeti states that professional consulting organizations define the STEEP analysis as an "audit of an organization's environmental influences with the purpose of using this information to guide strategic decision-making". The method helps to obtain a detailed overview of present and future opportunities and threats faced by in this case the PoR chlorine cluster [164]. By identifying key driving forces on a societal, technological, economic, environmental and political level, policies and uncertainties can be identified that drive change in the system under this study. Here the STEEP analysis is used to determine the future opportunities and threats regarding policies and uncertainties that have to be taken into account during the model application & analysis. The third step determines the scenario logic. This step results in a 2X2 matrix where the key drivers from the STEEP analysis are placed on the y and x axis. Next, a description is given about the scenario assumptions. This part elaborates on the configuration of internal and external system variables, like the specific parameter values of the evaluation metrics and values for energy prices. The last step is dedicated to the assessment of scenario outcomes. Here is assessed what we can conclude from these results regarding the impact of the market & behavioural barriers on investment decisions at the chlorine cluster.

2.4. Research flow diagram

The research flow diagram (RFD) in figure 2.4 gives a visual representation of the research design that follows from the previous sections. The diagram distinguishes five main phases and shows how the various research activities contribute to the answering of the sub-questions. The first phase starts off with the desk research. During this phase the conceptualisation of a decision protocol and evaluation metrics 2.2.5, plant-process-product inventarisation, zero emission technology inventarisation 2.1.2 are conducted. Followed by the second phase 2.1.4 where we conduct the empirical research. The empirical research is conducted via expert elicitation 2.2.7, where interviews are used to help determine the heterogeneity within the evaluation metrics 2.2.5 fit best to one of the companies at the chlorine cluster. This assignment will later be used as one of the scenario's during the model use. The expert elicitation is also used to validate the case study on the PoR chlorine cluster. The third phase is dedicated to the model design. During this phase the CCI model is designed. Hereafter, the model use phase aims to answer sub-question three, by model experimentation and analysis. The last phase concludes with a conclusion, future research and recommendations.

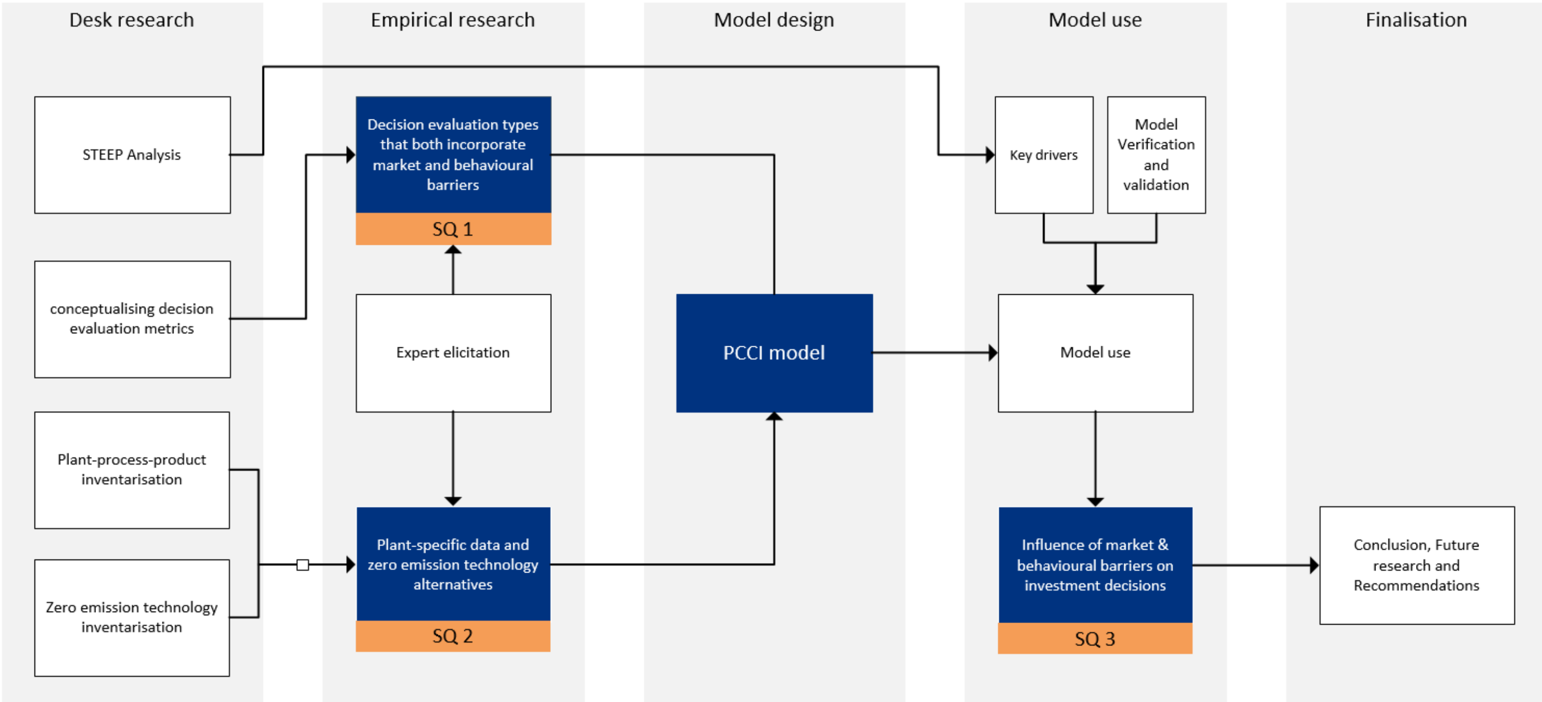

Figure 2.4: Research flow diagram

2.5. Reflection on research activities

This section reflects on the research activities of this master thesis, that have been elaborated earlier this chapter. In table 2.9 an overview of the research activities, corresponding data sources and the respective strengths/limitations are shown.

Table 2.9: Reflection on research activities

Research activities	Research data sources	Strengths/limitations
Plant-process-product inventarisation	MIDDEN-database & desk research	**Strength**: Gives a highly detailed overview of the current state of the technical system. **Weakness**: may prove to be difficult to quantify all the processes and prices accurate for the specific companies
Zero-emission technology inventarisation	MIDDEN-database & desk research	**Strength**: the combination using the MIDDEN-database which is filled by experts within the field and desk research for omissions leads to a good overview. **Weakness**: the MIDDEN-database might be biased by the contributing researchers and companies
Conceptualisation decision evaluation types	Literature review	**Strength**: Many other researches use the same way of representing barriers. Also, flexible method to add more forms of representation of barriers. **Weakness**: gives a selected overview of market & behavioural barriers. Also, all decisions will be made with the same protocol rather than various decision heuristics.
Expert elicitation	Interviews	**Strength**: retrieves information right from the source, leads to more accurate data **Weakness**: the interviewees might not have all the specific information that is required. Besides, the interviewees might opt not to share certain information.
Scenario analysis	Desk research	**Strength**: the scenario gives a good overview of the most likely futures. **Weakness**: does not lead to robust solutions and a thorough exploration of possible futures.
STEEP analysis	Desk research	**Strength**: the STEEP analysis is a common used method. It helps to structure and identify the key drivers that influence and change the PoR chemical sector. **Weakness**: it is difficult to gain a complete overview of all the key drivers based on desk research.
Model experimentation	Computer model	**Strength**: Fast and flexible way of representing simplified version of reality. **Weakness**: all models are wrong and therefore might lose practical relevance for this specific case.

3

Case: The PoR chlorine cluster

This chapter is dedicated to the PoR chlorine cluster, of which specifically Nobian, Shin-etsu, Westlake and Huntsman are considered. First an introduction 3.1 to the chlorine cluster is given where the history and important connections & dependencies are explained. Next, two types of analysis are conducted, the plant-product-process inventarisation 3.2 and zero emission technology inventarisation 3.3. In the last section 3.7 of this chapter, a complete overview of the technical system and technology alternatives is given and answers the sub question:

1. *What are possible zero-emission technologies that can be implemented at the PoR chlorine cluster?*

3.1. Introduction to the PoR chlorine cluster

3.1.1. History of the PoR chlorine cluster

The PoR chlorine cluster consists out of companies located in the Botlek and Pernis areas. These areas are both important harbour as industrial areas. Both these areas were chosen for development, due to it's strategic location [130]. Around 1900, the first companies started to use the area t store their goods and later on production sites were built at the Waalhaven. The development grew westwards and resulted in the completion of the Pernis petroleum harbours in 1933 and 1941. This area is still renowned, mainly because of the large Shell refinery located in Pernis. After the end of the war, plans were developed to develop the Botlek are. The construction started in 1954 with the arrival of DOW chemical and was further on built between 1960 and 1980 [130]. Where the Pernis area was mainly a petroleum area, the Botlek area was settled by chemical companies. This eventually resulted in the current chlorine cluster, taking up a part of both the Botlek and Pernis areas.

3.1.2. Important connections and dependencies of the PoR chlorine cluster

As earlier introduced in chapter 1, the PoR industrial cluster is a highly interconnected area. There have been developed several infrastructures, including the electricity network, steam pipelines, residual heat pipelines and a hydrogen pipeline [130]. The Botlek and Pernis areas contains are a more locally connected area, which contains a chlorine network, industrial gas network, steam network. These local networks lead to interconnections and dependencies between companies in the connected area. It is important to note the difference between a connection and a dependency. When a company is dependent on another company, there will be significant consequences if one of them changes its process. For example, company A supplies company B with the main feed stock for their process, and company B aims to substitute its feed stock. If in that case company A is forced to stop its production; this is a strong dependency. If company A is able to find alternative customers for its product and can continue producing, there is a connection but no strong dependency. A connection can be seen as an optimization of the closely located independent plants from an economic perspective [130].

Steam networks

The PoR chlorine cluster is connected to three steam networks, the Nobian - Shin-etsu network in the Botlek and the Shell steam network in Pernis where Westlake and Shin-etsu are connected with. Thirdly, Huntsman is connected tot he Botlek-Rozenburg steam exchange network. The steam dependency between Nobian and Shin-etsu is based on the utilization of residual heat. Nobian produces steam with it's CHP for Shin-etsu. In return, Shin-etsu returns lower temperature steam that can be used in Nobian's low temperature production processes [130]. On the right side of figure 3.1, the Shell refinery steam network is shown. Shell's Pernis refinery is the main user of Pergen's steam. After using the high temperature steam, Shell sends low temperature steam to Westlake and Shin-etsu Pernis. Westlake uses the low temperature steam in it's epoxy resin production. At Shin-etsu Pernis, the steam is used during the PVC purification process. The third steam network has Huntsman at it's center. Huntsman acquires high temperature steam from Air liquide and Eurogen. This is used during the MDI purification process. After utilization, lower temperatures steam is exchanged with Ducor, Wilmar, Lucite and Invista, via private steam pipelines [130].

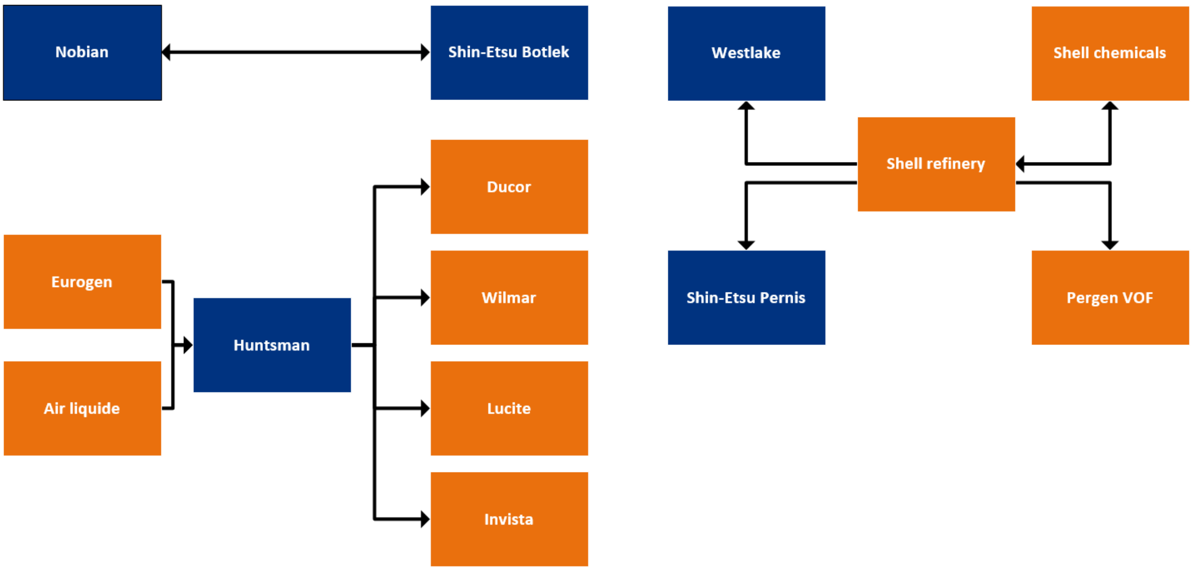

Figure 3.1: Steam Networks Botlek, Pernis and Rozenburg [130]

Industrial gas network

Two types of industrial gasses are exchanged with companies at the PoR chlorine cluster, namely refinery gas and carbon monoxide. Shell supplies Shin-etsu and Westlake with refinery gas that is considered waste from it's refinery processes. The refinery gas consists out of multiple types of small hydrocarbons and a small amount of hydrogen C. Shin-etsu uses the refinery gas during it's cracking process, which uses a gas fired cracker. Westlake uses the refinery gas in it's gas fired steam boiler. Lastly, Hunstman receives carbon monoxide from air liquide, which is used during phosgene production.

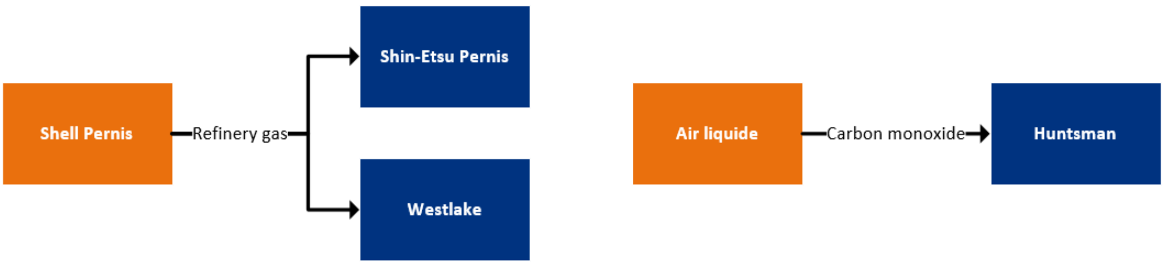

Figure 3.2: Industrial gas network Botlek & Pernis [130]

The Chlorine network

The chlorine network has Nobian at it's center of the material exchange network 3.3. This network interchanges chlorine, HCl caustic soda and hydrogen. With a yearly production of 640 kt, Shin-etsu, Westlake and Huntsman are provided with locally produced chlorine for their production processes. HCl, which is produced as a by product by Huntsman and Westlake, is used at Shin-etsu Botlek and Nobian. Shin-etsu uses HCl during the oxychlorination process. Nobian can use the waste HCl to produce chlorine. Next, caustic soda is produced by Nobian and transported to Huntsman and Shin-etsu. Huntsman uses caustic soda for MDA production and Shin-etsu

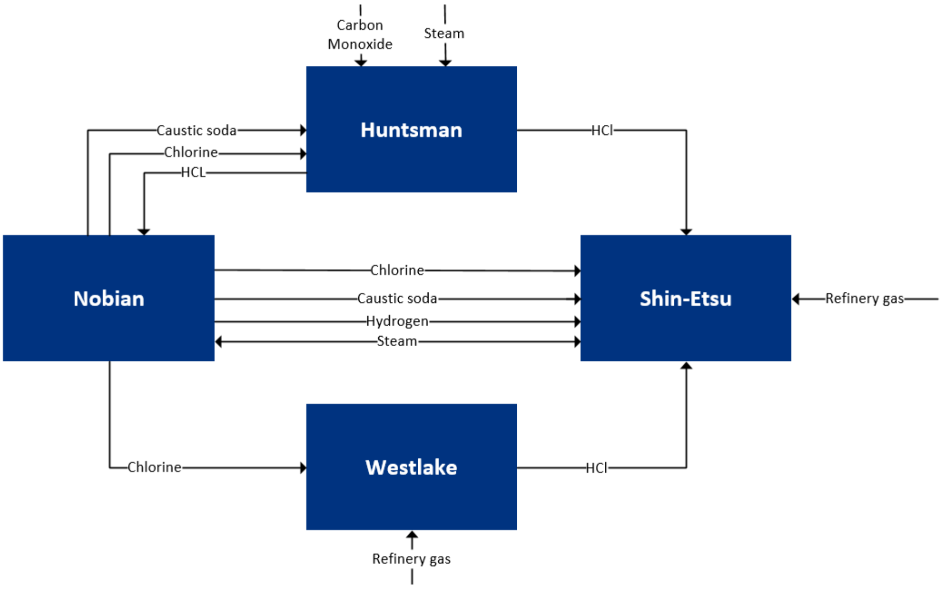

Figure 3.3: Overview of the integrated chlorine chain at industrial site Botlek [154]

3.2. Plant-product-process inventarisation

3.2.1. Nobian

Nobian Plant data: Chlor-alkali manufacturing

Nobian is a producer of chemicals for the industry and located in the Botlek area of the PoR. According to the MIDDEN database, Nobian has been classified as a producer of anorganic basic chemicals. As, Nobian produces chlorine, caustic soda and hydrogen. Chlorine is produced by the electrolysis of salt (NaCl). Besides chlorine, also caustic soda and hydrogen are produced during the electrolysis of natrium chloride. The overall reaction equation of natrium chloride electrolysis is shown in the equation (3.1).

$$2NaCl + 2H2O \rightarrow Cl2 + H2 + 2NaOH \tag{3.1}$$

From this equation follows that for every ton of produced chlorine, 1100 kg of caustic soda and 28 kg of hydrogen is produced. Where it is easy to produce caustic soda and hydrogen via other processes, it is not the case for chlorine. Therefore, the production of chlorine is entangled with the production of caustic soda and hydrogen. That is why plants like the botlek Nobian one are called chlor-alkali manufacturing plants, as they produce these three products under one roof. The table 3.1 shows the production of the three products and their quantity at the Nobian botlek site. A more detailed explanation of the production process is given in the next paragraph on Nobian's process data.

The production of chlorine is an energy-intensive process. For every megaton of chlorine produced at Nobian, around 3.5 PJ of heat energy is needed. Besides the thermal demand also 3000 GWh of electricity are needed. The heat demand is equivalent to the yearly natural gas consumption of around 85 thousand households and an electricity usage comparable to yearly electricity use of Utrecht. That makes Nobian a large CO_2 emitter with it's current technology configuration, see table 3.2.

Table 3.1: Overview of Nobian's material and energy flows [130]

	In/out	Capacity (kt/yr)	Energy (PJ/yr)
Salt	Input	1024	n/a
Water	Input	1472	n/a
Steam use	Input	n/a	1.2
Natural gas consumption	Input	n/a	2.3
Electricity use	Input	n/a	5.5
Chlorine	Output	640	n/a
Hydrogen	Output	17.9	2.1
Caustic soda	Output	723	n/a
Steam production	Output	n/a	1.9

Table 3.2: CO_2 emissions of Nobian per year [178]

	Direct CO2 emissions in 2017		
Plant	**CO2 [kton/year]**	**Share of CO2 within PoR [/&]**	**Share of CO2 within chlorine cluster [%]**
Nobian Botlek	157.7	0.8	57.8

Nobian Process data: Chlor-alkali manufacturing process

The central part of chlor-alkali manufacturing of Nobian is the electrolysis of natrium chloride (NaCl). This production process is surrounded by a series of subprocesses that allow for the right proportions of sodium chloride and caustic soda to flow into the electrolyser at one time [154]. As such, the chlor-alkali manufacturing process can be conceptualised as a series of the following sub-processes[154]:

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

The sub-processes are further elaborated below, figure 3.5 gives an overview of the complete process.

Steam generation
Low-temperature steam (150°C, 3-4 bar) is needed for the processing of caustic soda. Nobian produces it's steam with an on-site gas-fired CHP. The low-temperature steam is needed for the caustic soda preparation, where the steam is used in a multiple effect evaporator. The caustic soda's concentration is brought to the desired level within the multiple effect evaporator by using the steam.

Caustic soda preparation
The caustic soda preparation process is needed to attain the correct concentration and temperature of caustic soda. From the electrolysis of natrium chloride, 32% concentrated caustic soda is produced. This stream of caustic soda is fed back to a dilution chamber [152]. In the dilution chamber the 32% caustic soda is combined with dilution water and depleted to 30% concentrated caustic soda. The lowered concentrated caustic soda is needed as an input for the electrolysis process. Waste heat from the electrolysers is first used to increase the temperature of the caustic soda to the required 90 °C [152]. Thus, this process is a constant loop of depleted and replenished caustic soda between the dilution chamber and electrolyser.

Brine preparation
The brine preparation process aims to produce saturated brine that can be used in the electrolysis process. From the electrolysis process, 17% depleted brine is sent back to be processed and replenished to a concentration of 23% brine. The depleted brine is treated and dechlorinated with large pumps, hydrogen chloride and a small amount of 32% cuastic soda [19]. Follwing this step, the dechlorinated depleted brine is mixed with diluation water and inudstrial salt. This new mixture is then heated up to 90°C with waste heat from the electrolysers. This process needs a large amount of heat, as it needs around half of all waste heat produced by the electrolysers. The last step passes the new concentrated brine

through resins to remove impurities like, calcium, magnesium and various metals that might damaging to the membranes in the electrolyser.

Electrolysis
The electrolysis at Nobian is conducted via the membrane method. An electrolytic cell is separated in two chambers by a membrane, see figure 3.4. The left side of the figure shows a positive anode and the right side a negative cathode. The electrolysis starts with the injection of saturated brine (23%) on the left side. Here the chloride ions are oxidized by the anode, where they lose electrons to form chlorine gas. See the equation 3.2 for the first process step.

$$2Cl^{-} \rightarrow Cl2(g) + 2e^{-} \tag{3.2}$$

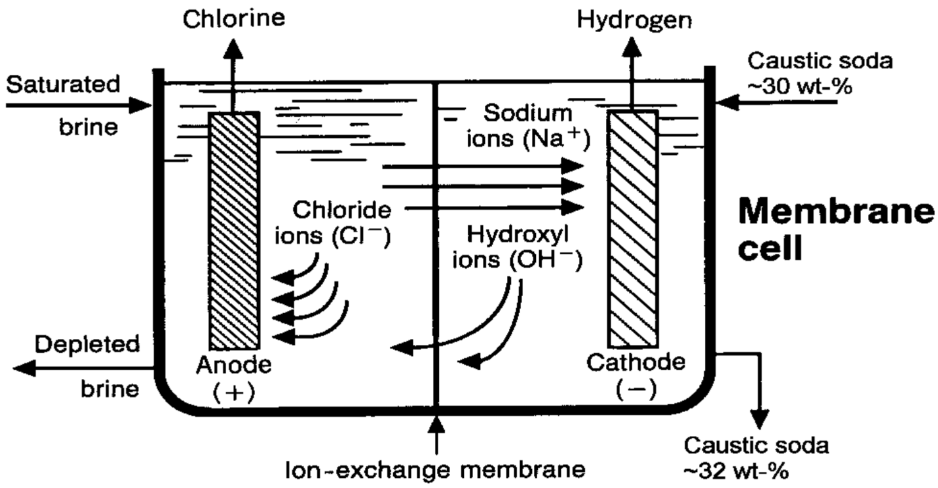

Figure 3.4: Overview of membrane based electrolysis [19]

At the same time caustic soda (30%) is fed into the right chamber at the cathode. The cathode reduced the hydrogen ions in the water, where they form in to gydrogen gas. At the same time hydorixde ions are rleased in the solution, see the equation 3.3 for an overview [19].

$$2H2O + 2e^{-} \rightarrow H_{2(g)} + 2OH^{-} \tag{3.3}$$

Only positive ions like the H+ and Na+ can pass through the membrane. The negative ions however, such as the Cl- or Na- cannot pass through the membrane. So, Na+ ions will move from the left side to the right side of the electrolytic cell where it combines with OH- to form extra caustic soda. In turn this leads to the brine concentration to decrease in the left side of the cell and the caustic soda concentration to increase in the right side of the cell [19]. An overview of this reaction in given in equation 3.4.

$$2NaCl + 2H_2O \rightarrow 2NaOH_{aq} + H_2(g) + CL_{2(g)} \tag{3.4}$$

Caustic soda processing
A large amount of the 32% caustic soda which is drained at the bottom right of the figure 3.4, is pumped back into the caustic soda preparation step. The rest of the caustic soda is used to produce higher concentrated 50% caustic soda, which is used by other partners at the PoR industrial cluster [19]. This is done trough multiple effect evaporation. A lot of heat energy is needed for the multiple effect evaporation, as almost 80% of the total steam demand for Nobian is used for this process [56].

Hydrogen processing
The high temperatures in the electrolysers lead to the mixtures of hydrogen gas and large amounts of steam [19]. The mixture consists out of 75% steam and 25% hydrogen gas, which is cooled in such a way that the steam condenses and only hydgrogen gas remains [56]. After this step the hydrogen gas is compressed by pumps and moved through piples to end-uses, which in this case Shin-Etsu.

Chlorine processing
The last process is dedicated to the chlorine processing. Chlorine gas that is obtained via electrolysis is

mixed with steam during the electrolysis process with a mix of 20% steam and 80% chlorine gas [19]. To remove the steam from this mixture and obtain pure chlorine gas, the mixture is cooled. By the cooling the mixture a large part of the steam condenses and seperates from the mixture. To remove the last part of steam, sulpheric acid is used [56]. Some parts of this pure chlorine gas is shared with Westlake and Huntsman. A total overview of this manufacturing process is shown in figure 3.5.

Nobian Product data: Chlor-alkali products

This subsection dives deeper into the three products that have been discussed in the section above namely, chlorine, caustic soda and hydrogen. First an overview of the market value and main applications is given per product. Secondly, a more detailed description is given per product.

Table 3.3: Chlor-Alkali production products by Nobian [19]

Product	Market value (EUR/ton)	Main applications
Chlorine	264	Production of plactics like, PVC and Teflon.
Caustic soda	165	Organic chemical production, food industry, water treatment, bleach.
Hydrogen	2340	Used in the Petrochemical industry, fertilizer production, electronics industry, fuel source.
Steam		

Chlorine
Chlorine is a chemical product with both applications for the consumer as chemical industries. Chlorine is for example used as a household cleaning agent or as disinfectant for drinking water and swimming pools, all though a negligible portion. A larger part of the total chlorine production of Nobian is used to produce plastics such as, polyvinylchlorice (PVC) and epoxy-resins. The chlorine of Nobian is used in production processes of Shin-Etsu, Westlake and Huntsman [152].

Caustic soda
Caustic soda is a highly used base in the industrial sector. The substance is used in various industries, like the organic chemical production, food industry, water treatment and bleach. At the PoR chlorine cluster, the caustic soda of Nobian is shared with Huntsman and Westlake. Huntsman needs the caustic soda for during the neutralization of MDA.

Hydrogen
The last product of Nobian is hydrogen (H_2). Hydrogen is one of the building blocks for industrial production and as of late being pushed as a energy carrier to be used in the mobility and energy sectors.

Steam
Steam

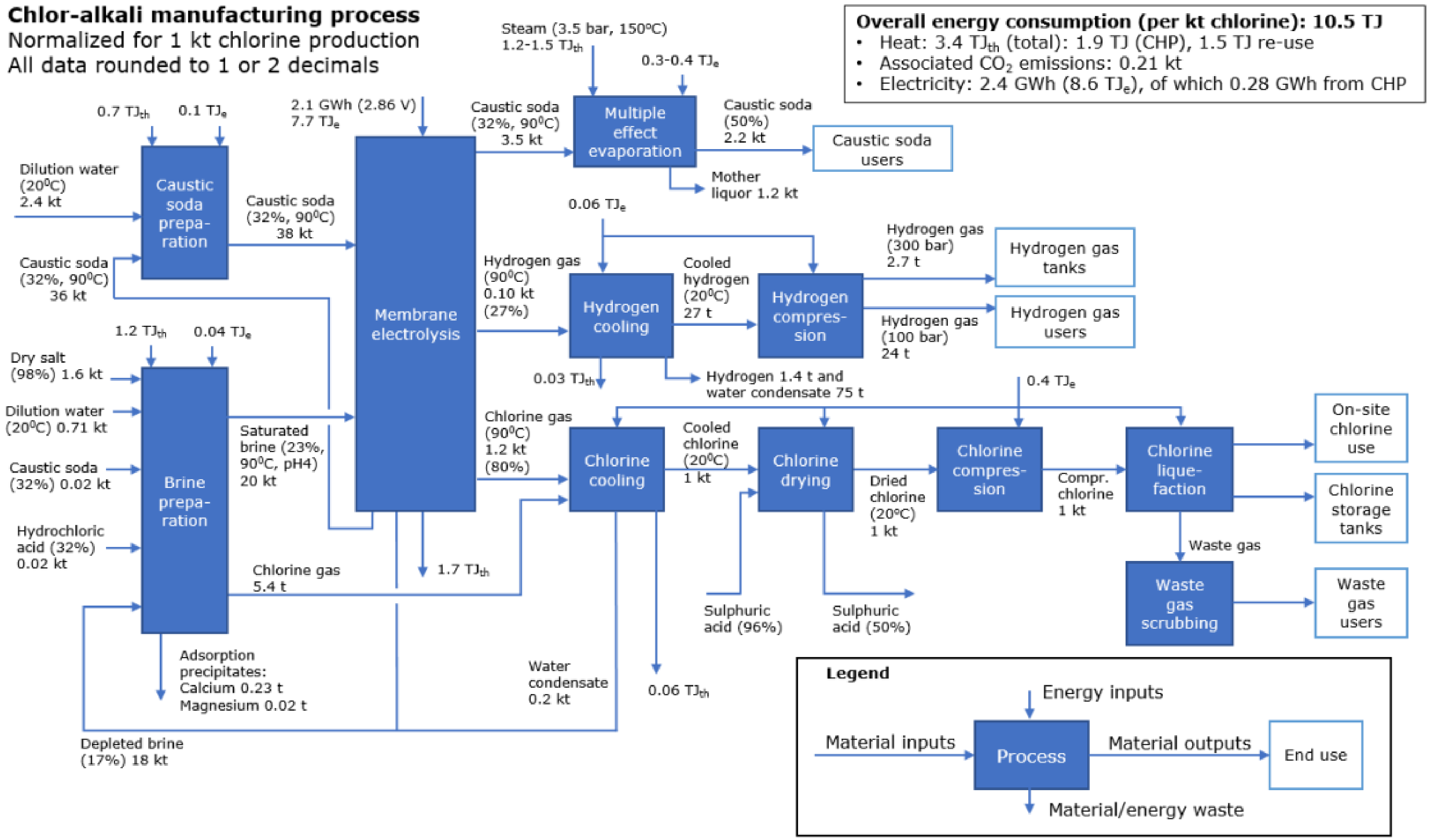

Figure 3.5: Chlor-Alkali production processes at Nobian [152]

3.2.2. Shin-Etsu

Shin-Etsu Plant data: PVC manufacturing

Shin-Etsu is a Japanese chemical producer and has the largest global market share for polyviniyl chloride (PVC), semiconductor silicon, and photomask substrates [43]. In the Netherlands, Shin-Etsu is one of the two PVC producers. Shin-Etsu operates two factories within the PoR chlorine cluster, which it bought back in 1999. The Botlek site is dedicated to Ethylene Dichloride (EDC) and Vinyl Chloride monomer (VCM) production. The second production plant, located in Pernis, produces polyvinyl chloride (PVC). Before Shin-Etsu bought these plants, they were operated by a joint venture of Shell and AkzoNobel [154]. The Plants produce around 670 kt of VCM, 80 kt of EDC and 520 kt of PVC per year. which makes Shin-Etsu the largest VCM, EDC and PVC producer in the Netherlands.

Table 3.4: Production figures of Shin-Etsu [154]

	In/out	Capacity (kt/yr)	Energy (PJ/yr)
Chlorine	Input	388	n/a
Ethylene	Input	308	n/a
Air	Input	489	n/a
Oxygen	Input	94	n/a
Steam use	Input	n/a	2.57
Electricity use	Input	n/a	0.94
Refinery gas use	Input	n/a	2.08
VCM	Output	670	n/a
EDC	Output	80	n/a
PVC	Output	520	n/a

Just like the production of chlorine, the VCM, EDC and PVC production processes are energy-intensive. The yearly direct CO_2 emissions of Shin-Etsu are shown in table 3.5. For every tonne of EDC a total of 6 GJ is needed. For VCM it is 0.9 tonnes and the PVC production part requires 4.1 GJ per tonne of product. The energy demand is built up in the form of electricity and steam.

Table 3.5: CO_2 emissions of Shin-Etsu per year [178]

	Direct CO2 emissions in 2017		
Plant	**CO2 [kton/year]**	**Share of CO2 within PoR [/&]**	**Share of CO2 within chlorine cluster [%]**
Shin-Etsu Botlek	101.6	0.5	34.2
Shin-Etsu Pernis	0	0	0

Shin-Etsu Process data: PVC manufacturing process

PVC is produced by polymerisation of the chemical vinyl chloride monomer (VCM). This chemical is obtained by thermal cracking (pyrolysis) of EDC. At Shin-Etsu, EDC is produced by a combination of direct chlorination and oxychlorination of ethylene. In general, the total PVC process can be divided in three main parts, each consisting of several subprocesses. The three main parts that are conducted at two production plants, produce three main products: EDC, VCM and PVC. An elaboration on the production processes is given below, to give an overview of how that production process looks like. A total overview of the EDC, VCM and PVC production is given in figure 3.6.

1. Direct chlorination (EDC)
2. Oxychlorination (EDC)
3. EDC Purification
4. VCM Cracking
5. VCM Purification
6. PVC Polymerisation
7. PVC Purification
8. PVC Drying

Direct chlorination
Shin-Etsu has three sources of EDC for the VCM production process. Direct chlorination and oxychlorination are two separate processes that are performed in parrellel to produce EDC. Thirdly, EDC is recycled back from the VCM purification to EDC purification [154].

At the direct chlorination production step, 1,2-ethylenedichloride (EDC) is produced. During this step, ethylene and chlorine react in order to form EDC [166].The chemical reaction of the chlorination goes following this equation:

$$C_2H_4 + Cl_2(g) \overset{FeCl_2}{\longleftrightarrow} C_2H_4Cl_2(l) \tag{3.5}$$

In this chemical reaction the ferric chloride acts as a catalyst. Also, to ensure the complete ethylene conversion, an excess of chlorine is used. This used chlorine at Shin-Etsu is produced by Nobian [154].

Oxychlorination
The oxychlorination is conducted parallel to the direct chlorination. During this process step, ethylene, hydrogen chloride and oxygen react to produce EDC and water. This process requires a high temperature and pressure and is therefore carried out on either a fluid-bed reactor or a fixed-bed reactor [154]. At Shin-Etsu, three fluid-bed reactors are used to conduct the following chemical reaction of oxychlorination:

$$C_2H_4 + 2HCl(g) + \frac{1}{2}O_2 \overset{CuCl_2}{\longleftrightarrow} C_2H_4Cl_2(g) + H_2O(g) \tag{3.6}$$

Oxychlorination is similar to direct chlorination, but at oxychlorination steam is produced as a by-product. The steam can later on be used during the distillation steps of EDC purification. The hydrogen chloride for the oxychlorination is retrieved from Westlake and Huntsman.

EDC Purification
The produced EDC from the previous two steps or from any unreacted EDC from VCM production, needs additional purification to attain the required purity [154]. The EDC from direct chlorination is washed with water to wash out the $FeCl_3$ catalyst. The washed out catalyst is then fed back into the direct chlorination process step. The EDC from oxychlorination is mixed with water vapor to condense the EDC from a gas to liquid phase. After this, the two EDC streams are mixed together and fed into the EDC dryer. Followed by the stream being fed into a distillation column, with removes by-products and tars [166]. The by-products are formed into hydrogen chloride through oxidation, which can then in turn be used again in the oxychlorination step.

VCM Cracking
The purified EDC is then decomposed in a furnace into VCM and hydrogen chloride, following this equation:

$$C_2H_4Cl_2(g) \longrightarrow C_2H3Cl(g) + HCl(g) \tag{3.7}$$

The cracking is conducted under a temperature of around 500 degrees Celcius and 1-4 MPa of pressure. The cracking process is an thermic reaction with a heat of reaction of +71 kJ/mol [45]. This energy is typically provided by burning natural gas. Also, it is expected that natural gas is burned in gas burners to reach the higher operating temperature of approximately 500°C [154]. This would mean that this step is a main source of CO2 emissions in the production process.

VCM Purification
The cracking gas from the previous step is purified during this process step. The hydrogen chloride, EDC and other by-products are two-stage distilled. The first distillation separates the hydrogen chloride together with a part of the by-products from the cracking gas. This stream is then recycled back to the oxychlorination process step [166]. The second distillation step separates VCM from the last by-products and is transformed into a liquid to be put in the VCM storage [154].

PVC Polymerisation
The VCM from the previous step is polymerized via the suspension technology method to form PVC

[154]. The Suspension method places small drops of VCM in water, that is consequently stirred in large reactors. In the reactors the polymerisation of VCM monomers happens. The polymerisation is shown in the equation below. Where n is the number of VCM molecules that are used to form the polymer.

$$nCH_2 = CHCl \longrightarrow (-CH_2 - CHCl-)_n + heat \tag{3.8}$$

PVC Purification
It is common practice to remove any leftover VCM from the PVC down to concentrations well below 1 ppm [154]. This is generally done by means of a steam stripping column. The slurry is blown down into a stripping column from the top recovered down to atmospheric pressure. Next, steam of approximately 100°C (between 100-120°C) is fed from the bottom of the column, which will evaporate VCM and part of the water from the slurry. The stripped slurry leaves the column from the bottom while the recovered VCM/water gas mixture is captured at the top. The VCM is recovered and recycled back to the polymerization reactor. The PVC slurry, still containing 50-60% water, is processed further in the next part of the process.

PVC Drying
The last process step aims to remove water that is present in the PVC slurry. This can be done by a mechanical and thermal drying drying step [154]. The slurry can be mechanically dried with a centrifuge, which separates a large fraction of the water from the slurry and brings the moisture content to 20-30% [140].

Shin-Etsu Product data

This subsection dives deeper into the three products that are sold by Shin-Etsu, EDC, VCM and PVC. First an overview of the market value and main applications is given per product. Secondly, a more detailed description is given per product.

Table 3.6: Chlor-Alkali production products by Nobian [19]

Product	Market value (EUR/ton)	Main applications
EDC	950 [27]	Raw material for VCM, paint thinners and cleaning solvents [12].
VCM	1302 [51]	Raw material for PVC, housewares and automotive parts.
PVC	808 [61]	Pipes, insulation electric cables, construction, clothing.

EDC
Around 95% of the world's EDC production is used for VCM production [80]. Besides that, EDC is used as a degreaser and paint remover. However, the use of EDC is phased out due to its toxicity. At the Shin-Etsu plant almost all of the EDC that is produced is used for VCM production. Around 3 percent of the EDC is sold to other companies.

VCM
VCM is also mainly used as a chemical intermediate. Due the toxic properties of VCM, there are no end products that use VCM in it's monomer form. Small amounts of VCM are used in houseware products and automotive parts, but in very small concentrations. At the Shin-Etsu plant, 470 kton of 620 kton the totally produced per year is used at the Pernis PVC plant. The remaining 150 kton of VCM is used at a Shin-Etsu plant in Portugal.

PVC
Almost half the world's produced PVC is used to produce pipes, like sewage pipes. PVC is also used for the insulation of electric cables, in construction and even clothes. The Shin-Etsu plant produces roughly 470 kton of PVC per year and that makes them the largest producer of PVC in the Netherlands.

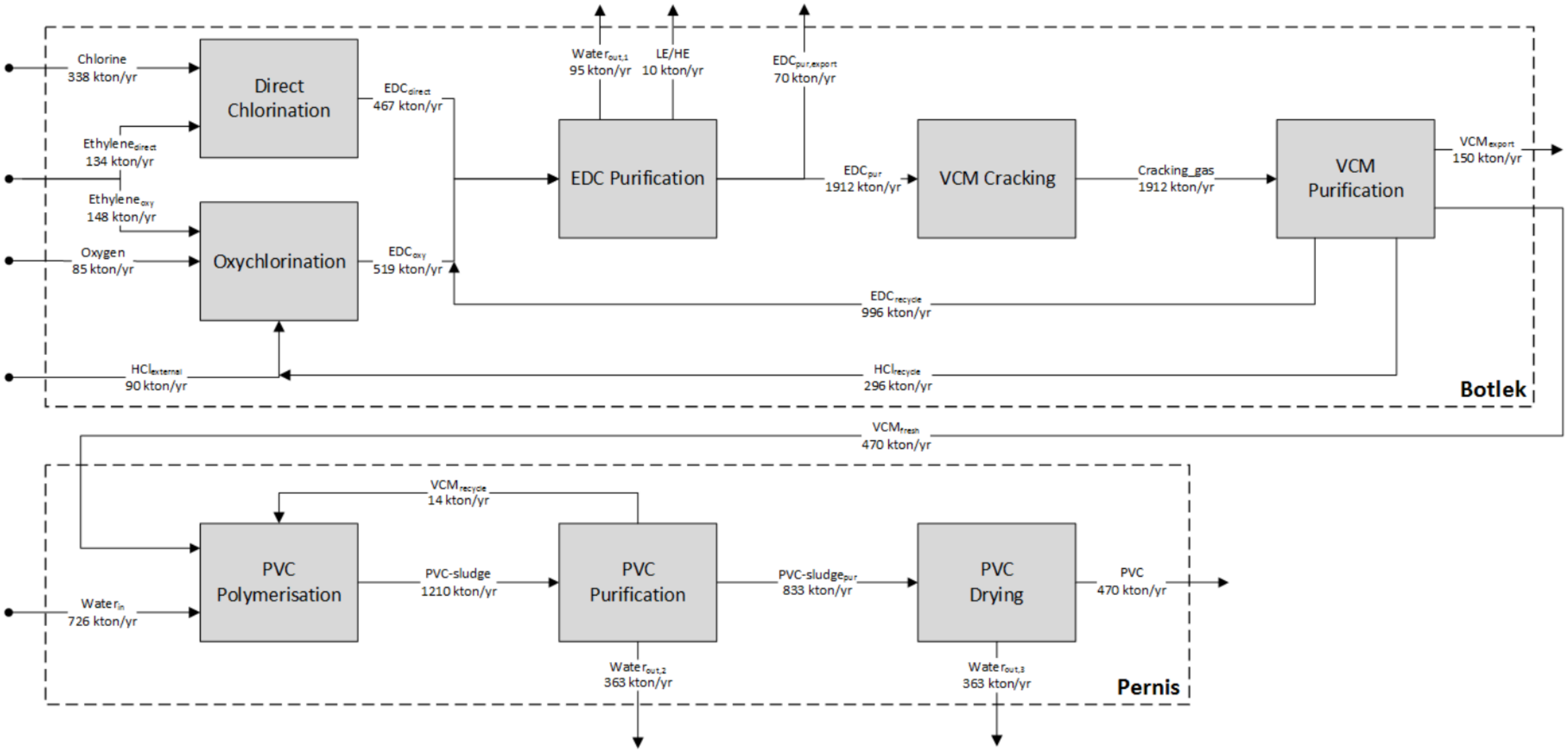

Figure 3.6: Shin-Etsu VCM and PVC process overview

3.2.3. Westlake

Westlake Plant data: MDI production

Westlake is an international producer and supplier of petrochemicals, polymers and fabricated building products. It was founded back in 1986 in Houston Texas. Westlake's presence in the PoR started when they took over Hexion. Hexion operated a epoxy production plant in the PoR, which Westlake acquired in the beginning of 2022. Westlake's main products are epoxy resins and hydrogenchloride. The hydrogen chloride is formed as a by-product during the production epoxy resin production process, see tab 3.7.

Table 3.7: Production figures of Westlake [108]

	In/out	Capacity (kt/yr)	Energy (PJ/yr)
Propylene	Input	59	n/a
Chlorine	Input	175,3	n/a
Acetone	Input	47,5	n/a
Phenol	Input	155,8	n/a
Steam use	Input	n/a	2
Electricity use	Input	n/a	0.2
Tars	Output	36	n/a
ECH	Output	100	n/a
BPA	Output	190	n/a
Epoxy resins	Output	170	n/a

Westlake is the third largest CO_2 emitter of the chlorine cluster, see tab 3.8. The direct CO_2 emissions are mainly for the heat supply needed for it's production process. The yearly direct CO_2 emissions of Westlake are shown in table 3.8.

Table 3.8: CO_2 emissions of Westlake per year [178]

	Direct CO2 emissions in 2017		
Plant	**CO2 [kton/year]**	**Share of CO2 within PoR [&]**	**Share of CO2 within chlorine cluster [%]**
Westlake Botlek	37.4	0.2	12.6

Westlake Process data: Epoxy resin production process

At Westlake, epoxy resin is produced by combining hydrogen chloride, ECH (Ethylene cyanate hydrene) and BPA (Bisfenol A). At westlake they produce around 170 kton of epoxy resin per year via this method. The several sub processes are elaborated below. A total overview of the EDC, VCM and PVC production is given in figure 3.7.

1. Chlorification of propylene
2. Production hypochlorous acid
3. Epichlorohydrin production
4. ECH production
5. BPA production
6. Epoxy resin production

Chlorification of propylene
By letting propylene react with chlorine, allyl chloride and hydrogenchloride are produced. The allyl chloride is later used to form epichlorohydrin. The hydrogenchloride is needed as a building block for epoxy resin. See the following equation for an overview of this reaction:

$$Cl_2 + C_3H_6 \longrightarrow C_3H_5Cl + HCl \tag{3.9}$$

Production of hypychlorous acid
In this process step, hypochlorus acid is formed by combining chlorine and water. As a by product, also hydrogen chloride is formed. See the following equation:

$$Cl_2 + H_2O \longrightarrow HOCl + HCl \tag{3.10}$$

Epichlorohydrin production
In this step, a mixture of hypochlorous acid and allyl chloride that forms epichlorodyrin. The epichlorohydrin is necessary to eventually produce ECH. See the following equation for the reaction:

$$HOCl + C_3H_5Cl \longrightarrow C_3H_5Cl_2(OH) \tag{3.11}$$

ECH production
The ECH follows from a reaction of epichlorohdyrin with caustic soda that is retrieved from Nobian. This reaction results in the formation of ECH, Natrium chloride and water. The natrium chloride and water are not needed in further reactions and are therefore currently treated as waste. The 'waste brine' is send off to Shell for waste treatment. However, this stream of brine could be an opportunity for Westlake as the natrium chloride as it is one of the main feed instocks for Nobian. Nobian uses natrium chloride to produce chlorine via electrolysis and thus could be recirculated with Nobian. Westlake probably pays 4000 euro per kton, following Lyu et al. [107].

$$2(C_3H_5Cl2OH) + NaOH \longrightarrow 2(C_3H_5ClO) + NaCl + 2H_2O \tag{3.12}$$

BPA production
The second main product of epoxy resin production is formed by mixing Phenol and acetone to form Bisfenol A (BPA) and water. Together with ECH, BPA is needed to form epoxy resin.

$$C_3H_6O + 2(C_6H_5OH) \longrightarrow C_15H_16O_2 + H_2O \tag{3.13}$$

Epoxy resin production
The last step of the process is where epoxy resin is formed by combining ECH and BPA. As a by-product HCL is formed, which is sold to Shin-Etsu and thirds. This step requires heat that is generated by the local gas boiler.

$$C_3H_5ClO + C_15H_16O_2 \longrightarrow [-C_18H_21O_3-] + HCl \tag{3.14}$$

Westlake Product data

This subsection dives deeper into the two output products of Westlake, epoxy resins and HCL. First an overview of the market value and main applications is given per product. Secondly, a more detailed description is given per product.

Product	Market value [EUR/ton]	Main applications
Epoxy resins	2580 [28]	Coatings, adhesives, composite materials and many more.
HCl	125 [29]	Formation to hydrochloric acid and vinyl chloride.

Epoxy resins
The applications for epoxy-based materials are very extensive and are considered to be very versatile products [22]. We also encounter epoxy-based products in every day life. Think of PET bottles and plastic bags.

HCl
Hydrogen chloride is mainly a product used to produce hydrochloric acid. Hydrochloric acid is the aqueous solution of hydrogen chloride and is used both as a product or used in industrial production processes. Hydrogen chloride is also used to produce vinyl chlorides, which is also produced in the chlorine cluster by Shin-Etsu.

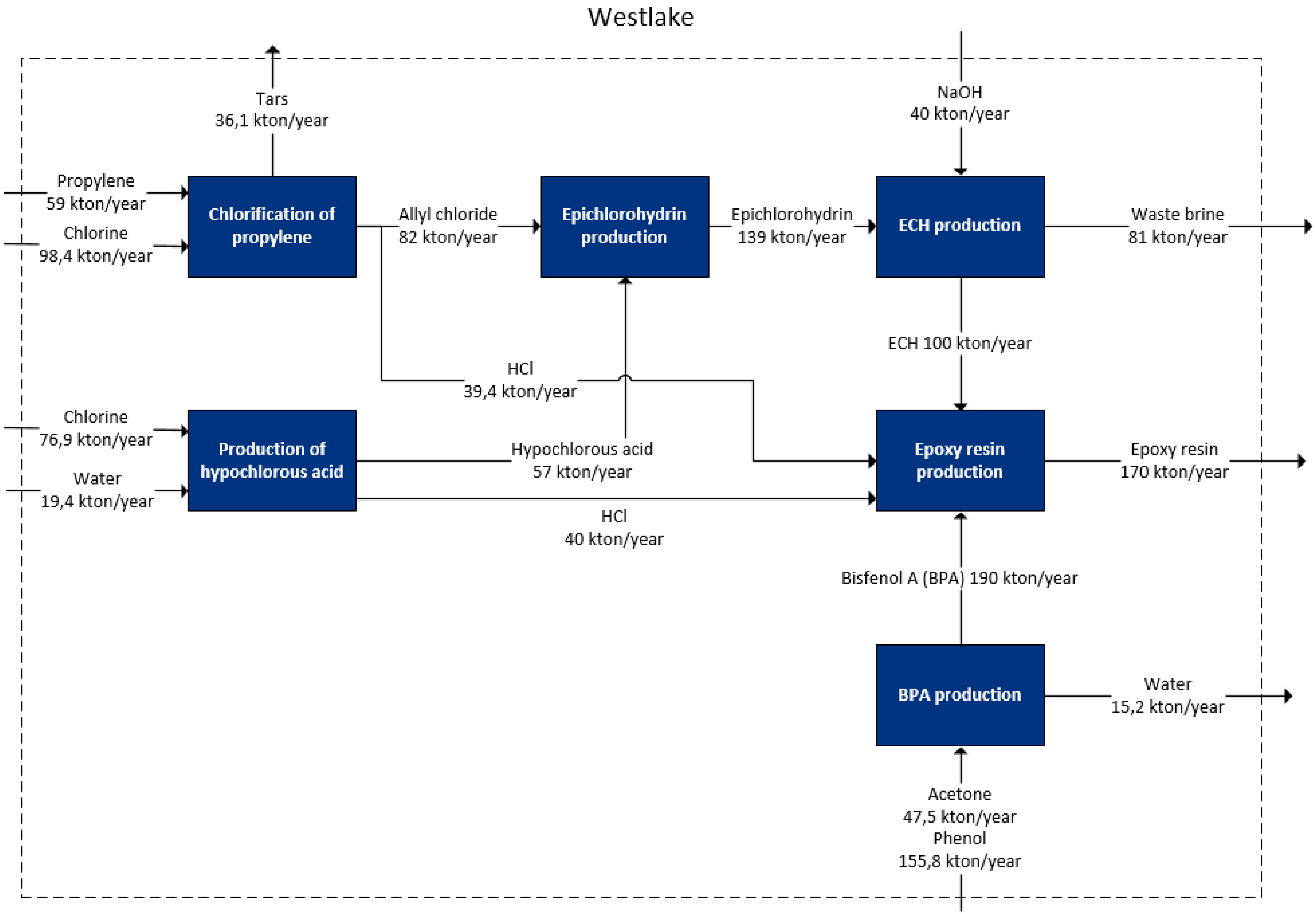

Figure 3.7: Epoxy resin manufacturing process

3.2.4. Huntsman

Huntsman Plant data: MDI production

Huntsman is an American manufacturer of chemical products for consumers and industrial customers, founded in 1970. In the PoR, Huntsman produces halffabricates that are used in the polyurethane industry. Huntsman uses chlorines as a feedstock to produce MDI (Methyl-diphenyl diisocyanate). The MDI is used as a raw material for the production of polyurethene. Polyurethene is processed in every day products like, mattresses, chairs and building materials. At it's Rotterdam plant, Huntsman produces MDI via the conventional phosgene route [169]. The plant produces around 400 kton MDI and 238 kton hydrogen chloride per year, see table 3.9.

Table 3.9: Production figures Huntsman

	In/out	Capacity (kt/yr)	Energy (PJ/yr)
Aniline	Input	297	n/a
Formaldehyde	Input	47.4	n/a
Chlorine	Input	227.5	n/a
Carbon monoxide	Input	63.7	n/a
Steam use	Input	n/a	2.0
Electricity use	Input	n/a	0.3
MDI	Output	400	n/a
HCL	Output	232	n/a

Huntsman does not have a lot of and direct CO_2 emissions because, they currently buy their steam from other companies at the PoR. The yearly direct CO_2 emissions of Huntsman are shown in table 3.5. The energy demand is mainly driven for the heat purposes in the process step of MDI purification.

Table 3.10: CO2 emissions of Huntsman [178]

	Direct CO2 emissions in 2019		
Plant	**CO2 [kton/year]**	**Share of CO2 within PoR [/&]**	**Share of CO2 within chlorine cluster [%]**
Huntsman	0.2	0	0.1

Huntsman Process data: MDI production process

The production process at the Huntsman plant are divided in to four parts, shown below [136].

1. Phosgene production
2. MDA production
3. Phosgenation of MDA to crude MDI
4. MDI purification

Phosgene production
Most of the production routes to MDI use phosegene to synthesize MDI from MDA [176]. During this process step, carbon monoxide and chlorine (from nobian) are reacted to form phosgene, see the equation below.

$$CO + Cl_2 \longrightarrow COCl_2 \tag{3.15}$$

MDA production
The raw product needed for MDI production is MDA. MDA stands short for Methylenedianiline. MDA is formed initially through the reaction of formaldehyde with analine. After this reaction, the mixture is neutralised by adding caustic soda. The caustic soda is bought from Nobian. This neutralisation parts results in a waste stream and crude MDA [136]. The reaction of formaldehyde and analine is shown below.

$$2(C_6H_5NH_2) + CH_2O \longrightarrow C_13H_14N_2 + H_2O \tag{3.16}$$

$$C_13H_14N_2 + H_2O + NaOH \longrightarrow X \tag{3.17}$$

Phosgenation of MDA to crude MDI
During this process step, phosgene is reacted with MDA to produce MDI and hydrogen chloride as a byproduct. The reaction equation is shown below.

$$C_13H_14N_2 + 2(COCl_2) \longrightarrow C_15H_10N_2O_2 + 4HCl \tag{3.18}$$

MDI purification
The last step is dedicated to the MDI purification. This step is performed by distillation, where all impurities are parted from the MDI. Also monomer MDI's are formed into polymer MDI chains.

$$MonomerMDI \longrightarrow PolymerMDI \tag{3.19}$$

Huntsman Product data: MDI and hydrogen chloride

This subsection dives deeper into the two products that are sold by Huntsman, MDI and hydrogen chloride. First an overview of the market value and main applications is given per product. Secondly, a more detailed description is given per product.

Table 3.11: MDI production products by Huntsman

Product	Market value (EUR/ton)	Main applications
MDI	2683 [162]	Raw material for polyurethane, paints and coatings.
HCl	141 [28]	Raw material for vinyl chloride, formation to hydrochloric acid.

MDI
The main application for MDI is for the production of polyurethane. It is also used in small quantities in paints and coatings. MDI isn't much used on it's own due it's hazardous properties. It is a very reactive material to for example water and results in a exothermic reaction.

HCl
Hydrogen chloride is mainly a product used to produce hydrochloric acid. Hydrochloric acid is the aqueous solution of hydrogen chloride and is used both as a product or used in industrial production processes. Hydrogen chloride is also used to produce vinyl chlorides, which is also produced in the chlorine cluster by Shin-Etsu. Just as Westlake, Huntsman sells it's HCl to Shin-Etsu.

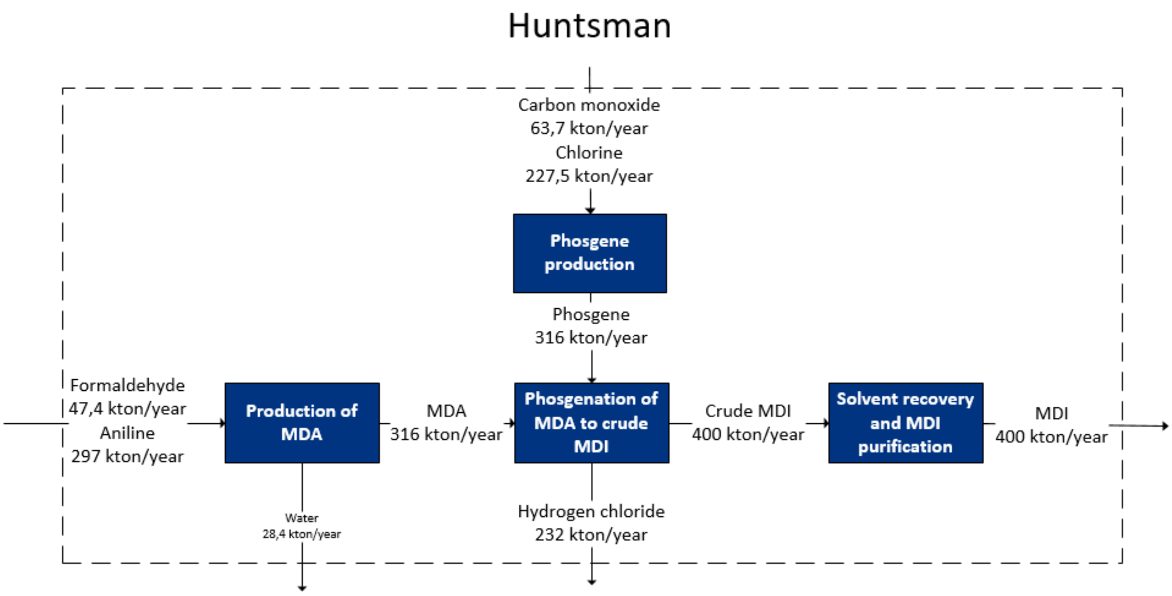

Figure 3.8: Huntsman MDI manufacturing process [136]

3.3. Zero emission technology inventarisation

This section shows the zero emission technologies for Nobian, Shin-Etsu, Westlake and Huntsman. This section gives per company a technology description of the zero emission technology alternatives and an overview of the techno economic characteristics. Also, the currently installed technology is described. The last subsection shows an overview of all the various alternatives and which companies are involved. Mainly The MIDDEN database [133] was used as a data source for this section.

3.3.1. Nobian

In this section, the currently installed technology and possible zero emission technology are discussed. First, the currently installed assets are shown. Followed, by the the zero emission technologies. The currently installed assets, that can be replaced by zero-emission technology alternatives are:

1. CHP
2. Finite gap brine electrolysis
3. Multiple effect vaporisation (2)

CHP

Nobian operates a large scale gas turbine combined heat and power plant (CHP), to produce electricity and low pressure steam (1-9 bar). As shown in figure 3.5, Nobian produces 10.5 TJ of energy per kton of chlorine via their CHP. With 640 kton of chlorine produced per year, Nobian produces a total of 6720 TJ of energy with their CHP. Assuming that they are using gas turbine CHP, with an efficiency of 69 % at 8760 load hours per year, the CHP has a required capacity of 85.5 MW. The rest of the characteristic values are shown in table 3.14.

Table 3.12: CHP at Nobian

Characteristic	Value	Comment
Capacity required	85.5	808 MWh per kton Chlorine
Efficiency	69%	[58]
Cost per capacity unit	1.25 MEUR/MW	[58]
CAPEX	106.8 MEUR	Capcity times the cost per MW
OPEX	1.7 MEUR/year	2% of CAPEX per year [152]
ELT	20	[133]

Finite gap brine electrolysis

Nobian currently operates finite gap electrolysis for their electrolysis production process. During the electrolysis process step, brine is used to produce to caustic soda, chlorine and hydrogen. They use a traditional cell configuration with two electrodes (- and +) split by an inter-electrodal gaps. These cells have inte-relectrodal gaps of a few millimeters (see fig 3.9).

Table 3.13: Finite gap brine electrolysis Nobian

Characteristic	Value	Comment
Capacity required	238 MW	2318 MWh per kton Chlorine
Efficiency	71%	[58]
Cost per capacity unit	0.8 MEUR/MW	[146]
CAPEX	190.4 MEUR	Capacity times the cost per MW
OPEX	3.8 MEUR/year	2% of CAPEX [62]
ELT	5	[133]

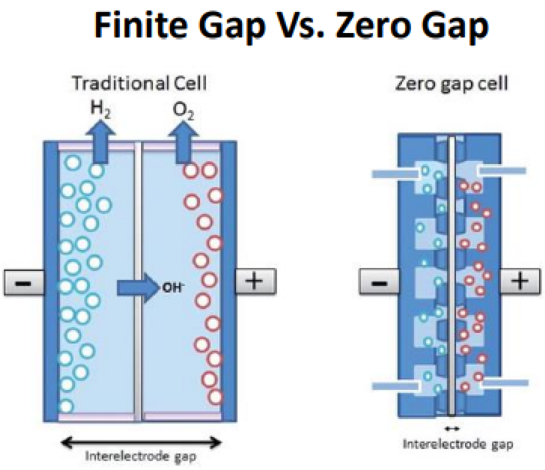

Figure 3.9: Finite gap vs zero gap electrolysers

Multiple effect vaporisation (3)

Multiple effect evaporation (MEV) is a device that efficiently uses heat from steam to evaporate liquids [50]. The MEV boils the water in a sequence of boilers and is commonly restricted to four evaporators, see figure 3.10. Multiple effect evaporation (MEV) is used at Nobian to increase the concentration of caustic soda from 32% to 50 % and produce mother liquor. The evaporation under high temperatures make it possible to increase the concentration of caustic soda. Currently, Nobian uses three evaporators in their MEV unit.

Table 3.14: Multiple effect vaporisaton (3) Nobian)

Characteristic	Value	Comment
Capacity required	19.7 MW	30% more than MEV(5) [152]
Efficiency	-	30% less efficient than MEV(5)
Cost per capacity unit	0.66 MEUR/MWth	[152]
CAPEX	13 MEUR	-
OPEX	0.26 MEUR/year	2% of CAPEX
ELT	20	[133]

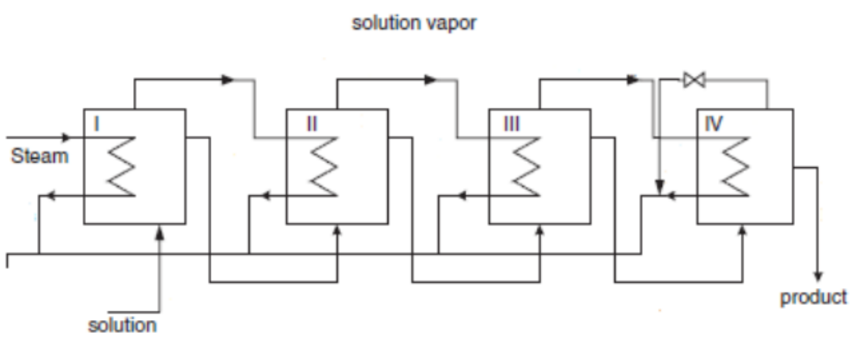

Figure 3.10: Multiple effect evaporator (4) schematic

Alternatives
The Nobian Botlek site has four sections in it's production process where alternative technology configurations are possible. In the utility, brine electrolysis, caustic soda processing and brine preparation sections. For Nobian there are four zero-emission technology alternatives:

1. Electric boiler
2. Biomass boiler
3. Zero gap membrane brine electrolysis
4. Multiple effect (5) vaporisation

Electric boiler

The current gas powered CHP produces both electricity and heat for Nobian. A decarbonisation alternative to the natural gas CHP would be to buy externally produced electricity and an electric boiler to produce heat. Under assumption that the electricity is produced renewable. This decarbonisation alternative is based on the SDE++ subsidy advice [133] for a large-scale electric boiler. In an electric boiler, electricity is run through a heating element that heats water via a heat exchanger [152]. The advice of PBL describes the capital expenditure (CAPEX) for the boiler, superheater, pump systems, on-site electricity infrastructure, piping, measuring equipment, civil works, scaffolding and cranes. To replace the CHP, a 38,4 MWth electric boiler would be needed at a price of 0.115 MEUR/MWth, would result in a 4.416 MEUR CAPEX investment. The annual OM costs lay at 2.3 kEUR/MWth and would total 88,230 kEUR/year. Lastly, the economic life time (ELT) is 15 years [133].

Table 3.15: Electric boiler Nobian [133]

Characteristic	Value	Comment
Capacity required	38.4 [MW]	To suffice the total heat demand of Nobian
Efficiency	99%	Stated by Scherpbier and Eerens [152]
Cost per capacity unit	0.25 MEUR/MWth	Price per MWth for upfront investment costs [40]
CAPEX	9.6 MEUR	Total upfront investment costs
OPEX	0.2 MEUR/year	2% of CAPEX
ELT [year]	15	-

Biomass boiler

The biomass boiler would function the same as the electric boiler described above, However, instead of using electricity to produce heat, the biomass boiler would use biomass as a feed in stock. Think of a wide variety of wood types, like pellets, chips and logs. 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 vaporisation process, cooled or condensed steam can be passed back into the biomass boilers where it can be heated again [152]. The difference between the electric boiler and biomass boilers are mainly seen in CAPEX, OPEX and ELT. Having a higher total CAPEX, lower OPEX and shorter ELT. Allthough having a far larger CAPEX and shorter ELT, a selling point for the biomass boiler is that the biomass has a far more stable price than gas and electricity [152].

Table 3.16: Biomass boiler Nobian

Characteristic	Value	Comment
Capacity required	40 MWth	To suffice total heat demand Nobian
Efficiency	90%	Stated by Scherpbier and Eerens [152]
Cost per capacity unit	0.88 MEUR/MWth	Price per MWth for upfront investment costs
CAPEX	35.2 MEUR	Total upfront investment costs
OPEX	0.7 MEUR/year	2% of CAPEX per year
ELT [year]	12	-

Zero gap brine electrolysis

The zero gap brine electrolysis is an energy efficiency alternative. During the electrolysis process step, brine is used to produce to caustic soda, chlorine and hydrogen. Currently, Nobian uses conventional electrolysis with a relative large gap between the membrane wall, anode and cathode. The zero gap membranes have reduced distances between the anodes and cathodes. The reduced distance leads to a voltage drop across the electrolyte and thus saves electricity use [152]. Since the electricity savings from the zero gap membranes, compared to the currently used finite gap electrolysers, are around 25% [174], Due to these savings, the technology is an attractive investment for Nobian under the right electricity prices.

Table 3.17: Zero gap brine electrolysis Nobian [133]

Characteristic	Value	Comment
Capacity required	175.3 MW	2138 MWh per ton chlorine
Efficiency	87.5%	25% more efficient than currently [152]
Cost per capacity unit	1.380 MEUR/MW	price per MW for upfront investment costs [146].
CAPEX	241.9 MEUR	Total upfront investment costs
OPEX	12.1 MEUR/year	5% of CAPEX [152]
ELT [year]	5	-

Multiple effect evaporation (5)

For Nobian, Scherpbier and Eerens [152] mention that MEV with 5 evaporators as an energy efficiency option. This alternative operates according to the same principle shown in figure 3.10. Compared to the currently installed MEV(3), the MEV(5) alternative has a significantly higher efficiency. The reduction would result in a 30% reduction in electricity useIn the table 3.18 an overview of alternative characteristics and corresponding values is given.

Table 3.18: Multiple effect evaporation (5) Nobian [133]

Characteristic	Value	Comment
Capacity required -	15.13 MW	Capacity needed for evaporation.
Efficiency	-	30% more efficient [133]
Cost per capacity unit	0.88 MEUR/MWth	price per MWth for upfront investment costs
CAPEX	13.3 MEUR	Capacity required times the cost per capacity
OPEX	0.66 MEUR/year	5% of CAPEX per year*
ELT [year]	20	-

Overview of zero emission technologies for Nobian

The table 3.19, shows an overview of all the zero emission technologies for Nobian.

Table 3.19: tab: Overview of zero emission technologies for Nobian

Type of technology	Section	CAPEX	OPEX	Economic lifetime [years]
CHP	Utility	85.5 MEUR	1.7 MEUR/year	20
Electric boiler	Utility	9.2 MEUR	0.2 MEUR/year	15
Biomass boiler	Utility	35.2 MEUR	0.7 MEUR/year	12
Finite gap electrolysis	Brine electrolysis	190.4 MEUR	3.8 MEUR/year	5
Zero gap brine electrolysis	Brine electrolysis	241.9 MEUR	12.1 MEUR/year	5
Multiple effect (3) vaporisation	Caustic soda process	13 MEUR	0.26 MEUR/year	20
Multiple effect (5) vaporisation	Caustic soda process	13.3 MEUR	0.66 MEUR/year	20

3.3.2. Shin-Etsu

In this section, the currently installed technology and potential zero emission technology are discussed. First, the currently installed assets is shown. Followed, by the the zero emission technologies.

Currently installed: Natural gas furnace EDC cracking

Currently, Shin-Etsu operates a natural gas fired furnace for it's EDC cracking process (see figure 3.11). A schematic of a natural gas fired fluid bed reactor is shown in figure 3.11. The reactor creates en environment with high temperatures and pressure to crack EDC. The cracking product is in turn used for VCM production.

Table 3.20: Electric cracking furnace [133]

Characteristic	Value	Comment
Capacity required	131.7 MW [MW]	3.1 GJ/ton VCM [154]
Efficiency	50%	Estimation by Semeijn and Schure [154]
Cost per capacity unit	0.9 [EUR/MW]	[64]
CAPEX	118.53 [MEUR]	-
OPEX	2.4[MEUR/year]	2% of CAPEX
ELT [year]	30	[154]

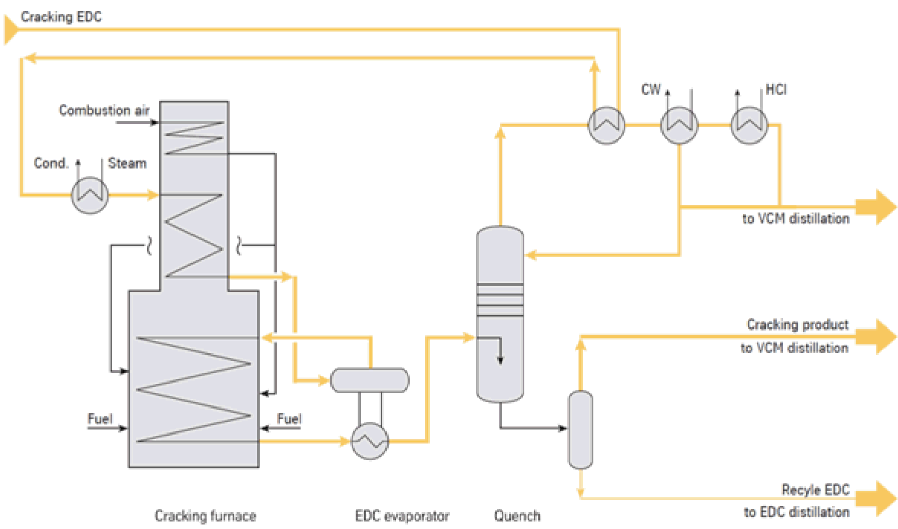

Figure 3.11: Schematic of EDC cracking

Alternatives
For Shin-Etsu there are two possible zero-emission alternatives. The two alternatives are both replacements for the current gas-fired EDC cracking installation. The two alternatives are a hydrogen cracking installation and electric cracking installation.

1. Hydrogen furnace EDC cracking
2. Electric furnace EDC cracking

Hydrogen furnace EDC cracking

Currently, Shin-Etsu uses a gas-fired Thermal cracking furnace to crack EDC in VCM. An alternative to the use of fossil fuels, would be to use hydrogen gas as an energy carrier to use in the thermal cracking furnace. Under assumption that the hydrogen is produced with renewable energy, this alternative would lead to the decarbonisation of this production process. In the cracker, the hydrogen gas is burned to supply the heat of reaction and to bring the reactants to the required reaction temperature of

500[U+1D52]C. With a conversion efficiency 55%, a total of 119.7 MW_{th} would be needed for this furnace. In table 3.21 and overview of the hydrogen's furnace characteristics and corresponding values is shown. H2 has a calorific value of 141.8 MJ/kg, so this means the hydrogen furnace would require kton on a yearly basis.

Table 3.21: Hydrogen furnace EDC cracking [154]

Characteristic	Value	Comment
Capacity required	119.7 [MW]	Required capacity to replace current cracker
Efficiency	55%	Estimation made by Semeijn and Schure [154]
Cost per capacity unit	0.4 (MEUR MW]	Estimation made by Semeijn and Schure [154]
CAPEX	47.9 [MEUR]	-
OPEX	0.48 [MEUR/year]	1% of CAPEX
ELT [year]	30	-

Electric furnace EDC cracking

Besides using hydrogen as an energy source for the cracking process, it is also possible to electrify the process with an electrical furnace. Under the assumption that the electricity is produced by renewable means, the electrification of the cracking process would result in the decarbonisation of the production process. Electrification of electric furnaces can be categorized in two main groups: direct and indirect heating technologies. Direct heating technologies include inductive and dielectric heating; indirect heating technologies include resistance, arc and infrared heating. Judging on the temperature ranges, indirect resistance heating and dielectric heating are most suitable for the replacement of EDC cracking furnaces, as the temperature in the furnace is typically 500°C. Especially indirect resistance heating is interesting for the PVC manufacturing industry, as it delivers heat in a similar way as gas-fired heating systems [154].

Table 3.22: Electric cracking furnace [133]

Characteristic	Value	Comment
Capacity required	66.5 [MW]	3.1 GJ/ton VCM[154]
Efficiency	99%	[154]
Cost per capacity unit	2800 [EUR/KW]	Estimation by Semeijn and Schure [154]
CAPEX	186.2 [MEUR]	-
OPEX	3.7 [MEUR/year]	2% of CAPEX
ELT [year]	30	-

Overview of technologies for Shin-Etsu

The table 3.23, shows an overview of all the technologies for Shin-Etsu.

Table 3.23: Overview of technologies for Shin-Etsu

Type of technology	Section	CAPEX	OPEX	Lifetime
Gas furnace	EDC cracking	118.53 [MEUR]	2.4 [MEUR/year]	30
Hydrogen furnace	EDC cracking	47.9 [MEUR]	0.48 [MEUR/year]	30
Electrification furnace	EDC cracking	136.2 [MEUR]	3.7 [MEUR/year]	30

3.3.3. Westlake

In this section, the currently installed technology and possible zero emission technology are discussed. First, the currently installed natural gas boiler is discussed. Followed, by the E-boiler as a zero emission technology.

Currently installed: Natural gas steam boiler Westlake

Currently, Westlake uses gas boilers to produce the steam needed for the production of epoxy resins. Westlake receives refinery gas from the Shell Pernis refinery, which Shell regards as a waste product. The steam production in the boiler is based on an exothermic reaction, where gas is ignited in burners with additionally added air. The burners heat up water via a heat exchanger, where water is vaporized and turned into steam. The steam at Westlake is consequently used for the production of epoxy resins.

Table 3.24: Natural gas steam boiler Westlake

Characteristic	Value	Comment
Capacity required	87 [MW]	To suffice the total heat demand for epoxy and BPA
Efficiency	69%	Following the efficiency from Nobians CHP [152]
Cost per capacity unit	0.187 [MEUR/MWth]	price per MWth for upfront investment costs [21]
CAPEX	16.3 MEUR	Total upfront investment costs
OPEX	0.33 Meur/year	2% of CAPEX per year
ELT	15	[152]

E-Boiler Westlake

The zero emission technology alternative for Westlake was retrieved from mail correspondence with Dick van Dam D. The only part that Westlake can directly decarbonize is the heat production. Therefore, Dick van Dam mentioned an E-Boiler as an zero emission technology alternative for Westlake's current fossil-based steam production. Also the recirculation project with Nobian is an alternative for Westlake, which is further elaborated in section 3.4.

The MIDDEN database unfortunately does not provide detailed information about this technology alternative specifically for Westlake. So, the values for the characteristics shown in table 3.26 are the combination of a MIDDEN report on another industrial plant ,called SABIC IP BoZ, and the information that was used for the e-boiler for Nobian. According to Mooij and Muller [100] per ton of Epoxy resin and BPA, respectively 6 GJ and 5 GJ of steam is needed. We know that Westlake produces 170 kton of epoxy resins and 190 kton of BPA on a yearly basis. Meaning that Westlake requires a total of 1.97 PJ per year for steam production. Assumed that Westlake operates a 24/7 continuous production process runs and an efficiency of 99% for the electric boilers [133], the boilers require a capacity of 60 MW. Using the same cost per capacity and OPEX costs, the values of table 3.26 are calculated.

Table 3.25: Electric steam boiler Westlake

Characteristic	Value	Comment
Capacity required	60 [MW]	To suffice the total heat demand for epoxy and BPA
Efficiency	99% [MW]	[152]
Cost per capacity unit [MW]	0.25 [MEUR/MWth]	price per MWth for upfront investment costs
CAPEX [EUR/MW]	15 MEUR	Total upfront investment costs
OPEX [EUR/year]	0.3 MEUR/year	2% of CAPEX per year
ELT [year]	15	[152]

3.3.4. Huntsman

Huntsman requires heat for it's distillation process during MDI purification. Currently, Huntsman buys steam from third parties for it's steam demand. An alternative for the externally bought steam, is to locally produce steam with an E-boiler.

Currently used: Externally bought steam

Currently, Huntsman buys it's steam from the PoR Botlek steam network. The steam networks makes it possible to exchange residual heat among industrial companies, in the form of steam [83]. The Botlek network is operational since 2013 and Huntsman has been reliant on the the network for some years. The main suppliers of the steam in the network are Air liquide and AVR, two companies situated in the Botlek area [161].

Huntsman requires 3.42 MJ/kg of heat for MDI production. With a total of 400 kton/year, Huntsman requires 136.8*107 MJ/year of heat [135]. The heat that is used at Huntsman, is steam at 70 Bar and 510 degrees celsius. Steam has a energy value of 3.41 MJ/kg at these characteristics. So, Huntsman has to buy 401 kton of steam per year. A typical practice is to consider 0,0085€/kg as a steam price value [142]. With that price, Huntsman pays 3.4 Million euro's for steam per year

E-boiler Huntsman

According to Dick van Dam C, Huntsman is planning on installing 50 MW e-boilers to produce their own steam. This is also announced in the 'Provinciaal Blad' of the Province of South - Holland. The announcement states that Huntsman intends to build electric boilers to produce the steam which is currently produced by thirds [84].

The heat that is needed for the MDI purification can be produced with E-boilers that work according to the same principle described in the Nobian and Westlake sections. The calculation for this alternative uses the same cost per capacity and OPEX as the Nobian and Westlake boilers. The characteristics and their corresponding values are shown in table 3.26.

Table 3.26: Electric boiler Nobian

Characteristic	Value	Comment
Capacity required [MW]	50 MW	According to Dick van Dam C
Cost per capacity unit [MW]	0.25 MEUR/MWth	price per MWth for upfront investment costs [40]
CAPEX [EUR/MW]	12.5 MEUR	Total upfront investment costs
OPEX [EUR/year]	0.25 Meur/year	2% of CAPEX [40]
ELT [year]	15	-

3.4. Shared zero emission technologies

This section presents two technologies, where two or more companies within the cluster are involved with. The brine recirculation between Westlake and Nobian is a project conducted within the EU water-mining project, which is accessed via WEI. The second alternative, for a shared CCS network, is a hypothetical shared connection to the larger Porthos project. The alternatives are elaborated in the subsections below.

1. Brine recirculation between Westlake and Nobian
2. Shared CCS network with Nobian, Shin-etsu, Westlake and Huntsman

3.4.1. Brine recirculation between Westlake and Nobian

Westlake currently produces a stream of wastewater containing natrium chloride. That waste stream is treated at Shell for a fee and afterwards disposed in the environment. The price for the waste water treatment was not publicly accessible, so the price is based on a scientific paper. Panagopoulos et al.

[128], estimate that the cost for brine disposal range between 0.54 EUR/ m^3 to 2.6 EUR/ m^3. However, as shown in figure 3.5 Nobian uses brine containing natrium chloride. Thus, instead of Westlake disposing the waste stream containing natrium chloride, it could be used as a feed-in for the production processes at Nobian. This alternative is currently being researched within the EU water-mining project as a demonstration project.. The process design consists of a High Pressure Oxidation unit (HPO), which aims to remove organics from the brine, see the coloured block in 3.12. The technical system comprises out of three major steps, the Brine conditioning, High pressure oxidation and Catalyst recovery/polising. During the brine conditioning process, brine is collected in a container and reacted with a HCl solution and catalyst provided by Westlake. The conditioned brine is consequently placed in the HPO, which increases the NaCl concentration of the brine. In the third step, the catalyst is removed from the brine to make it ready for shipment to Nobian.

Unfortunately, it is not possible to use the CAPEX and OPEX data from the water mining project, so the cost estimation is based on desk research. It is assumed that the CAPEX cost consists out of the HPO unit a pipeline connection between Westlake and Nobian. According to Keefe [156], a HPO unit has a capital cost of 150 thousand euros with comparable capacity requirements as the one proposed in the watermining project. Next, the pipeline connection should be around 2.3 km long. The distance is based on the google maps road distance between the Westlake and Nobian plants. Based on the average pipeline size and average construction cost for land based pipelines of 3 million euros/km [117], the CAPEX of the pipeline would cost 6.9 million euros. In total the CAPEX costs would total 7.05 million euros. Following the other zero emission alternatives from the previous sections, a yearly OPEX of 2% of the CAPEX is used. Lastly, the ELT is assumed to be 30 years.

Table 3.27: Brine recirculation between Westlake and Nobian

Characteristic	Value	Comment
Capacity required	0.1 $M^3/hour$	Water mining project info
CAPEX	7.05 MEUR	2.3 km of pipeline and HPO unit
OPEX	0.14 MEUR/year	2% of CAPEX
ELT [year]	30	Assumption made

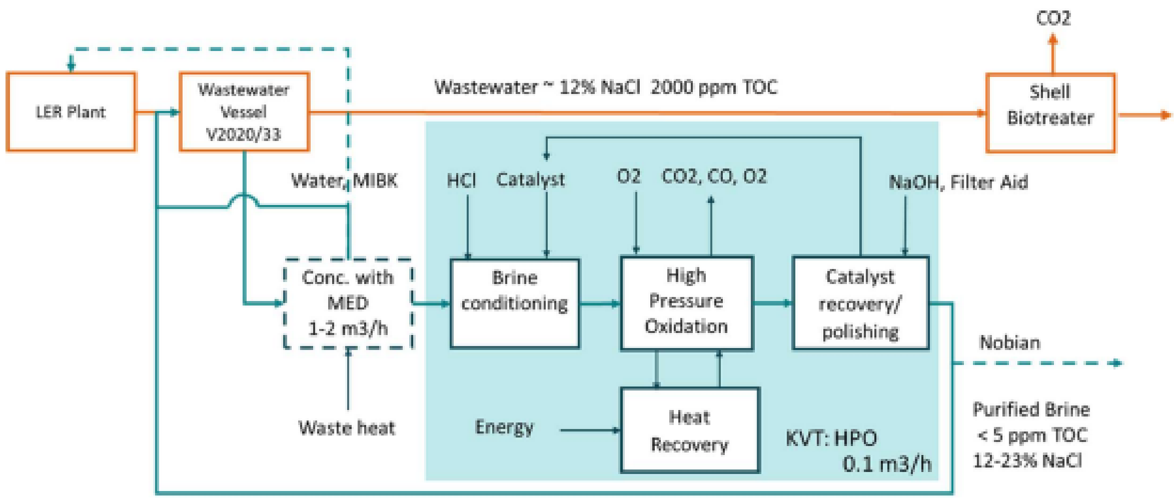

Figure 3.12: Demonstration project Brine circulation (IMPETUS project)

3.4.2. Connection to Porthos CCS network

This alternative is based on a suggestion made by Semeijn and Schure [154]. They have calculated the techno-economic characteristics for a Carbon, capture and storage (CCS) installation at Shin-Etsu's VCM plant. In this subsection we expand further on this suggestion by presenting a shared chlorine cluster connection to the Porthos CCS network. Where the alternative would comprise out of a plant based CCS installation and a shared cluster connection to the Porthos main pipeline. This alternative has to compete with the current fees that are paid to emit CO_2.

Porthos, short for Port of Rotterdam CO_2 Transport Hub and Offshore Storage, is a project where CO_2 from the industry in the PoR is transported and stored in empty gas fields under the north sea. They plan on building a pipeline starting from the Vondelingenplaat, following the A15 highway, to gas fields several tens of kilometers from the coast.

In figure 3.13, an impression is given of the CCS pipeline. The blue line represents the main pipeline and the orange lines the connections from the respective plants that directly emit CO_2 to the main pipeline. All of the The techno-economic characteristics, besides the CAPEX, are based on the estimations made by Semeijn and Schure [154] and shown in the table below. The CAPEX costs are divided into the plant based CCS installation and the pipeline connections. The CAPEX of the plant based CCS installation depicted in a price per captured CO_2, shown as the first OPEX value. The CAPEX row of the table solely represent the pipeline costs that have to be paid by the four companies together, the OPEX values are company specific. Based on figure 3.13, The blue line between Westlake and Huntsman is 7.5 km. Using the same price per kilometer pipeline as the brine recirculation example, the cost for the main pipeline would be 22.5 MEUR. The orange part from Huntsman to the main pipeline is 100m, Nobian and Shin-etsu share a 700m pipeline and Westlake also has a pipeline connection length of 100 meters. This would mean that Huntsman's part would cost 0.3 MEUR, the share Nobian & Shin-etsu pipeline 2.1 MEUR and Westlake's pipeline also 0.3 MEUR.

For the exploration of multi-agent interaction within the chlorine cluster, this alternative assumes that the chlorine cluster has to contribute to the financing of the main pipeline running between Westlake chemical and huntsman. The cost division is conceptualized in later chapters. In reality however, a large part of the financing for the main pipeline is funded by the European Union and the Dutch government [144] and companies are only responsible for the financing of their own CCS installations.

Table 3.28: Shared CCS network

Characteristic	Value	Comment
CO2 emissions	[14kt CO_2/PJ]	[154]
Theoretical amount of electricity required	12.5 [GWhe/PJ]	Post-combustion, capture, treatment and compression
CAPEX	22.5 MEUR	Shared pipeline CAPEX costs
OPEX	115 [EUR/t CO_2 captured] and 5.5 [EUR/t CO_2 captures/year]	Estimation made by Semeijn and Schure [154] and 4% of CAPEX per year [154]
ELT [year]	30	-

Figure 3.13: Impression CCS pipeline at Botlek

3.5. Expert elicitation

The expert elicitation among Nobian and Westlake was conducted via interviews, which are described in appendix C. The expert elicitation was used for this chapter to validate the plant-process-product and zero-emission inventarisations. Unfortunately, it was not possible to validate results for Huntsman and Shin-etsu. So, only Nobian and Westlake are discussed in this section.

3.5.1. Nobian

Nobian was not able to give a detailed overview of their production process at the Botlek plant, but was able to send the overview of 3.14. This figures shows the Nobian salt solution mining, their Chlor-alkali process in the Botlek and the brine recirculation suggestion with Hexion (now Westlake). Although this overview depcits the processes on a higher aggregation level, it is still useful as a validation for the conceptualized process so far. The streams and white process blocks correspond to what was shown in the previous sections.

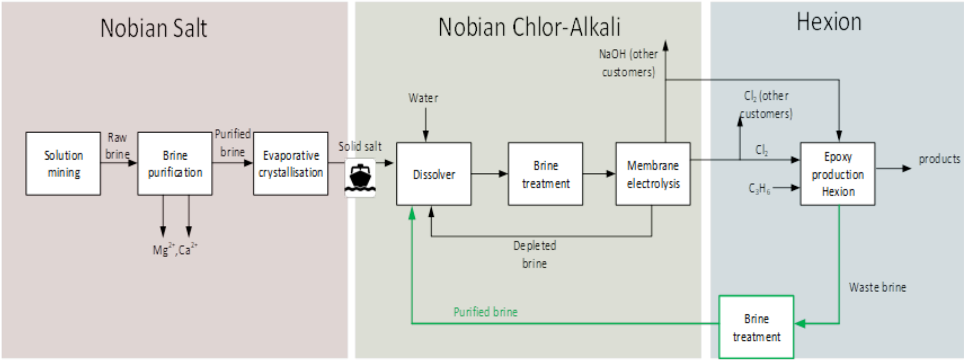

Figure 3.14: Nobian expert information

3.5.2. Westlake

The expert from Westlake was able to validate the main processes, mass flows and decarbonisation alternatives. He stated that all of the processes and alternatives were correct and the same for the decarbonisation alternatives. One comment was made about the current production of heat. In the conceptualisation was assumed that natural gas is used for the heat production. The expert explained that Westlake currently receives refinery gas from the Shell Pernis refinery. The refinery gas is a mixture of multiple hydrocarbons and a very small amount of hydrogen. He mentioned hydrocarbons like methane, ethane and propane.

3.6. Reflection on plant-process-product and zero emission technology inventarisation

This section reflects on both on the plant-process-product and zero emission technology inventarisation. The reflection elaborates on the strengths & limitations of the inventarisations. The following strengths of the inventarisations is observed:

- Generated a detailed understanding of the PoR chlorine cluster's technical system.
- Allows for the identification of emission reducing opportunities.

By using these two methods to analyse the PoR chlorine cluster a very highly detailed understanding of both the current state and possible future configurations of the cluster's technical system is gained. This made to possible to identify emission reducing opportunities, beside the already mentioned alternatives in the MIDDEN database. For example the connection to the Porthos CCS network and brine recirculation project. However, there are also some limitations to the used methods:

- Limited access to case specific data.
- Results in a static representation of the technical system and possible future configurations.

For the PoR chlorine cluster's specific companies there is not a very detailed overview of their technical systems, the same for the potential zero emissions technologies. The MIDDEN database did have detailed overviews of the Nobian and Shin-etsu plant's, but not of the Westlake and Huntsman plants. Beside the MIDDEN database there were no publically accessible sources for both of these companies. So, for this thesis the generally used production processes for Epoxy resin and MDI are used. This leads to a less accurate depiction of the chlorine cluster and a more time consuming process. The lower accurate depiction in turn leads to less accurate depiction of modeled energy and raw material use. Lastly, this method leads to a static representation of the technical system and possible future configurations. This could potentially lead to the model losing it's relevance over time, as the configuration of the technical system changes and the set of possible zero emission technologies.

3.7. Total overview of results

This section aims to give a total overview of both the plant-process-product and zero emission technology inventarisations. In the first subsection 3.7.1, an overview of the PoR chlorine cluster is given. The second section 3.7.2, gives an overview of all the zero emission technologies.

3.7.1. PoR chlorine cluster overview

The figure 3.15, shows a diagram the four companies at the PoR chlorine cluster and their major in - and out - puts.

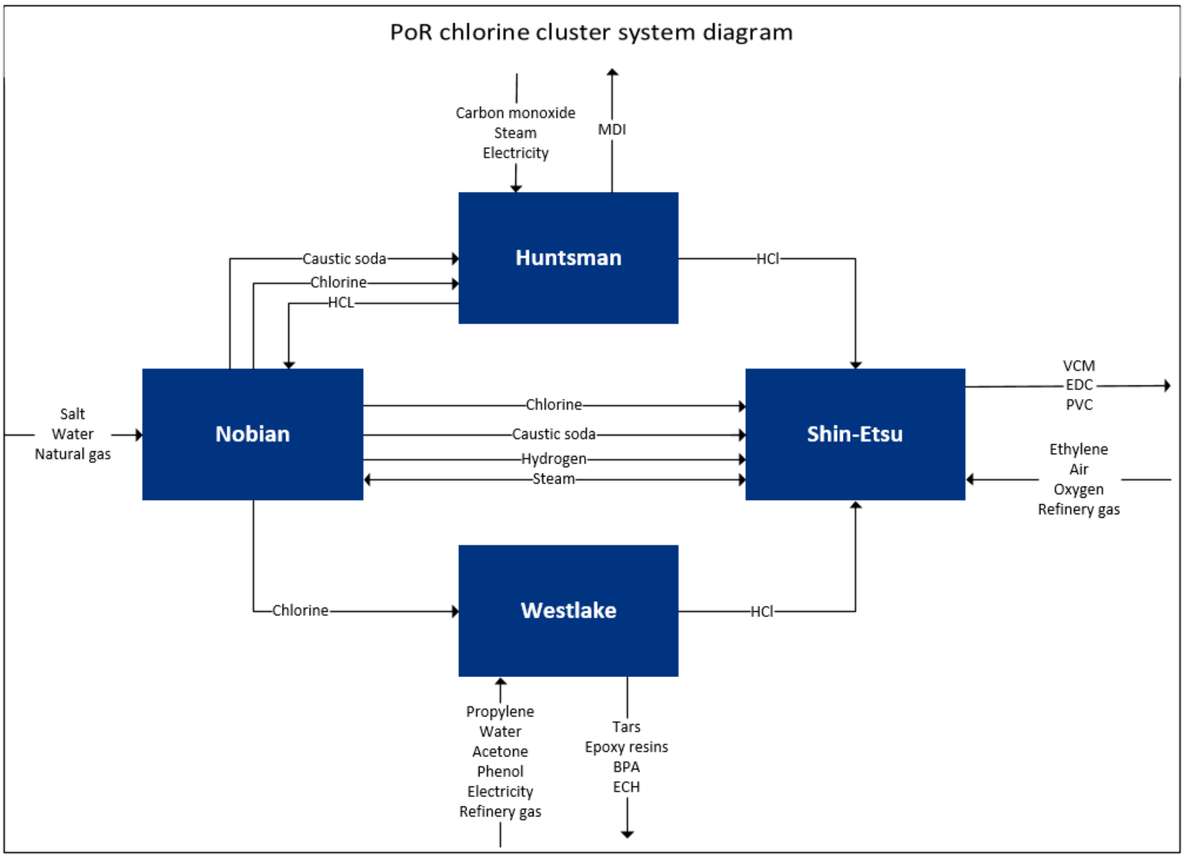

Figure 3.15: Diagram with all in-flowing and out-flowing mass flows PoR chlorine cluster

3.7.2. Overview of alternatives

The first table 3.29 shows all the zero emission technology alternatives and their corresponding CAPEX, OPEX and ELT. The second table 3.30 shows which companies are involved per alternative. There are only two alternatives where multiple companies are involved, which are the brine recirculation and shared CCS network. This overview of alternatives is used as input for the CCI model, so possible future configurations of the Por chlorine cluster can be simulated.

Table 3.29: Overview of all zero emission technologies

Alternative	CAPEX [MEUR]	OPEX [MEUR/year]	ELT	section	Company
CHP	85.5	1.7	20	Utility	Nobian
E-Boiler	9.2	0.2	15	Utility	Nobian
Biomass boiler	35.2	0.7	12	Utility	Nobian
Finite gap electrolysis	190.4	3.8	5	Process	Nobian
Zero gap brine electrolysis	241.9	12.1	5	Process	Nobian
MEV(3)	13	0.26	20	Process	Nobian
MEV(5)	13.3	0.66	20	Process	Nobian
Natural gas furnace EDC cracking	118.5	2.4	30	Utility	Shin-etsu
Hydrogen furnace EDC cracking	47.9	0.48	30	Utility	Shin-etsu
Electric furnace EDC cracking	136.2	3.7	30	Utility	Shin-etsu
Natural gas boiler	16.3	0.33	15	Utility	Westlake
E-Boiler	15	0.3	15	Utility	Westlake
E-Boiler	12.5	0.25	15	Utility	Huntsman
Brine recirculation	7.05	0.14	30	Process	Shared
Connection to Porthos CCS network	22.5	55 [EUR/ton CO_2/year	30	Process	Shared

Table 3.30: Overview of currently installed & zero emission technologies and involved companies

Alternative	Nobian	Shin-Etsu	Westlake	Huntsman
CHP Nobian	X			
E-Boiler Nobian	X			
Biomass boiler	X			
Finite gap electrolysis	X			
Zero gap brine electrolysis	X			
MEV(3)	X			
MEV(5)	X			
Natural gas furnace EDC cracking		X		
Hydrogen furnace EDC cracking		X		
Electric furnace EDC cracking		X		
Natural gas steam boiler Westlake			X	
E-Boiler Westlake			X	
E-Boiler Huntsman				X
Brine recirculation	X		X	
Connection to Porthos CCS network	X	X	X	X

4

Representing market & behavioural barriers

This chapter is dedicated to answer sub-question two, which is depicted below. The first section 4.1 conceptualises a decision protocol. The second section 4.2 shows a way to represent both market & behavioural barriers in an investment model, by the conceptualisation of decision evaluation types. As mentioned in the chapter 2, the decision evaluation types are conceptualised both using the methodology of Knobloch & Mercure [97] and incorporating the market & behavioural barriers shown in chapter 2. Thirdly, section 4.3 shows the decision acceptance criteria. Followed by the expert elicitation, which shows the key-take aways from interviews that have been conducted with Nobian and Westlake 4.4. The last section 4.5, reflects on the conceptualised representation of market & behavioural barriers.

2. *How can we represent market & behavioural barriers in an investment model at the PoR chlorine cluster?*

4.1. Conceptualising the decision protocol

As mentioned in chapter 2, the decision protocol determines how investment decisions regarding technology replacement and expansion are made. The decision protocol follows the logic of both the BRAIN and GPM models, which were reviewed in chapter 2. This means that technology adoption can be conducted both before and after the economic life time of the asset that is to be replaced. It is assumed for simplicity that all of the modeled companies have a binary choice to adopt a zero emission technology or not, see figure 4.1. Which is compared to the default emission technology with respect to the perceived CAPEX and perceived future cost-savings. Next, it is assumed to invest in a zero emission technology, the value retrieved from the profitability analysis has to suffice the decision acceptance criteria stated in section 4.3. From that leads that either an asset is installed or not. This decision protocol is run through on a yearly basis between 2022 and 2050. So based on the investment logic as described above we assume that our investor is a rational investor who always looks to pursue an investment option that gives him the value needed to accept an investment.

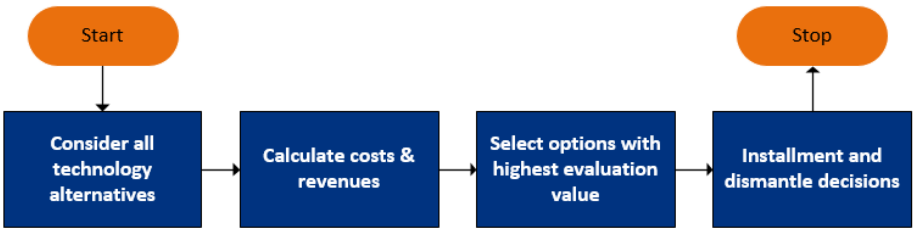

Figure 4.1: Decision protocol

4.2. Representation of barriers with decision evaluation types

This section elaborates on the decision evaluation types that are used during the evaluation of alternatives, shown in the flowchart of figure 4.1. As introduced in chapter 2, the evaluation types are conceptualised following the methodology of Knobloch & Mercure [97].

Their model is based on the combination of perceptions, heterogeneity and risk. They state that perceptions can differ between decision makers. Where the same information on an investment project may be perceived in different ways. What they want to make clear with this point, is the subjectivity upon which decision-making is based. Secondly, the heterogeneity of economic characteristics and decision-making procedures imply heterogeneous decisions. The investment of a homogeneous technology may be viable for the average company, but not for all companies, due to the various contexts and diverse characteristics of the respective companies. Lastly, risk affects the decisions made by companies. There are various aspects that make an investment risky, for example the uncertainty about future profitability or future demand. Table 4.2 shows different investment levels of decision-making, following the methodology of Knobloch & Mercure [97].

Table 4.1: Types of actors and their defining question

Actor	Defining question
Engineer	What is cost optimal for a representative company?
Heterogeneous firms with unbounded rationality	What should be perceived as optimal for a profit-maximising heterogeneous company?
Heterogeneous firms as organisations with bounded rationality	What should be perceived as optimal for a profit-maximising company, given organisational structures and limited decision resources?

Given that companies and the decision makers within them apply heterogeneous decision making rules, it is generally not possible to forecast individual choices according to Knobloch and Mercure [97]. However, by using the likely values of parameters used for investment decision making across companies and individual decision makers, it becomes possible to simulate how choices are made. So, this thesis proposes to simulate the investment behaviour of three types of actors. Each actor corresponds to the perspective and decision criteria a specific hypothetical actor can have. For this thesis, three types of actors have been defined: engineer, heterogeneous firms with unbounded rationality and heterogeneous firms as organisations with bounded rationality. Per actor a defining question is defined, see table 4.1. If companies were to make investment decisions according to the criteria of level X, what would be the aggregate system level outcome? The three different actors represent different amounts of variations (distributions around classic economic theory) and biases (systematic deviations from classic economic theory). This representation of barriers with can be used to obtain quantitative insight on likely aggregate outcomes of decision-making. This insight can then be used for two purposes:

- To estimate the technology adoption at the PoR chlorine cluster between 2022 and 2050.
- To classify impacts of various barriers on system outcomes.

For each actor, different subjective decision evaluation types are formalised. The different levels of decision making and assumptions, various barriers have been represented with either a NPV metric or pay-back period formula. These formula's are used in the CCI model to conduct the evaluation part of technology alternatives. In the table 4.2, 8 different levels of decision making are shown. Varying from no market & behavioural barriers at the baseline level, to all the barriers represented in the behavioural level. Every level incorporates one more barrier or another combination of barriers, to be able to determine the effect of various barriers on technology adoption at the PoR chlorine cluster. The configuration of the barriers are used to represent certain types of decision makers, which are shown in the second column. These barriers are in turn represented by parameters, shown in the third column of the table. There has been chosen for 8 different levels, and not for a full factorial design, as some of the barriers are dependent on the presence of other barriers. For example, imperfect information can't exist without risk and uncertainty. Or hidden costs can't exist without the representation of imperfect information. Also, because otherwise the amount of scenario's would become very large. Every barrier is represented by a parameter, shown in the fourth column. Where these parameters are eventually depicted in the formulas of the NPV or pay-back period. Underneath the table, every level of decision making is explained. The incorporated barrier(s), how they are represented with the respective parameter and the evaluation formula that follows from that.

Table 4.2: Levels of decision-making and their parameters, following Knobloch & Mercure [97].

Level	Actor	Assumptions	Barriers	Parameters	Metric
4.2.1 Baseline	Engineer	- Homogeneous decision makers - No risk or uncertainty - Perfect information - Unbounded rationality	-	-	NPV
4.2.2 Risk	Heterogeneous firms with unbounded rationality	- Heterogeneous decision makers - Risk and uncertainty - Perfect information - Unbounded rationality	- Risk	- Discount rates (ri)	NPV
4.2.3 Imperfection	Heterogeneous firms with unbounded rationality	- Heterogeneous decision makers - Risk and uncertainty - Imperfect information - Unbounded rationality	- Risk - Imperfect information	- Discount rates (ri) - Expectation values (Ei)	NPV
4.2.4 Hidden costs	Heterogeneous firms with unbounded rationality	- Heterogeneous decision makers - Risk and uncertainty - Imperfect information - Unbounded rationality	- Risk - Imperfect information - Hidden costs	- Discount rates (ri) - Expectation values (Ei) - Different upfront costs and benefits (delta Ct, delta Bt)	NPV
4.2.5 Access to capital	Heterogeneous firms with unbounded rationality	- Heterogeneous decision makers - Risk and uncertainty - Imperfect information - Unbounded rationality	- Risk - Imperfect information - Access to capital	- Discount rates (ri) - Expectation values (Ei) - Restricted acces to credit (ci)	NPV
4.2.6 All Market barriers	Heterogeneous firms with unbounded rationality	- Heterogeneous decision makers - Risk and uncertainty - Imperfect information - Unbounded rationality	- Risk - Imperfect information - Hidden costs - Access to capital	- Discount rates (ri) - Expectation values (Ei) - Different upfront costs and benefits (delta Ct, delta Bt) - Restricted acces to credit	NPV
4.2.7 Satisficing	Heterogeneous firms as organisations with bounded rationality	- Heterogeneous decision makers - Risk and uncertainty - Imperfect information - Bounded rationality	- Risk - Imperfect information - Hidden costs - Access to capital - Bounded rationality	- Discount rates (ri) - Expectation values (Ei) - Different upfront costs and benefits (delta Ct, delta Bt) - Restricted access to credit - Critical thresholds (bt) - Technological preference (tp)	Payback criterion
4.2.8 Behavioural	Heterogeneous firms as organisations with bounded rationality	- Heterogeneous decision makers - Risk and uncertainty - Imperfect information - Bounded rationality	- Risk - Imperfect information - Hidden costs - Access to capital - Split incentives - Bounded rationality	- Discount rates (ri) - Expectation values (Ei) - Different upfront costs and benefits (delta Ct, delta Bt) - Restricted access to credit - Critical thresholds (bt) - Technological preference (tp) - Level for cooperation	Payback criterion

4.2.1. Baseline

The first decision evaluation type represents the baseline. The baseline type is used to determine the optimal outcome and acts therefore as a baseline reference point. This type assumes a representative firm that makes investment decisions according to a perfectly rational decision making process with perfect foresight and information. Furthermore, the decisions are made without risk or uncertainty. This follows from the assumptions and barriers shown in table 4.2. Given the assumptions and barriers, this level follows the net-present-value (NPV) calculation as a metric without discount rate. As according to neoclassical economic theory, the right decision metric for a profit-maximising company is a NPV calculation [33]. For this level, the relevant cash flows are the upfront capital investments (ΔC) in the current period (t=0) and the annual gains (ΔB) that are made throughout the economic lifetime (n) (from t = 2022 up to t = 2050) [97]. The (ΔC) represent the difference in upfront costs compared to the existing asset (in case of technology replacement). The (ΔB) is defined as the cost-savings relative to the existing asset. Where ΔQ the change in required electricity or other input represents, multiplied by it's market price p_t, resulting in : $p_t * \Delta Q_t$. As this decision type assumes a risk-free investment, there is no discount rate used. The above mentioned, results in the following equation:

$$NPV = -\Delta C + \sum_{t=0}^{n} p_t * \Delta Q_t \tag{4.1}$$

4.2.2. Risk

The level risk introduces the assumptions of heterogeneity and risk & uncertainty. This is depicted in the first market barriers, risk. Previously was explained that risk can manifest itself in many forms, due to the uncertainties caused by imperfect foresight. Think of sources like macro economic trend, government policy and many more. To incorporate risk in this evaluation type, the barrier is represented by discount rates in the NPV formula that follows the same principles as explained in the baseline type. The heterogeneity is shown in the varying levels of discount rates r_i among decision makers, as their perception of risk may vary from each other. Next, the risk and uncertainty of potential investment projects is depicted by division part $(1+r)^t$. The r-value is determined by the level of risk and uncertainty per decision maker and per type of investment.

$$NPV_i = -\Delta C_+ \sum_{t=0}^{n} \frac{p_t * \Delta Q_t}{1 + {r_i}^t} \tag{4.2}$$

4.2.3. Imperfection

This type introduces imperfect information on top of the strategic level. Examples of the effects of imperfect information in the industrial sector are, the unawareness of available technology but also about it's characteristics like costs and saving potentials. During this thesis, the characteristics of cost savings are considered. The imperfect information regarding the actual cost savings are represented with the parameter expectation values (Ei). The expectation values might have influence on the realised efficiency of a technology alternative. As for example the fuel requirements turn out to be higher than anticipated when making the investment. This results in the following formula:

$$NPV = -\Delta C + \sum_{t=0}^{E_i(n_i)} \frac{E_i(p_i, t) * E_i(\Delta Q_i, t)}{1 + r^t} \tag{4.3}$$

4.2.4. Hidden costs

This type introduces hidden costs and also represented by expectation values E_i. There are roughly three main possible sources of hidden costs: the general overhead costs of energy management, the costs which are specific to an individual investment or the choice of a technology and it's potential loss of utility [159]. For this PoR chlorine cluster, this could mean that the companies may be subject to hidden costs concerning the actual OPEX costs that only manifest themselves after a certain period of time. So, these costs maybe differ from the moment of investment. This results in the following equation:

$$NPV = -\Delta C + \sum_{t=0}^{E_i(n_i)} \frac{E_i(p_i, t) * E_i(\Delta Q_i, t)}{1 + r^t} \tag{4.4}$$

4.2.5. Access to capital

This type builds forth on level tactical, where access to capital c_i is added. The access to capital can be restricted by the inability to access internal funds and/or attain external funds. Therefore, in the CCI model every company has their own specific amount of capital that can be used to invest in new technology. The access to capital is not represented in the NPV formula, but is rather modeled in the CCI model as a constraint. So, this type follows the same NPV formula as optimizing 2, but is modeled differently in the CCI model. See the equation:

$$NPV = -\Delta C + \sum_{t=0}^{E_i(n_i)} \frac{E_i(p_{i,t}) * E_i(\Delta q_i, -t)}{(1 + r_i)^t} \tag{4.5}$$

4.2.6. All Market barriers

This level of decision making combines levels operational 1 and 2, as both hidden costs and restricted access to capital are added. As mentioned in the explanation of optimizing four, the restricted access to capital is not represented in the NPV formula. Therefore, the NPV formula is the same as optimizing Operational 1 for the representation of these barriers.

$$NPV = -\Delta C + \sum_{t=0}^{E_i(n_i)} \frac{E_i(p_i, t) * E_i(\Delta Q_i, t)}{1 + r^t} \tag{4.6}$$

4.2.7. Satisficing

This is the first type where a behavioural barrier is represented. As Simon suggests, bounded rationality takes into account the cognitive limitations of decision-makers of both knowledge and computational capacity [158]. These limitations of the decision makers are represented in the model by a pay back period criterion b_t and a technological preference.

Allthough the pay-back period method in itself is a rational way to cope with limited information and limited cognitive abilities, it has it's deficiencies. The method does not account the time value of money, it does not account for the cash flows after the return of investment and the defined time period might be prone to bias. A survey conducted by Graham and Harvey [75] on budgeting behaviour by companies in the United States, concluded that 'always or almost always' the pay-back time criterion is used to make investment decisions. So instead of determining if the NPV value over the economic life time of an asset, the NPV is considered over a set pay-back time. According to Anderson and Newell [6], this threshold for payback is commonly found between one and five years. This threshold can also vary among the decision makers at the PoR chlorine cluster.

To also account for the cognitive limitations of decision makers, following bounded rationality theory, technological preference is also introduced.According to a study by Allais [4] on the irrationality of decision making, he found that personal preference of decision makers play a large role in the decision making process. He found that individuals will not always opt for the most utility maximising alternative, but rather choose the alternative of it's own personal preference.

This can also be the case for certain technological preferences of decision makers at the PoR chlorine cluster. This is not modeled in to the NPV formula by the factor tp that influences the perceived upfront investment costs. So that certain alternatives can be perceived as more or less expensive than they are in reality, depending on the preference of the decision maker. See the following equation:

$$NPV = t_p * -\Delta C + \sum_{t=0}^{b_i} [E_i(p_{i,t}) * E_i(\Delta q_{i,t})] \tag{4.7}$$

4.2.8. Behavioural

For this decision type, all of the market & behavioural barriers are incorporated. In addition to the Satisficing type, the split incentive barriers is added. As mentioned in chapter 2, the landlord-tenant problem examples shows that differences in incentives within companies or between companies can effect the adoption of technology. Following that problem, cooperating companies at the PoR chlorine cluster might have varying incentives when it for example comes to energy-efficiency. During this thesis, this barrier is used when considering technologies where multiple companies are involved with. Where the split incentives are represented in the willingness to cooperate. Therefore this leads to the same NPV formula and pay back criterion as satisficing, but the willingness to cooperate will be added in the CCI model.

$$NPV = t_p * -\Delta C + \sum_{t=0}^{b_i} [E_i(p_{i,t}) * E_i(\Delta q_{i,t})] \tag{4.8}$$

4.3. Decision Acceptance criteria

The decision makers evaluate investment opportunities based on an NPV calculation or pay back period. Both of these calculations have certain acceptance criteria. These acceptance criteria determine whether an investment is accepted or rejected. The NPV values can either be larger than zero, zero or smaller than zero. If an investment option has an NPV higher than zero, the decision maker selects the options with the highest expected NPV value among the alternatives that have an NPV higher than zero. When the NPV value is zero or smaller than zero, the investment is rejected. For the pay back period there are two values, either the evaluated alternative has a pay back period larger than X or equal/smaller than X. Where X is the value that the decision maker has set as a reference. When an investment is accepted, this means that the existing asset is replaced with another asset. When an investment is rejected, the currently installed asset remains operational.

Table 4.3: Overview of decision acceptance criteria

If value	This means	Decision
NPV >0	If the NPV value is larger than zero, than the investment would result in added value to the company.	The investment is accepted
NPV <0	An investment, with a NPV lower than zero, leads to a decreased value to the company.	The investment is rejected
NPV = 0	When the NPV is equal to zero, the company would neither gain nor lose value from this investment.	The Investment is rejected
Pay back period ≤ X	When pay back period is smaller than the value X , which is determined by the preference of the decision maker, then the investment is accepted.	The investment is accepted
Pay back period >X	If the pay back period is larger than the value X, then the investment is rejected.	The investment is rejected

4.4. Expert elicitation

Two out of four companies at the PoR chlorine cluster have been contacted for this thesis. The questions for this specific chapter were asked to gain insight about the decision protocols at the companies, their perceived risks and how do they make investment decisions. A more detailed description of the interview is given in appendix C. The key-take aways from the interview for this section are shown in the subsections below.

4.4.1. Nobian

The interview for with Nobian for this chapter focused on the perceived barriers to investment, the decision making process, the evaluation types and what role models have in the decision making process. Regarding the barriers, Nobian perceives the lack of economically viable technological alternatives as their main barrier to investment. They argue that the writing off costs of currently installed assets and large capital investment costs for replacement alternatives, are the main concerns. They incorporated this barrier in their investment calculations as a risk factor.

Regarding the decision making process, Nobian uses the FEL method. FEL, short for Front-end loading, is a common practice used to plan and design early in a project's life cycle. The FEL method is usually used in industries with high capital intensive and long lifecycle projects. During the interview they mentioned that they used this method and relied heavily on quantitative decision support models. The models, were split into two categories: the plant process model and an investment model. That might also be due to the fact that Nobian uses a very strict decision acceptance criteria. Nobian finds investments acceptable when the pay-back period is equal or smaller than three years or an internal rate of return (IRR) of 30% is reached. To conclude, the key-take aways for this chapter:

- Barriers are recognized but not thoroughly incorporated in Nobian's investment models.
- Quantitative investment models play a central role in Nobian's decision making process.
- The acceptance criteria are either a pay-back period of 3 years or 30% IRR.
- Cooperation with other companies and the division of benefits & costs is determined per project and not a specific division rule.

4.4.2. Westlake

When asked about the perceived barriers to investment, the expert from Westlake mentioned that the two main concerns for them were the lack of economically viable options and uncertainty. The reason for the lack of economically viable, was mainly due to the uncertainty in energy prices, commodity prices and government. As mentioned by the expert of Westlake, the uncertainty what the relative attractiveness of for example electrical powered heat production compared to refinery gas powered heat production refrains them from investment. Adding the uncertainty about government policy regarding subsidies and CO_2 costs, makes it very difficult for Westlake to make decarbonisation investment decisions. Next, the conversation shifted to the relevance of quantitative models in general regarding investment decision making. The expert from Westlake stated that models play a central role in their decision making process and are the basis of their economic viability analysis. For an alternative to be economically viable, Westlake uses acceptance criteria values that are representative for the industrial sector. Therefore, it is assumed that Westlake also uses a pay-back period of three years and IRR of 30%. The last topic that was addressed, was about investments that are conducted in cooperation with other companies. According to the expert, the barrier for cooperation is information assymmetry between companies. A lot of necessary information for companies to cooperate is difficult to share, because of the confidentiality of that information. To conclude, the key-take aways from the Westlake elicitation:

- Barriers are recognized, but do not have a significant effect on Westlake's case and therefore not incorporated in used investment models.
- Quantitative investment models play a central role in Westlake's decision making process.
- The acceptance criteria are comparable to the norm used in the industrial sector.
- Cooperation with other companies is mostly difficult due to information assymmetry.

4.5. Reflection on representing market & behavioural barriers with simple decision rules

This section reflects on the conceptualised method of representing the market & behavioural barriers. The reflection elaborates on alternative representation methods that could have been chosen and the strengths & limitations of the currently conceptualised representation method. The table 2.6, shows that all of the reviewed models base their representation of barriers on a similar way as in this thesis. However, an alternative to the simple decision rules are investment heuristics. Investment heuristics, also called 'rules of thumb', have been defined by Gerd Gigerenzer [70] as follows:

> *"A strategy that ignores part of the information, with the goal of making decision more quickly, frugally, and/or accurately than more complex methods"*

The heuristics can be used as tools to depict strategies that ignore parts of information and the cognitive limitations of decision makers. Gigerenzer's research mentions multiple types of heuristics for decision making, like the recognition heuristic, take-the-best heuristic and Fast-And-Frugal Trees. The recognition heuristic for example, exploits the cognitive ability of recognition to make inferences about unknown quantities in the world. When considering two alternatives, the heuristic would works as follows: If one of two alternatives is recognized and the other not, then infer that the recognized alternative has the higher value with respect to the criterion [73]. These heuristics have their own specific decision protocol, decision evaluation and acceptance criteria, which differs fundamentally from the approach chosen in this thesis.

For this thesis, a deliberate choice was made to use the same decision protocol for every level of decision making and only differentiate in the decision evaluation part. We acknowledge that the parameterisation of market & behavioural barriers is a simplified way of truly capturing various investment behaviours. As, this method limits the way of completely capturing variations in methods for decision making like heuristics. As these also differentiate in decision protocols and acceptance criteria. However, there are also various strengths to the chosen representation of market & behavioural barriers:

- The representation in the form of evaluation types is interchangeable and can be used in various heuristics that contain an evaluation process.
- Can be expanded with other/more parameters to represent the barriers.
- Can identify whether it is necessary to conduct a more detailed investment analysis.

5

Model conceptualisation and application to the PoR chlorine cluster case

This chapter gives the conceptualisation of the CCI model and a detailed explanation how the model works. First, section 5.1 defines all the requirements of the CCI model. Followed by section 5.2, which defines all the elements that are included in the model. Third, section 5.3 discusses the main assumptions that are made. Section 5.4 explains why Linny-R is chosen as a modeling tool and it's key concepts. Next, section 5.5 elaborates on the implementation of the previously mentioned elements and assumptions in Linny-R. The last section 5.6, is dedicated to the model verification and validation.

5.1. Requirements of the CCI model

This subsection defines the functional and non-functional requirements of the CCI model. The functional requirements are, "the services and functions that the system should provide, the things it should do, or some action it should take", following the definition of Faulconbridge, et al. [60]. The non-functional requirements on the other side are defined by Faulconbridge, et al.[60] as "the qualities, properties, or attributes that the system must posses". To make the distinction between the two types of requirements we reference to functional requirements as something the model 'must do' and the non-functional requirements as something the model 'shall do'. The requirements that are discussed later on this section, are based on the input and output flows of figure 5.1.

Table 5.1: Requirements of the CCI model

Requirements CCI model	Description
1.	The model must be able to represent the plants, processes, products and zero emission technologies of the chlorine cluster
2.	The model must make decisions on installing new assets every year
3.	The model must make decisions on dismantling existing assets every year
4.	The model must be able to model heterogeneous decision evaluation types
5.	The model must be able to model heterogeneous entities
6.	The model must output transition pathways, CO_2 emissions and cash flows.
7.	The model shall be computationally feasible

The main function of the CCI model is to simulate technology adoption made by the PoR chlorine cluster under various market & behavioural barriers and exogeneous factors. The table 5.1 above, shows all the requirements of the CCI model. These requirements reflect how the primary goal of the CCI is realised. Requirement one reflects the necessity to model the technical system of the PoR chlorine cluster on a highly detailed level. This is necessary to be able to model investment decision making on an asset level. Requirements two and three reflect the functionality of yearly investment decision making, as reflected in the figure 5.1. Replacement and expansion investment need to be considered every year and accepted investments need to be installed. Besides, the replaced 'old' assets need to dismantled.

Next, requirements four and five reflect the necessity to incorporate market & behavioural barriers in the form of the conceptualised heterogeneous decision evaluation types. For requirement number four this means that the model must be able to incorporate risk & uncertainty, imperfect information, hidden costs, access to capital, bounded rationality and split incentives. Also, the model must be able to model heterogeneous entities. Where the entities can be specified at various scales on the perception of risk & uncertainty, how they treat imperfect information, hidden costs and access to capital. Also, how the biases towards technology represent their bounded rational behavior. Lastly, also the behavioural differences in the form of values connected to split incentives. Requirement six is necessary to answer sub question 3, as this is the main output parameter to determine the effect of market & behavioural barriers on zero emission technology adoption. Where transition pathways must be depicted as a set of installed and dismantled assets over time (2022-2050). The last requirement is a non-functional argument about the computational feasibility. Because of limited time and computational limitations, the run time of the model should not be too long. This eventually is a trade-off between the level of accuracy and practicality of the model.

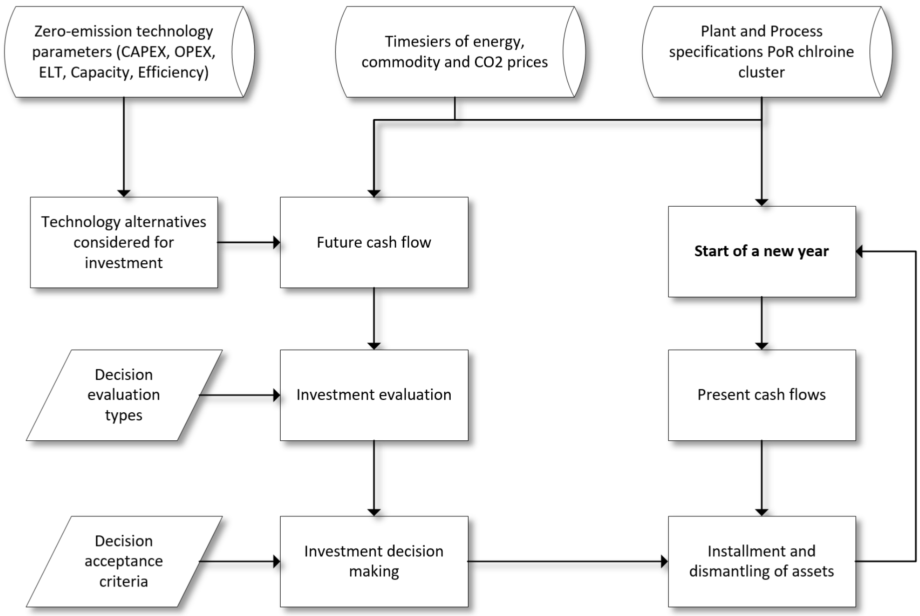

Figure 5.1: CCI model flows, ammended from MIDO model flows [149]

All of the requirements are visually represented in the figure 5.1. The top part of the figure represent externally inputted data. The parallelograms depict information streams within the model and the square boxes processes within the model. The top left box contains information regarding the techno-economic information of the zero emission-technology alternatives. The middle top box represents the exogenous information, like the market conditions in the form of energy prices, commodity prices, CO_2 prices. The top right box contains the specifications of the current state of the technical system. The left two columns represent the investment decision making for zero emission technology alternatives and the third column depicts the alteration of the current configuration that is changed on a yearly basis.

5.2. Included elements in CCI model

This section makes explicit which elements are considered, that form the main components that in this model. The elements that are included follow from chapters 3, 4 and the elements needed to answer sub-question three. Therefore the following elements are included in the CCI model:

1. PoR chlorine cluster's technical system
2. Investment decision-making
3. The chlorine cluster's companies
4. Exogenous environment

5.2.1. PoR chlorine cluster's technical system

The first element that is built in the CCI model, is the technical system. This incorporation of this element suffices requirement number one. The technical system is based on the plant-process-product inventarisation and zero-emission technologies from chapter 3. The five plants of Nobian (1), Shin-etsu (2), Westlake (1) and Huntsman (1) are included on a highly detailed level. This means that the five plants have been modeled on a input, process and output level. When it comes to the technology alternatives, all the alternatives shown in the last section of 3 have been incorporated. This element allows for the change in current configuration of the technical system to possible future configurations.

5.2.2. Investment decision-making

The investment decision-making element, is included by incorporating simple decision rules. The element is based on a decision protocol, decision evaluation types and decision acceptance criteria. The decision protocol determines how investment decisions regarding technology replacement and expansion are made. Within that protocol, one of the steps is dedicated to the evaluation of investment projects. This part is represented by the decision evaluation types that have been thoroughly explained in chapter 4. Lastly, the values that are derived from the investment project evaluation lead to an investment being accepted or rejected. This part is represented by decision acceptance criteria, further explained in section 5.5.2.

5.2.3. The chlorine cluster's companies

The techno-economic characteristics of four companies of the chlorine cluster are incorporated in the model. The companies differ from each other through their heterogeneous parameter configurations on the decision evaluation types and techno-economic characteristics. This element is suffices the fifth requirement, shown in the first section of this chapter. The heterogeneity between these decision makers is based on their varying perspectives to the barriers. Also, the techno-economic parameters differ between the decision makers. As a company can only evaluate investments to which he is involved with, following table 3.30

5.2.4. Exogenous environment

Lastly, the exogenous environment represented by the model for the in/out - going mass & energy flows, commodity buyers, energy suppliers, technology suppliers and policy makers. The supply of of mass & energy flows that are needed for the chlorine cluster are not specifically modeled, but modeled as an exogenous environment. The same counts for the supply of technology of the zero-emission technology alternatives, as well for the actors that buy commodities like chlorine, PVC, etc, from the chlorine cluster.

5.3. Main assumptions

This part follows the third point of the model approach structure introduced in 2.3.2. Here, the treatment of space, time, uncertainty, entities and resolvement are discussed.

Space

Following the definition of Kelly [94], which was earlier introduced in chapter 2, this model treats space as compartmental space. As this thesis focuses solely on the compartmented PoR chlorine cluster's four companies and their interconnections, in the Botlek area. The companies represent certain homogeneous characteristics, in this case the production of chemical products. So when looking at figure 5.2, only the locations of the companies is considered. Not the surrounding roads or waterways, etc. The mass and energy flows that come from third parties, such as NaCl for Nobian and steam for Huntsman are treated as exogenous incoming flows.

Figure 5.2: The locations of the four PoR chlorine cluster's companies.

Time

This model uses a discrete temporal treatment of time. The model assumes a time frame between 2022 and 2050 and takes a yearly time step to compute the model. Therefore, all the input and outputs are based on yearly averages. So, for instance electricity prices are used in the model based on the yearly averages and do not account for variations of the prices within a year.

Uncertainty

The uncertainty that is taken in to account in this model is based on the inputs for model runs. These inputs are the uncertainties incorporated in the decision evaluation types, the heterogeneity of the decision makers (agent-granularity) and the exogenous environmental uncertainties like energy and commodity prices. Furthermore, it is assumed that the market demand for the products produced at the cluster is constant over the time frame defined above. Commodity prices can change in the model, but commodity input and outputs remain stable.

Treatment of entities

As mentioned in chapter 2, models can treat entities in various ways. In this model, the four companies are treated as individual entities based on their company specific characteristics. Therefore, in the model, four aggregated decision makers are incorporated and their interactions with each other and their environment. The interaction with each other is based on their interchanging of products and the zero emission technology alternatives where two or more decision makers are involved.

Resolving the model

The resolvement of the model is scenario-based with a comprehensive discrimination between technology alternatives. This approach makes it possible to explore the effect of the decision evaluation types, heterogeneity of decision makers and the exogenous environment on investment decision at the PoR chlorine cluster. The investment decisions are based on representative years, where the model performs a simultaneous optimisation regarding installment and dismantling decisions.

Table 5.2: Main assumptions

Assumption	Description
Space	Confined to the PoR chlorine cluster's physical location. The four companies are represented as four compartments that are interconnected among eachother.
Time	Discrete temporal treatment of time, with a timeframe between 2022 and 2050. A yearly timestep is used to compute the model.
Uncertainty	The uncertainties considered are based on the inputs for model runs. Uncertainties incorporated in the decision evaluation types, heterogeneous entities and exogeneous environment (energy prices e.g.). It is also assumed that the market demand for products is static over the modeled time period.
Entities	Treated as four unique entities and external actors.
Resolving	Scenario-based resolvement. With simultaneous investment decision making based on a representative year.

5.4. Linny-R

This section is dedicated to the chosen modeling software. The rationale behind this choice is explained in subsection 5.4.1. Followed by a explanation of Linny-R itself in subsection 5.4.2.

5.4.1. Rationale for using Linny-R: solving a MILP problem

This subsection explains why Linny-R is chosen as a modeling tool. First, it is introduced why the research can be seen as a Mixed Integer Linear Programming (MILP) problem. Followed, by explaining why Linny-R is a suitable tool to solve MILP problems.

As mentioned above, the model aims to optimize the adoption of zero-emission technology at the PoR chlorine cluster under varying representations of market & behavioural barriers, agent granularity and exogenous factors. This is comparable to unit commitment (UC) problems in electrical power production. In UC problems, the production of a set of production plants is coordinated to achieve a certain common target. Most of the time those targets might be matching energy demand at minimised costs or maximisation of gains from production. The decisions that can be made usually are, commitment, production or network decisions. To commit whether a producing unit is turned on at a certain moment in time. Second, to determine which level of production that unit is producing at a moment in time. Lastly, how much of that production is flowing from A to B. The same can be said for the investment problem for the PoR chlorine cluster. Between the time period of 2022 and 2050, yearly is decided whether to commit, produce and transport. Production units are invested in or not, in order to match product demand while minimizing investment costs. The production units can have certain production levels and transport certain levels of product from A to B.

This problem can be solved with a MILP based approach [92]. MILP is a form of mathematical programming that is commonly used for the optimisation of complex linear systems [125]. In a MILP model, a value of the objective function is optimised by changing the values of the decision variables. This function is subject to constraints on the values that the variables can hold. The objective function and constraints are subsection 5.5.2. The MILP problem in this thesis is mainly a simultaneous UC optimization problem, with the objective to minimize investment costs, where the system is represented by a number of *units* belonging to set **U**. These units (zero technology alternatives), can supply, demand or convert material and energy *streams* ($\in$ S). The set of *units* can be further divided into *process units* (PU $\subset$ U) and *Utility units* (UU $\subset$ U). The process and utility units (See all overview of alternatives in chapter

3) can be optimized in terms of existence. This is because it is assumed the value of an alternative can either be 1 or 0, meaning it can be operating at it's maximum capacity or not operating at all. This follows from the main assumption that the market is static and demand for products does not change over time.

There are various tools to solve MILP problems, for this thesis Linny-R is chosen as the modeling method to make the CCI model. Linny-R is an executable graphical specification language for MILP (Mixed-integer linear programming) problems, developed by Pieter Bots at the TU Delft [15]. Linny-R's is a user friendly tool, mainly because of it's graphical representations and ease of modelling. It is also a tool that has been used for master theses for the CoSEM programme with success before. Examples of thesis which have used Linny-R are for example Advani's [2] on finding robust transition paths for industrial ecosystems. He used Linny-R to find ways to determine optimal investment paths for industrial clusters under specific constraints like: investments should contribute to sustainability, provide a positive return for the clusters as a whole and allow for a distribution of costs and benefits. Another thesis that used Linny-R, is Desideri Perea's thesis on the analysis of cooperative relationships in the transition of the energy-intensive industry [44]. In her thesis she was able to provide insights in the effects of contractual structures on the transformation of industrial clusters with Linny-R. So to summarize, two reasons for choosing Linny-R:

- Linny-R allows to solve MILP problems.
- Linny-R is a user friendly tool because of it's graphical representation and ease of modelling.
- Previous success of other CoSEM students using Linny-R.

5.4.2. Key Linny-R concepts

In Linny-R, entities are the main building blocks. They are identified by their unique name and have various attributes Linny-R has sixentity types: process, product, actor, link, constraint, cluster and dataset. Underneath, the Linny-R entities are further explained.

Processes

A process, shown in figure 5.3, transforms a product into another product. In Linny-R, the processes are depicted as rectangular shapes with 5 types of information visible. First off, the process name in the middle. Followed by the 'owner' of the process, shown in the figure with 'actor'. Next, a processes can be constrained with lower and upper bounds. In the top left corner the upper bound of the production capacity of a process is shown. When the model is run, the solver of Linny-R will compute the optimal production level (top right corner) for each process, per time-step. Additionally, a initial production level can be specified for the process. Lastly, when the model settings have been ticked to infer cost prices, the process will show the cost price in the bottom left corner.

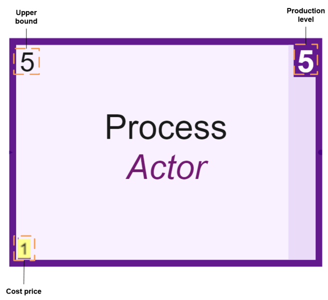

Figure 5.3: Linny-R process

Products

A product represents something that can be produced and/or consumed by a process. What the products represent can be something tangible like chlorine, but also something intangible like information [16]. Products can be limited to a lower and upper bound, shown on the left side of the figure below.

Additionally, an initial stock level can also be specified. On the right bottom corner, the cost price is shown. Underneath the top product oval, four specified types of products are shown. Starting from the left, a stock is shown with a double lined edge. Stocks are able to aggregate their inflows and outflows over time. Next, the sink is shown with the gray downward facing triangle at the top of the product. A sink can be used as the 'exit' flow from a model. Next, the source with the gray triangle facing upwards can spwan product from outside of the 'system'. Last, on the far right side a data product is shown. It is recognizable by the dashed rim. With this product it is possible to distinguish between goods and information.

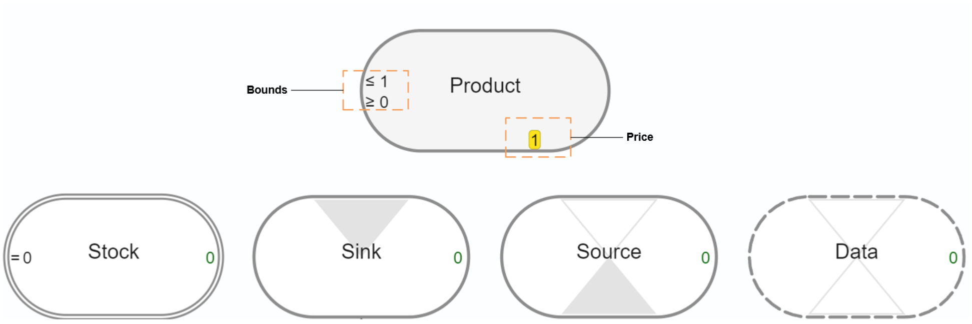

Figure 5.4: Linny-R product and product specifications

Actor

An actor is mainly used to assign 'owners' to processes. During each run, the model solver aims to maximize the weighted sum of the cash flows of all the actors. By default the weight factor of every actor is equal to 1, if necessary it is possible to modify the weight. The cash flow of an actor is calculated as the sum of the cash flows at a certain time step, of all the processes where the actor has been assigned to.

Links

A link, shown in figure 5.5, depicts a product flow or data flow. The flows that run over the links are equal to the level of producing by the processes, multiplied by the rate of the link (see right side of the figure) hen the model is run, the realized flow is shown in blue (see left side of the figure below). When the link is a data flow instead of a product flow, the link is shown with a dashed shaft. These links can have particular information, which is indicated by the symbol that is near the head of the arrow. The information that the link can throughput is shown on the right side of the figure below.

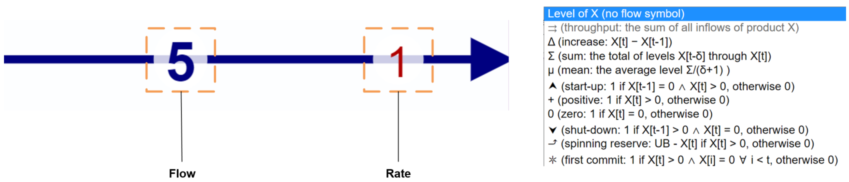

Figure 5.5: Linny-R link

Cluster

A cluster makes is possible to group processes and make the graphical representation of the model look more appealing. Every process can only be part of one cluster, also known as it's parent cluster. Unlike processes, products and links, clusters do not affect the optimization problem. Lastly, although the clusters can be associated with an actor (see figure below), this is only a 'cosmetic' feature. As, it does not affect the ownership of the processes that are grouped within the cluster.

Dataset

Datasets make it possible to group data that can be used in variables in expressions. Most of the time, the data sets are comprised of a numbers over a certain time series. Where every line in the data set represents a timestep of the time series.

Figure 5.6: Linny-R cluster

Simple representation of a production process

In the figure below, a simple representation of a production process is shown with products, a process and links.

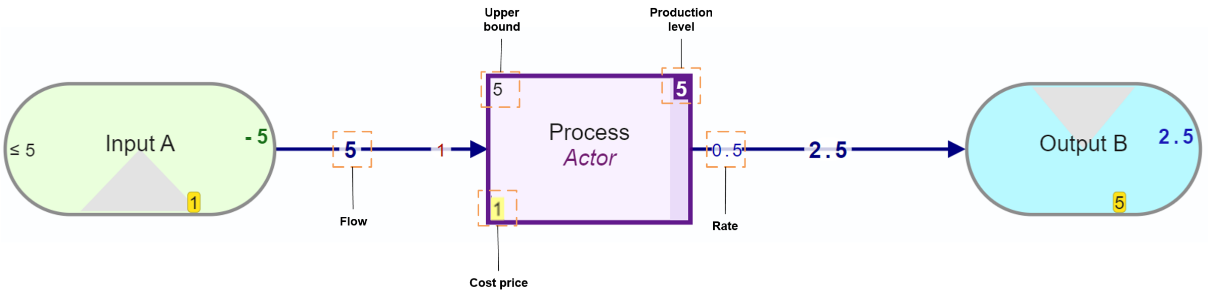

Figure 5.7: Simple representation of a production process in Linny-R

5.4.3. Time and optimization in Linny-R

Here is explained how time is represented in the Linny-R and how the solver uses a "rolling time horizon" to solve optimization problems. Linny-R uses a solver called Gurobi. The Gurobi solver allows for the solving of major problem types like, Linear programming, Mixed-integer linear programming, Quadratic programming. The solver usually sets up to calculate the model in a chain of smaller parts of time, also called 'chunks' [16]. The size of the chunks is equal to the block length of n time steps and a look-ahead period of 1 time step. Where the specification of the block length and look-ahead period is specified in the model settings dialog. An example of a Linny-R timeline is shown in figure 5.8. Here it is shown how Linny-R runs a "rolling time horizon", where a overlapping series of chunks is optimized of which the sum covers the entire optimization period.

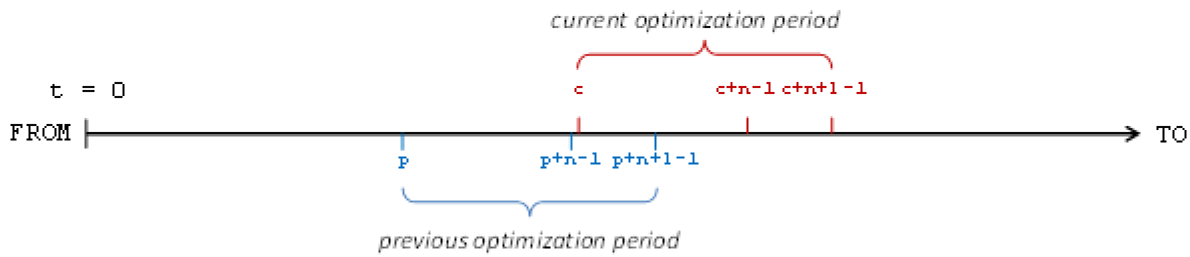

Figure 5.8: Optimization periods in Linny-R

After solving the model for the previous chunk of n+1 time steps, which started at time point p, and then having solved the model for the previous chunk of n+l time steps starting at time p, and then having calculated the values of all model attributes for that period while advancing the simulation time t from p to p+n+l-1, Linny-R moves t back to c = p+n, being the first time step of the now current chunk. After this is completed, Linny-R then sets up the optimisation problem for a new period (n+1 time step), where it uses the calculated stock values and production levels at time c-1. This is where the constraints are represented. Lastly, Linny-R then solves the optimization problem for the currently run period and calculates all the model attribute values for this period.

5.5. Implementing the CCI model in Linny-R

This section gives a explains how the model has been implemented in Linny-R. First, subsection 5.5.1 explains how the plant-process-product and zero emission technology inventarisation are modeled in Linny-R. Next, subsection 5.5.2 elaborates on how the market and behavioural barriers are implemented in Linny-R. The last subsection 5.5.2, how the four companies are modeled as decision makers.

5.5.1. Modeling the technical system in Linny-R

As earlier mentioned, the technical system of the model consists out of the plant-process-product and zero emission technology inventarisations. The first inventarisation makes it possible to model the current state of the technical system. The technology alternatives, make it possible to model possible future configurations of the PoR chlorine cluster. Underneath is explained how the two have been represented in Linny-R. The data for the techno-economic characteristics was retrieved from chapter 3.

The plants, processes and products in Linny-R

The plant-process-product inventarisation from chapter 3, resulted in manufacturing overviews of the five plants (Nobian (1), Shin-Etsu (2), Westlake(1) and Huntsman(1). These have been modeled in Linny-R, following the previously explained key-concepts of Linny-R. The Plants have been represented in clusters, the processes with processes and products with product entities. The mass and energy flows have been represented by rates and flows via links. This resulted in a highly detailed technical overview of the PoR chlorine cluster. See the online appendix for a visual representation.

Zero emission technologies in Linny-R

All the technical alternatives shown in table 3.29, are modeled in Linny-R. Every alternative is represented by the four distinct elements and their respective representations, see table 5.3.

Table 5.3: Modeling alternatives

Element	Representation	Info input	Link in/out
Alternative	Process	Name, actor, bounds	Mass link (flow/year)
CAPEX	Sink product	Dataset with CAPEX placed in price of product	Start-up link
OPEX	Sink product	Dataset with OPEX place in price of product	Positive link (yearly +1)
ELT	Stock product	Upper bound with max ELT and initial level	Positive link (yearly +1)

The alternatives are modeled with a processes, containing the name, actor and bounds. Where the bounds represent the minimal and maximal production capacities of the alternative. Also, all of the alternatives that are considered are linked with mass flows that go in and out. As mentioned before, the alternatives are either replacement or expansion alternatives. If it are replacement alternatives, the alternative is placed in the same process section as the currently installed asset (see figure 5.9). The expansion alternatives in the case of this thesis, totally new production processes.

Next, the CAPEX & OPEX are modeled with sink products and the ELT with a stock product. The CAPEX price is included in the price segment of the product, with a dataset. The dataset contains a negative numerical value, in order to represent the up front investment costs. The CAPEX cost is only paid once, so only for the first start-up of the alternative the link will between the process and CAPEX is activated. The OPEX is also represented as a sink product and it's price is placed in the product with a dataset. The OPEX represents the yearly costs of an alternative, so the link connected between the process and OPEX product is the positive link. This link is activated with value 1 at the end of every year. The last characteristic of an alternative, is the economic lifetime. The ELT is represented by a stock product that can be filled with years, until the upper bound with the max ELT is reached. Just as the CAPEX and OPEX, the ELT data-input is sufficed with a dataset placed in the initial level and upper bounded. In the figure below, an example of two alternatives is shown (natural gas boiler and E-Boiler). The boiler is depicted with a process that produces heat. The boiler has three links, showing the CAPEX, OPEX and ELT with their start-up and positive links.

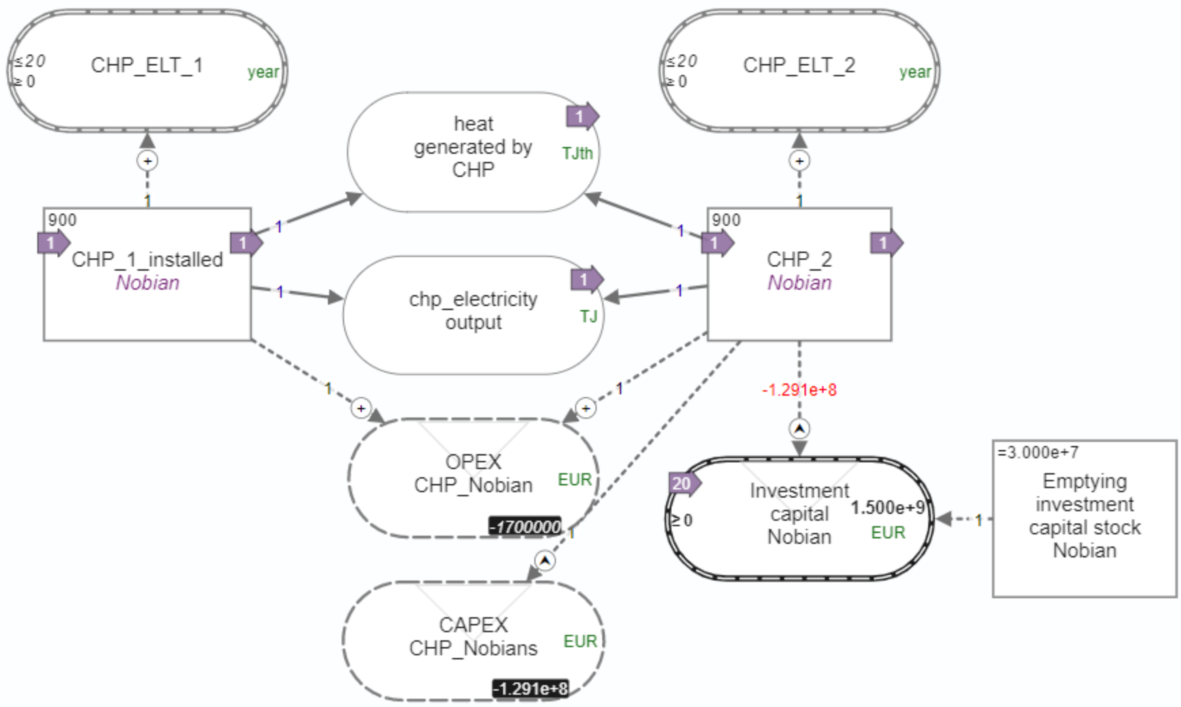

Figure 5.9: Example of two alternatives modeled in Linny-R

5.5.2. Investment decision making in Linny-R

The aim of this section, is to show the logic of the investment decision part of the CCI model. First the objective function and constraints are given, following the earlier introduced MILP problem. Followed by, the investment decision part. This part is broken up into the decision protocol, decision evaluation types, decision acceptance criteria and the decision makers.

Mathematical formulation of the MILP problem

As mentioned above, the system is represented by a number of *units* belonging to set **U**. These units (zero technology alternatives), can supply, demand or convert material and energy *streams* (∈ S). The set of *units* can be further divided into *process units* (PU ⊂ U) and *Utility units* (UU ⊂ U). Beneath, these sets are used in the objective function and constrainst for the Linny-R model.

Objective function
Following the decision protocol, the model seeks to optimise the technology alternatives and already installed assets. The investment of a zero emission technology is accepted, if the installation of an alternative saves the total system more than the investment cost. Therefore the objective function is based on the minimisation for investment costs:

$$C^{inv} = \sum_{u \in U} \sum_{p \in P} (c_u^{inv,fix} + c_u^{inv,var} * y_{u,p} * \Delta t_t^{op} \tag{5.1}$$

where $c_u^{inv,fix}$ and $c_u^{inv,var}$ are the fixed and variable investment costs of unit $u \in U$ in period $p \in P$. Where $y_{u,p}$ represents the binary variable to use a unit.

Constraints
The objective function is subjected to the following constraints. The heat/electricity/product production of modeled processes cannot exceed their standard generation capacity:

$$G_{u,y,t} \leq S_{u,y,t} \tag{5.2}$$

Where $G_{u,y,t}$ represents the generation of a unit given in a certain time period, being smaller or equal to the maximum generation capacity $S_{u,y,t}$.

The technology alternatives cannot exceed their ELT:

$$LT_{u,y,t} \leq ELT_{u,y,t} \tag{5.3}$$

Where the current lifetime in period t $LT_{u,y,t}$ is smaller or equal to the maximum economic life time of an asset $ELT_{u,y,t}$.

The decision protocol in Linny-R

This section explains how the decision protocol of figure 4.1 is modeled in Linny-R, which is used in every time step of the model run. The first step states that all technology alternatives should be considered. This is achieved by using the logic shown in figure 5.9. By using this structure, the Linny-R solver has alternative possibilities to produce a certain product produced by a process. For instance considering a gas furnace, e-furnace and hydrogen furnace at Shin-etsu. The next step of the decision protocol aims to calculate costs and revenues. Linny-R can optimise between the considered alternatives, given the specific characteristics of an alternative. So it compares the CAPEX, OPEX, production capacities and does this for all the alternatives, over the period that the model is supposed to optimize. This period is reflected in the chosen block length in the model settings. The evaluation, depending on the used evaluation metric, gives a NPV value or Pay-back period. The values of the considered alternatives is consequently used as input for the question 'Suffice acceptance criterion'?. Here the NPV's/ Pay-back periods are ranked in order from high to low. If the value of the NPV/Pay-back period is high enough to out compete the currently installed asset and/or out compete the other alternatives, then the investment is accepted. If not, the currently installed asset will continue to operate or another alternative from the considered alternatives is installed.So, this protocol aims to maximize either the NPV or Pay-back period, allows for investment before the end of the ELT and allows for only one installed alternative for the production of a certain asset. Subsequently, the solver of Linny-R will select the alternative that results in the optimal outcome for the entire modeled system. This is reflected by the installment of an alternative (process in Linny-R) and the dismantlement of a previously installed asset. In the model's graphical representation, this is shown by production levels.

Used model settings

The model settings of Linny-R allow to define the time resolution of the model, the period over which the solver should optimize and the look-ahead period given to the solver. For the model's time resolution, a yearly time-step is used between 2022 and 2050. Therefore, every model run contains 28 time-steps. Next, the block length and look-ahead period that are used per actor type are shown in table 5.4. The engineer actor uses a block length and look-ahead period of 28 time-steps. This gives this actor type perfect foresight between 2022 and 2050, over which the solver will optimize the model's entire modeled time resolution. These settings result in the most optimal system outcome. The second actor type is the heterogeneous firms with unbounded rationality. Following Lenoir, et al., a heterogeneous firm should optimize over a period of ten years, during which the actor is able to for see three years.

Table 5.4: Model settings Linny-R

Actor	Blocklength	Level of foresight
Engineer	28	28
Heterogeneous firms with unbounded rationality	10 [101]	3
Heterogeneous firms as organisations with bounded rationality	3 [C]	3

The third actor has a block length of three years and foresight of three years. This represents an actor with bounded decision resources and cognitive limitations. A period of three years was retrieved from the interviews with both Nobian and Westlake. Both of the companies stated that they used a three year pay back period as their main decision acceptance criterion. This represents the period of which they optimize their investments. These three model settings are in combination with the corresponding decision evaluation types depicted in chapter 4.

Decision evaluation types in Linny-R

Underneath is explained how the market and behavioural barriers are implemented in the CCI model. The explanation uses table 4.2 as a reference.

Risk
As mentioned in the second chapter, risk can have a variety of sources for the industrial sector. Think of uncertainties caused by imperfect foresight like technical risks, macro economic trends and government policy. This market barrier, is represented by discount rates in a NPV formula. The NPV formula in Linny-R is represented as a monadic operator. The operand looks like: npv(r;N;CF). It evaluates as the npv of a constant cashflow (CF) for a period of N time steps and a discount rate r. The npv formula's are placed in the processes reflecting the CAPEX investment, as that resembles the alternative that is evaluated. Next, the discount rates are placed in actor-specific data sets. These values are in turn placed in the npv formula. The values for the discount rates are based on benchmark rates for the industries where the companies are part of.

Imperfect information
The imperfect information should represent the difference between expected cost savings and realized cost savings. The zero gap electrolyser for example should result in a 25 % reduction in electricity consumption compared to the finite gap electrolyser. However, when actually installed, it is possible that the reduction in electricity consumption turns out to be lower. To represent this imperfect information about expected and realized performance of the alternative, two datasets are used. The two data sets, the perfect information and imperfect information dataset. The idea is to 'fool' the Linny-R solver with these two data sets. The expression shown in figure 5.10 starts with bt=1?. The ?-mark is the same as an if-statement. The bt=1 resembles the condition, is the block length equal to one. If that is true, the imperfect information dataset is used to represent the link efficiency of an alternative. If that is not true, so after the investment has been made the actual value of efficiency is placed in link with the perfect information dataset. So, in a run where the solver optimizes over a period of X, the imperfect information dataset is used in that period X. After installment, the perfect information dataset is activated. This ways the solver is fooled, because the actual value over which it should have optimised is revealed after investment.

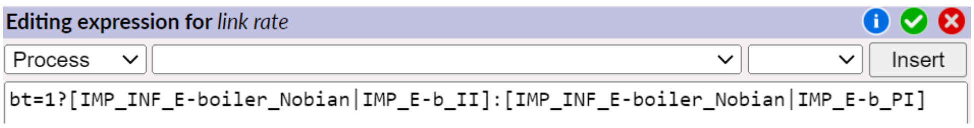

Figure 5.10: Imperfect information in Linny-R

Access to capital
Access to capital is represented by a product stock, which can be filled up with capital until a certain upper bound is reached (see figure 5.11). If an investment is accepted, like the CHP of Nobian, the stock of investment capital for Nobian is emptied by the CAPEX value. The CAPEX value is placed in the link rate, which is only activated in the time-step when the alternative is installed. Besides the emptying of the capital stock, the stock is also filled on a yearly basis with a certain rate. The rate is based on the respective companies their reported yearly CAPEX investments and the relative contribution of the modeled plants to the revenue of the overarching companies. The emptying is represented by a process and a positively linked (yearly activated) product. This rate of 'emptying' the investment capital stock is again actor-specific.

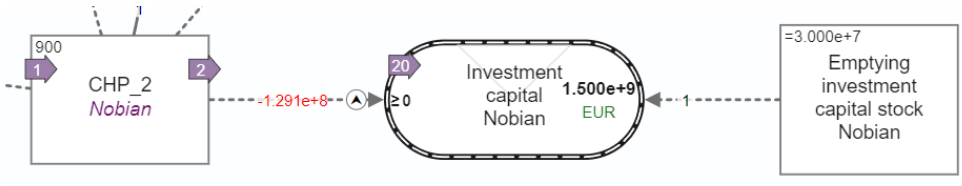

Figure 5.11: Access to capital

Hidden costs
Hidden costs represent the expected and realized OPEX of technology alternatives. The OPEX costs per alternative are placed in product containing an expected value dataset selector and realized set in the price definition. The approach is comparable to the approach explained for the imperfect information barrier. Here again, the actually realized OPEX is activated depending on the modeled block length. Both of the data sets are placed in the OPEX cost stock before and after investment, see the following product expression:

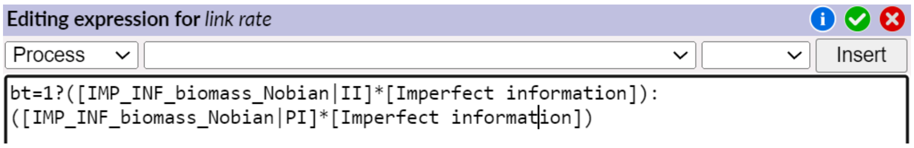

Figure 5.12: Hidden costs in Linny-R

Bounded rationality
Bounded rationality is represented by critical thresholds and technological preference, to resemble the limited cognitive capability of decision makers. In this model the critical threshold is the pay-back period. The pay-back period can be modeled, by optimizing over a certain block period in Linny-R. The pay-back period is resembled in the model experiment settings. Three types of block length are resembled by the three selectors. The baseline optimizes over a period of the entire run length, followed by the optimizing selector that optimizes in periods of 10. Lastly, the satisficing and behavioural evaluation types use a pay back period of 3 years represented by the block length of three years. The technical preference is reflected higher or lower prices for zero emission technology alternatives. The preference is implemented as a data set with a factor that influences the CAPEX cost. The technical preference set is placed in the process's price properties of alternatives In this case, the factor that multiplies the CAPEX cost is either larger or smaller than 1. A value larger than one represents a technological preference for the non zero emission technologies and a value smaller than one represents a preference for the zero emission alternative.

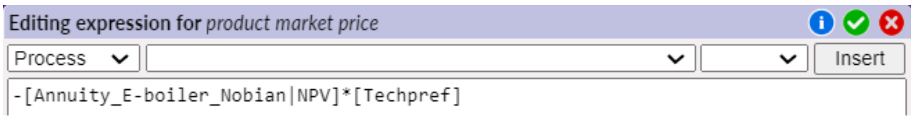

Figure 5.13: Technological preference

Split incentives
The split incentives between firms is addressed, by varying the assignment of CAPEX and OPEX costs between companies for cooperative investments. The division of these costs is based on their relative cash flows. Consequently these relative cashflow rates are placed in the links to both OPEX and CAPEX processes (see figure 5.14). The recirculation alternative, shown in figure 5.14, depicts the used logic for investment as the costs and benefits for this alternative is split over more than one actor. The alternative itself is shown in the centre of the figure where the process is modeled without an actor assigned. On the left side of the picture, the recirculated brine is shown and on the right side the CAPEX & OPEX. For these three parts, separate processes were added to assign the costs and benefits to the two different actors. The CAPEX costs for instance is connected with two links and two processes, where the sum of the two links must be 1. The same is done for the OPEX and recycled brine products.

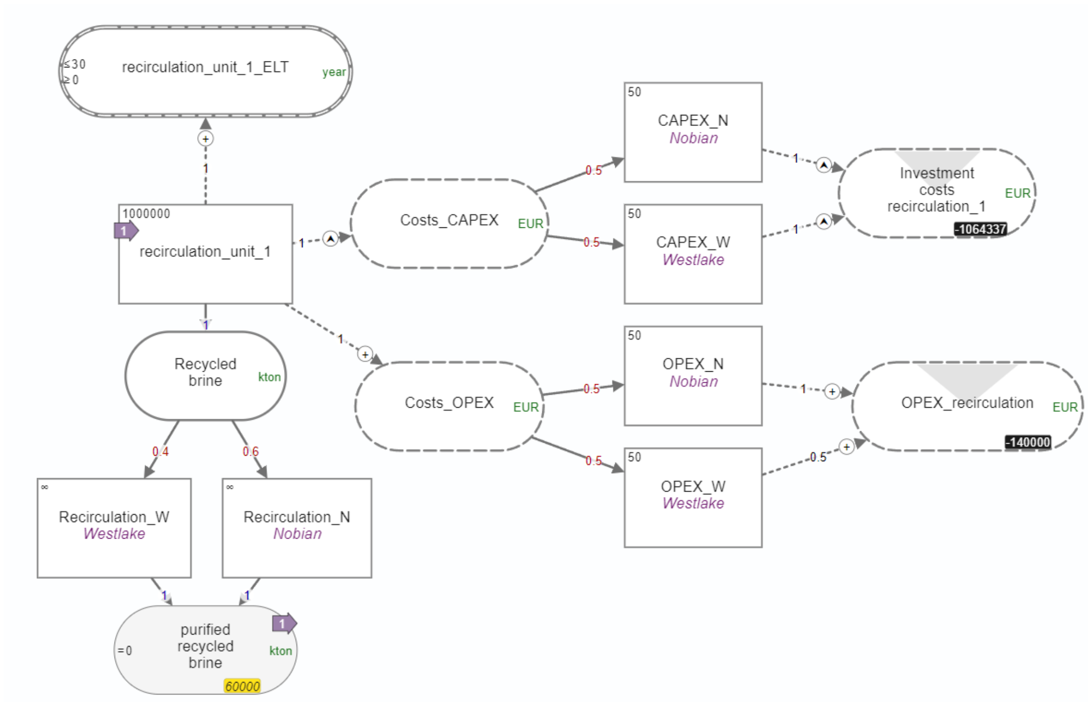

Figure 5.14: The recirculation alternative between Nobian and Westlake

Decision Acceptance criteria in Linny-R

This subsection explains how the decision acceptance criteria, shown in table 4.3, have been modeled in Linny-R. The NPV criterion is modeled using the NPV formula in Linny-R, at the CAPEX cost products. Furthermore, the Linny-R solver aims to minimize the cost of technology adoption in this model. This means that the highest NPV value is chosen when the solver compares alternatives among each other. Secondly, the pay-back periods are modeled by altering the model settings dimensions. This is also shown in the 'bounded rationality' barrier explanation.

Actors in Linny-R

The four companies, in the form of Nobian, Shin-Etsu, Westlake and Huntsman, have their specific values for the decision evaluation types. For all the barriers, their perception of risk & uncertainty, level of imperfect information, hidden costs, amount of capital available, technological preference and willingness to cooperate through split incentives are decision maker specific. For every barrier there are actor-specific data-sets, that are in cooperated in the processes, products and links. In the appendix D, an overview is given of the heterogeneous data-sets.

5.6. Model verification and validation

In this section the model verification and validation (V&V) is performed. A visualisation of the V&V process is depicted in figure 5.15, containing three assessment activities and modeling & simulation activities. The model verification determines whether the implemented computer model accurately represents the conceptualised mathematical model. Followed by a validation to check if the model is an accurate representation of the real world, from the perspective of the intended purpose of the model [165]. For the verification a static verification is performed and the validation is conducted via an extreme value test.

5.6.1. Model verification

For this section, a numerical sanity check is performed to determine whether the Linny-R model accurately represents the conceptualised model intended. A model numerical sanity check is test to determine

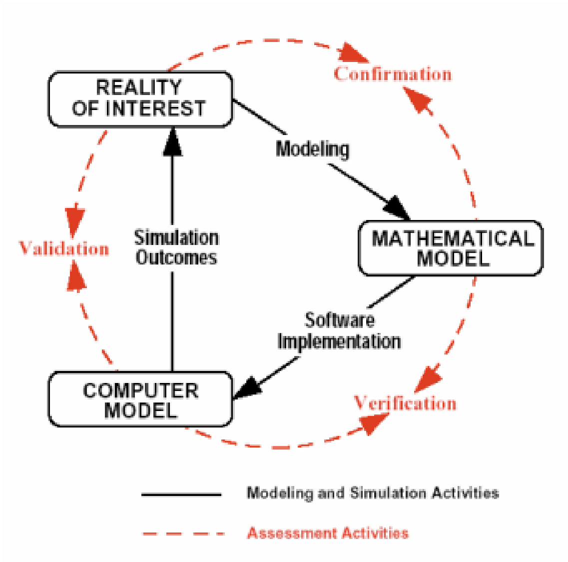

Figure 5.15: Simplified visualisation of the model verification and validation process [165]

whether the result of a model calculation can possibly be true. The main point of this test is to rule out certain types of logically false results. This verification test does not catch all possible errors but it is a fast and simple method to discover a lot of possible model faults. The check is performed by running the model under baseline conditions. So, without barriers and price scenario normal (see appendix C. The following points are checked with a 'back-of-the-envelope calculation:

- Yearly CO_2 emissions
- Mass flow for Epoxy resin production
- Maximum ELT of assets

First, the CO_2 emissions were considered for the Nobian production plant. According to the plant-process-product inventarisation of chapter 3, the yearly direct emissions of Nobian should result in 157.7 kton/year. Where the local heat and electricity production, via the gas fired CHP are the only source of emissions. The table 5.5 shows the descriptive statistics of Nobian's CO2 emissions. N, shows the 28 time steps which verifies that the model runs for 28 time steps. The min value gives 0, so when all the CHP's at Nobian are dismantled for zero emission technology alternatives the CO_2 emission goes to zero. The maximum value shows a value of 157,7 kton, which corresponds with the yearly emission output of Nobian. The sum over 28 timesteps gives 2050 kton. This corresponds with the fact that the CHP's were turned on for 13 years. Thirteen times 157.7 equals 2050 kton.

Table 5.5: Verification CO2 emissions

Variable	N	Min	Max	Mean	Sum [kton]	#Not zero
CO2 emission (Nobian) | L	28	0	157.7	73.2	2050	13

The second test looks at the maximum ELT of assets. As mentioned in the zero-emission technology inventarisation, technology alternatives have a maximum ELT. In the model it has been modeled as a stock that is filled per time step until a certain upper bound is reached. For this run, all the heat assets from Nobian were considered and verified whether the maximum ELT value is not exceeded. The MAX column shows the maximum value this stock product has had during the 28 time steps (N). Following the max ELT values shown in chapter 2, we see that the maximum value of the alternatives that were active was not exceeded.

Next, the mass flow for epoxy resin production at Westlake is verified. The production process goes according to this reaction:

Table 5.6: Maximum ELT heat assets at Nobian

Variable	N	Max
CHP_ELT_1 | L	28	13
CHP_ELT_2 | L	28	0
e_boiler_1_ELT | L	28	15
e_boiler_2_ELT | L	28	0
biomass_boiler_1_ELT | L	28	0
biomass_boiler_2_ELT | L	28	0
biomass_boiler_3_ELT | L	28	0
biomas_boiler_4_ELT | L	28	0

$$C_3H_5ClO + C_15H_16O_2 \longrightarrow [-C_18H_21O_3-] + HCl \tag{5.4}$$

Here, ECH + Bisphenol A is reacted into Epoxy resins and hydrogen chloride. Following the following calculation of mass balance, the reaction would be: 92.52g/mol : 228.29 g/mol –> 285.36 g/mol + 36.46 g/mol. This would result in the ratio of 0.32 : 0.8 –> 1 : 0.13. This means that for every kton of produced epoxy resin, 0.32 kton of ECH and 0.8 kton of Bisphenol A would be needed and 0.13 kton HCl produced. With a yearly production of 170 kton of epoxy resins, there would be a 54.4 kton of ECH, 136 kton of Bisphenol A and 22.1 kton of HCl. Following the mass flows depicted in figure 5.16, the model corresponds with the flows that were calculated by hand.

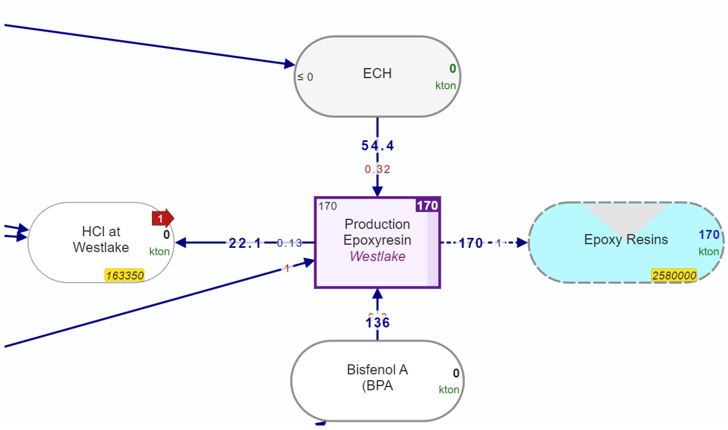

Figure 5.16: Mass flows production epoxyresin at Westlake

To conclude, the sanity check verified that the conceptual model and model in Linny-R correspond. With this test the output product in the form of CO_2 was tested, the internal mass flows and an investment constraint, were deemed to be consistent with the conceptual model.

5.6.2. Model validation

Now that we verified that the model accurately represents the conceptualised model, we can proceed with the model validation. The validation aims to assess whether the computer model and reality of interest are aligned. The reality of interest is relationship between independent variables: market & behavioural barriers in the form of decision evaluation types and the exogenous environment on the transition pathways of the PoR chlorine cluster, CO_2 emissions and cash flows. The validation consists out of three tests: a base case test, extreme value test with exogenous parameter values and decision evaluation type test.

Validation test 1: base case

For the first validation test, we assume the input data shown in table F.1. All of these parameter values are fixed in the initial value settings in Linny-R. With this input data, the model should converge toward an equilibrium states between 2022 and 2050. We consider the following hypotheses:

- We should see dominant investments towards a certain type of energy source for utility alternatives after the ELT of the initially installed assets is reached. Unless the relative attractiveness of alternatives to the initially installed technology are more favourable.
- Cash flows should stabilize between the time investments are made.
- We should see CO_2 levels correspond with the installment/dismantling of CO_2 producing assets.

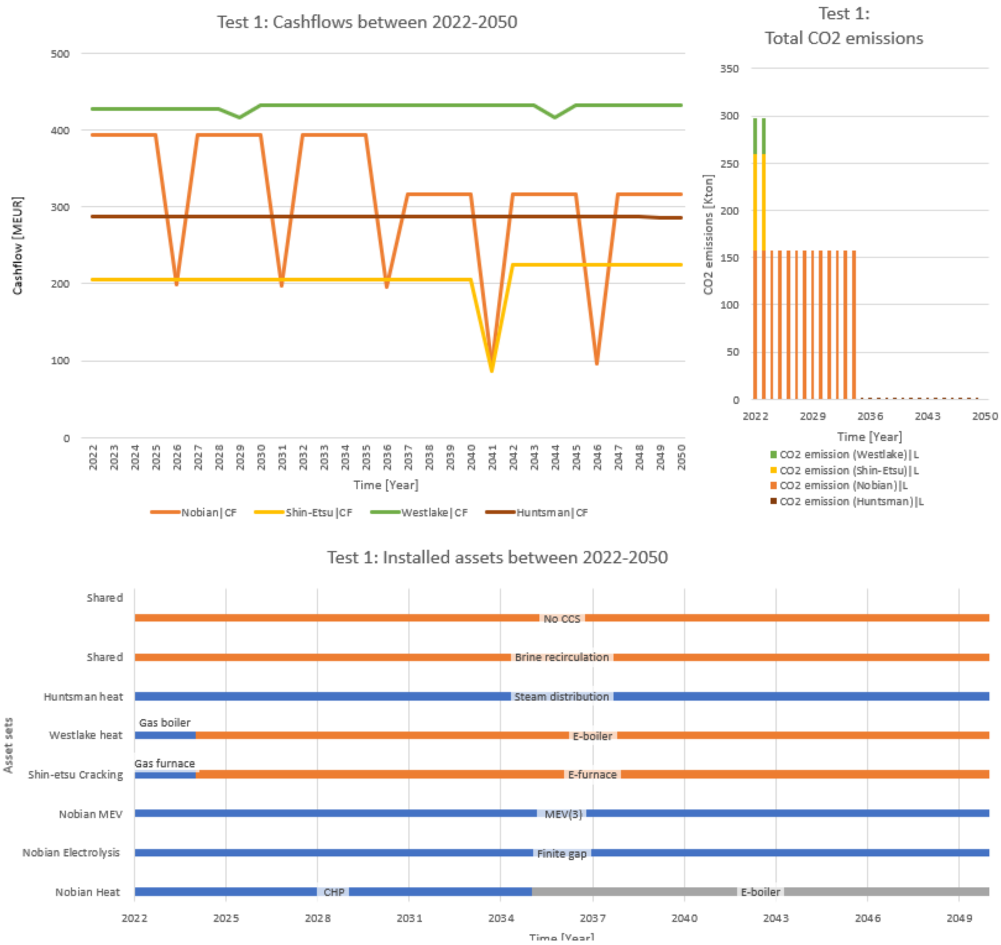

Figure 5.17: Model validation base case

The results from this validation test are shown in the three graphs of figure 5.17. The three graphs show the cash flow, CO_2 emissions and transition pathway results. For the first hypothesis we consider the 'installed assets between 2022-2050 graph'. This graph shows what kind of asset is installed over time, where the data labels specify which asset specifically. As we can see, all of the asset sets dedicate to a specific type of asset, apart from Westlake heat, Shin-etsu cracking and Nobian heat. Both the Westlake gas boiler and Shin-etsu gas furnace are replaced before the end of their ELT. Nobian's already installed CHP is replaced after it has reached the end of it's ELT. This is due to the alternative to the CHP being not competitive enough to replace earlier over the chosen optimisation period. So, when it comes to this part of the test, the model performs according to the stated hypothesis.

The second hypothesis states that cash flows should stabilize between investments. As shown in the top left graph the cashflows indeed stabilize between investments and investments can be noticed where the cashflow dips towards down. The model 'writes off' all of the CAPEX in the year of installment, so that is why we can see the significant lowering of cashflows over time. For the Nobian line, we see two different levels for the cash flow. One of the cashflow levels is around 4000 MEUR/year and the second level around 3100 MEUR/year. The second level for the cashflow is lower, because during this phase the CHP is replaced by an E-boiler. Under the configuration shown of F.1 this leads to more expensive steam production. Also a periodical dip is seen between 2022 and 2050 for Nobian. These are the moments the finite gap electrolyzers are replaced, which have a considerable CAPEX cost. To conclude, also for this hypothesis the model performs according to what is expected. The last hypothesis states that we should see CO_2 levels correspond with the configuration of installed assets. The top right graph shows the CO_2 emissions per company between 2022-2050 and corresponds to the installed assets in the installed assets graph. For Shin-etsu and Westlake, the CO_2 emissions drop after their gas furnace and boiler are replaced with non-emitting assets. The same is observed after Nobian's CHP is replaced with an E-boiler.

Validation test 2: extreme value test exogenous parameters

For the second validation test we assume the input data shown in table F.2. All of these parameter values are fixed in their initial values in the Linny-R products. With this test we aim to validate that the model performs logically when extreme values are used. For this test we, consider an extremely high CO_2 and natural gas prices. At the same time, very low biomass, hydrogen and electricity prices are used. The energy and CO_2 prices are important for the relative attractiveness of an alternative. That is because besides the attractiveness is determined by a combination of the CAPEX, fixed yearly OPEX and the variable costs made due to the use of energy or CO_2 emissions. As Linny-R optimizes for the optimal system outcome, the lower the total costs, the better. In this case we consider the following hypotheses:

- We should see a rapid dismantlement of natural gas assets and rapid installment of non CO_2 emitting alternatives.
- We should see low CO_2 levels, because the polluting assets should be dismantled rapidly.

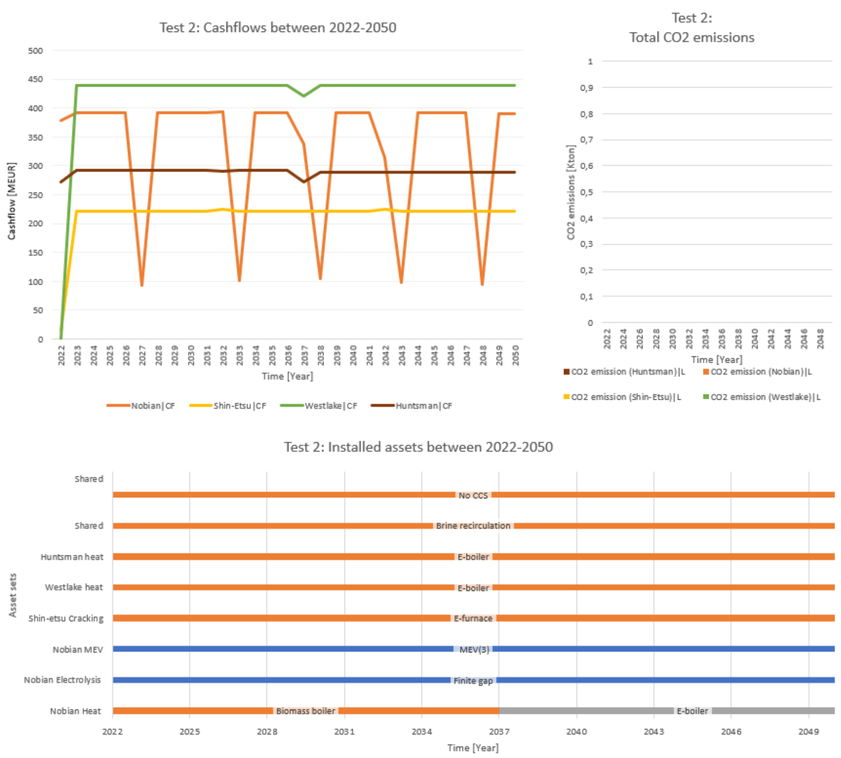

Figure 5.18: Model validation test 2

During this test we examine whether the the model responds to changes in relative attractiveness between assets. As shown in figure 5.18 the model works accordingly. Nobian's CHP is uninstalled and immediately replaced with a biomass boiler. The same for Westlake's gas boiler and Shin-etsu's gas furnace, which are replaced with electrified options after one year. This leads to a rapid decline in total CO_2 emissions

Validation test 3: decision evaluation types

For the first validation test, we assume the input data shown in table F.3. For this test we validate whether every parameterization of the barriers and reality of interest are aligned. Therefore, we will consider all the barriers and that function accordingly. The following hypotheses are tested:

- High discount rates for zero emission technologies should lead to a lower amount of installment years
- The lack of capital should lead to no investments.
- High tech preference for zero emission technologies should lead to higher amount of installment years.

Figure 5.19: Model validation test 3

The effect of high discount rates for zero emission technologies is shown in the top bar graph of figure 5.19. The orange bars represent the amount of installed years per asset between 2022-2050 with the 'normal' discount rates for zero emission technologies. The blue bars represent the high discount rates for zero emission technologies. As can be observed, the high discount rates lead to lower amount of installed years for zero emission technologies. In the model, a higher discount rate leads to higher CAPEX values. As the high CAPEX value for zero emission technologies lead to less relative attractability compared to the non sustainable assets, the amount of installed years between 2022-2050 decrease. This shows that the model performs according to the stated hypothesis and the reality of interest. Next, the lack of capital is shown in the second graph of figure 5.19. This graph represents the results of a model run, without the accessibility to capital. As stated in the hypothesis, the lack of capital should lead to no investments. As shown in the graph, the installed assets only run until 2027. This is the first moment an investment is needed, as the finite gap electrolyzer at Nobian reaches the end of it's Economic Life Time. Because it is not possible to invest in another electrolyzer, due to the lack of capital, the production of chlorine comes to a stop. Because there is a lack of chlorine within the cluster, the other industrial plants cannot produce their products and all the other assets are also shut down. This behaviour follows logically from the way access to capital is modeled and the reality of interest. As in reality it is impossible to invest without capital. The last graph shows the influence of technical preference settings. As explained earlier in this chapter, the technical preference parameter is modeled as a factor is multiplied with the CAPEX values of alternatives. The blue bars represent a run where the technical preference favours the zero emission technologies and the orange line represents a run without technical preference. As shown in graph, the number of installed years for the zero emission technologies increases when the technical preference favours these type of alternatives. Apart from Nobian's MEV(3), all of the zero emission technologies are installed for more years between 2022-2050. This follows logically from the way technological preference is modeled. Therefore, the last hypothesis is met as well during this validation test.

5.6.3. Conclusion

From the model verification & validation, we can conclude that the quantitative model in Linny-R works according to the earlier conceptualised model. Where both the technical and investment behaviours acted according to the needed functionalities and the tested hypotheses. The validation test show us that:

- Validation test 1 shows that under base case conditions the CCI model result in the intended purpose of the model. The test shows investments are made over time and the CO_2 emission values correspond with the configuration of technology over time.
- The electricity, biomass, hydrogen, gas and CO_2 prices affect the investmentment behaviour in the CCI model in the expected way. Where the extreme value test shows that extreme configurations of these prices result in the change of relative attractiveness of alternatives.
- Investment behaviour influenced by parameters from the decision evaluation types result in the expected outcome. The change in discount rates affects the relative attractiveness, no access to capital result in no investments and technological preference result in more relative attractiveness to the less preferred technologies.

6

Model use and results

This chapter is dedicated to the model use and results. The first section 6.1, elaborates on the scenario analysis set-up. The focal question, key drivers, scenario logic and scenario assumptions are addressed. Secondly, section 6.2 assesses the results from the performed scenario analysis.

3. *What is the influence of market & behavioural barriers on investment decisions, at the PoR chlorine cluster?*

6.1. Scenario analysis

The model experimentation is performed via a scenario analysis and it's results aim to determine the effect of market & behavioural barriers on zero emission technology adoption at the PoR chlorine cluster. There are various scenario development techniques. During this thesis the intuitive logics methodology is used following bradfield et al [18]. The STEEP analysis is conducted in section 6.1.2, where the key drivers and uncertainties are acquired to determine the influencing factors. Followed by the scenario logic in section 6.1.3. Lastly, the principles and assumptions for alternative futures is described in section 6.1.4.

6.1.1. Focal question scenario analysis

In order to determine the influence of the barriers on investment decisions at the PoR cluster between 2022 and 2050, we can make a distinction between independent and dependent variables. By manipulation of the independent variables, we can test the cause-and-effect relationship with the dependent variable. Where the independent variables is the variable we can manipulate or vary to explore it's effects. It is called independent, because it is not influenced by any other variables within this study. A dependent variable on the other hand changes as a result of the independent variables manipulation. The following categories of independent variables and dependent variables are considered.

- Independent variables
  - Decision evaluation types
  - Exogenous environment
- Dependent variables
  - Transition pathways
  - Cash flows
  - CO_2 emissions

6.1.2. Identifying key drivers with the STEEP analysis

The key drivers are identified with a STEEP analysis. The drivers are analysed according to their impact and level of uncertainty, ranging from low to high. The complete analysis is shown in appendix E. From that analysis, the drivers in the table 6.1 were found. The key drivers are bundled in three categories called: energy prices, commodity prices and government policy.

The first driver is a combination of multiple energy prices. The energy prices comprise all energy carriers needed for the technology alternatives that are considered. So, that are natural gas, electricity, biomass and hydrogen prices. All of these price largely influence the costs made at the chlorine cluster's production process and also influences the relative attractiveness of considered alternatives. Besides, these prices are subject to large uncertainties. This is due to the fact that both the supply and demand side, which together form the price, are hard to predict over a large time period like 2022-2050. Three major supply-side factors affect these prices: amount of production, level of storage and volumes of imports and exports. Also, three major demand-side factors affect prices: variations in seasonal effects, level of economic growth and availability and prices of other energy sources [54].

The second key driver consists out of commodity prices. The commodity prices reflect the prices for all the major outputs of the four companies, thee prices for chlorine, caustic soda, PVC, epoxy resins and HCl. These prices have a large impact on the financial situation at companies at the PoR chlorine cluster, as they are the main sources of revenue. The prices of these commodities are determined by their production costs, total supply and on the other side the demand for these products. Therefore, commodity prices are a key driver With both an uncertain price for the production costs and uncertain demand for the product between 2022-2050.

Lastly, government policy is represented by CO_2 prices per kton. The CO_2 prices are based on the EU emission trading system (ETS) and the "CO_2-heffing" for the Dutch industry [3]. This policy mechanism has a high impact on the relative attractability of polluting assets compared to non polluting assets. Besides the high impact, the government policy has proven to be a highly uncertain factor. For a long time, the Dutch government did not implement an additional national tax on top of the market based EU ETS price. So for a long time the Dutch industry was first of all not sure of how the ETS price was going to develop and whether an additional national tax would be implemented.

Table 6.1: Key drivers STEEP analysis

Key driver	Parametrisation
Energy prices	Electricity price Natural gas price Biomass price Hydrogen price
Commodity prices	Chlorine price HCl price VCM price PVC price Epoxy resin price MDI price
Government policy	CO_2 pricing

6.1.3. Scenario logic

For the model is ran in a full factorial experiment, however due to the large amount of results (8192 runs) four specific scenario's are highlighted. These scenarios represent the vertices of the solution space. The key drivers from the previous section have been bundled into two axis: governmental decarbonisation priority and zero-emission technology attractability (see figure 6.1). The X-axis ranges from low to high, which determines whether the scenario is attractable to zero-emission technologies or not. The Y-axis is dedicated to governmental decarbonisation policy, which is represented by CO_2 prices. With this configuration it is possible to determine what the relative impact of the modeled barriers and the exogeneous environment is.

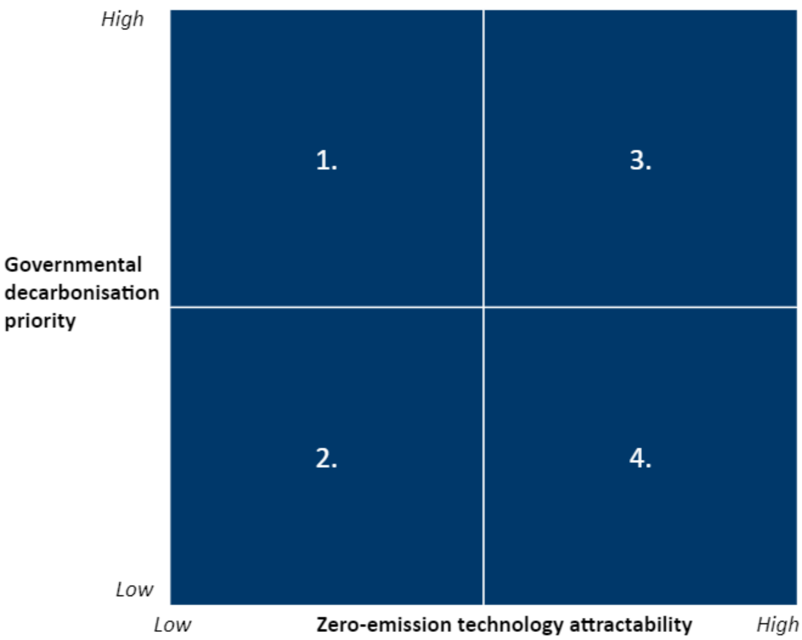

Figure 6.1: Scenario logic

The four scenarios are named as follows:

1. High priority at unfavourable circumstances
2. Slow decarbonisation
3. High priority and favourable circumstances
4. Give the industry more incentives

The independent van dependent variables of this scenario analysis are shown in figure 6.2. The three independent variables are manipulated to see how they affect the three dependent variables. Multiple levels of of the independent variables are used, in order to determine to what extend the independent variables affect the dependent variable. Especially, the decision evaluation types and parameter calibrations are of interest and to what extent they affect the transition pathways, cashflows and CO_2−eq emissions.

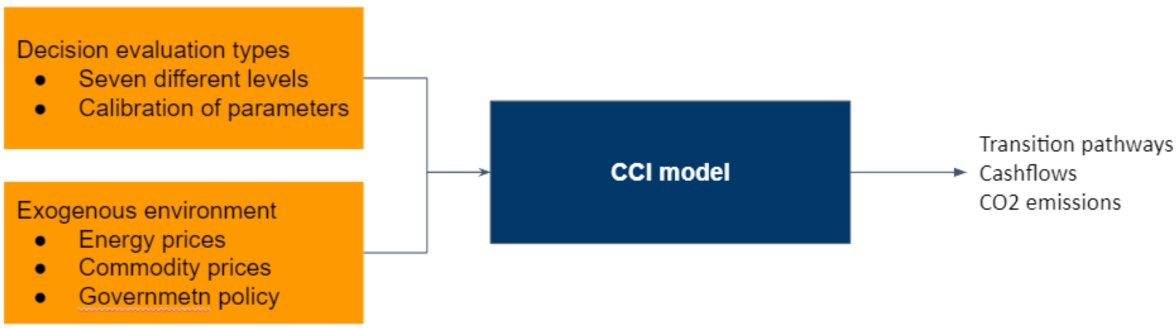

Figure 6.2: CCI model inputs and outputs for the scenario analysis

6.1.4. Scenario assumptions

The scenario specific assumptions describe the principles and assumptions for the alternative futures using qualitative story lines and trends of the key drivers [18]. In appendix D, the corresponding model settings that follow from the scenario assumptions are shown. Underneath, the scenario assumptions are described per scenario.

Baseline: setting the normative baseline benchmark

The baseline scenario aims to determine the optimal solution for technology adoption at the PoR chlorine cluster. Therefore, this scenario runs the model under normal circumstances without any barriers. The results from this run is used as a benchmark compared to the other runs. The model settings are set with a level of foresight and block length of 28 years. This represents the perfect foresight and perfect rationality.

Scenario 1: High priority at unfavourable circumstances

This scenario is dedicated to illustrating the optimal situation for decarbonisation at the PoR chlorine cluster. It represents a possible future where the gas and CO_2 prices are high while there are simultaneously low electricity, hydrogen and biomass prices. This might be a future where there is a strong governmental push to increase the speed of decarbonisation with CO_2 pricing and a large surplus of renewable electricity production. This surplus of cheap electricity make hydrogen production via electrolysis and biomass more attractive. In this future, the relative attractiveness of CO_2 polluting gas technologies is very low. Also, in this scenario all the barriers are turned off.

Scenario 2: Slow decarbonisation

These circumstances are very unfavourable for zero emission technology adoption. The relative attractiveness of zero emission technologies compared to currently used technology is low, due to low CO_2 prices and unfavourable energy prices. This scenario could represent a situation where there is a over supply of natural gas and a low priority for decarbonisation on a governmental level.

Scenario 3: High priority and favourable circumstances

This is a favourable situation for technology adoption, because the relative attractiveness of zero emission technologies is high. High CO_2 and gas prices make it cheaper to operate alternatives that run on electricity, hydrogen or biomass. This scenario could be possible under a large supply of cheap renewable energy production and a high priority from the government. This is the first scenario where the barriers are turned on, which should result in lower zero emission technology adoption and more CO_2 emissions compared to scenario 1.

Scenario 4: Give the industry more incentives

Allthough the energy prices are very favourable for the transition to other energy carriers than natural gas, the government does not prioritize further incentives for the decarbonisation of the industry. Therefore, the scenario name: give the industry more incentives! From the perspective that we want to realize a fast emission reduction. During this scenario the barriers are turned off. This should result in lower zero emission technology adoption and more CO_2 emission compared to scenario 2.

6.2. Model Results

This section shows the model results that are retrieved from the scenario analysis. First the normative benchmark is set with a baseline run. This run gives us the optimal technology adoption between 2022 and 2050. The next section elaborates on the differences between the baseline benchmark and the various decision evaluation types. Per decision type, the earlier conceptualised scenarios have been run in the CCI model. These results can be consulted in appendix F. From the model results, the following points regarding the investment behaviour in the model can be observed:

- The market & behavioural barriers lead to less zero emission technology adoption, compared to the normative baseline benchmark.
- A limited access to capital forces Nobian to invest in an E-boiler instead of a CHP.
- The CCS alternative only operates under long postponement of investments in zero emission technology. Also, the model results suggest that the CCS alternative is not a viable option, even though the national push for the adoption for CCS in the industrial sector.
- The Zero gap electrolyzer is only installed when sustainable utility alternatives are not installed.
- Shin-etsu's Hydrogen boiler is only installed under favourable environmental conditions and technological preference.
- Westlake's E-boiler installment is strongly dependent on imperfect information.
- Huntsman's E-boiler is less installed under the pay-back period of three years.
- The pay back period strongly influences the postponement of investments in zero emission technology.

The figure 6.3 shows the results from the four conceptualised scenario's. The first two columns show the company, the unit and the associated technologies. The technologies are depicted as $technology_X$, where the X represents the scenario number. The columns show all the decision evaluation types. All of the baseline values are the same, as that are the values that show the normative benchmark values. The first point that was noticed, is the large difference between the first column 'Baseline' and the other columns representing one or more barriers. The difference is noticed by the higher amount of years that non sustainable assets are installed and the higher total (CO2) levels between 2022 and 2050. We can observe the difference when comparing the columns per row and see that for instance the CHP of Nobian is installed for more years between 2022-2050 and the E-boiler is installed less. Where the higher amount of years installed imply an earlier adoption of the technology between 2022-2050. Another point of interest, is the effect the access to capital type has. We see that the CHP is less installed compared to the imperfect information and hidden cost types and the e-boiler is earlier adopted. The reason that this happens is due to the difference of CAPEX costs between the CHP and E-boiler. Due to the limited access to capital, the model forces Nobian to adopt the cheaper E-boiler. This is also seen in scenario number four, where the biomass boiler is installed more instead of the CHP. Thirdly, is noticed that the CCS is only installed when there the CO_2 polluting technologies are installed for longer periods. The attractiveness of the CCS is modeled as the difference in cost for the investment in the CCS alternative compared to paying for emitted CO_2. So, only during scenario's where the polluting assets are installed for long enough and/or the CO_2 price is high enough, the CCS is installed. Also, the model results show that the CCS alternative is not a likely alternative to be installed. This is result stands opposed from the national push for the introduction of CCS in the industrial sector. A large part of the national emission reduction should result from this alternative. However, the model results argue that the adoption of zero emission alternatives would be a more cost effective option. The low results for CCS in this scenario analysis compared to the plans made in the real world, might be due to the assumptions were made for the costs. The model does not account for risk reduction in the form of subsidies and lowered CAPEX costs for the chlorine cluster. So, the assumptions might represent higher costs than they in reality might be. Next, we see that the zero gap electrolyzer is only installed under conditions when sustainable utility alternatives are not installed. In these circumstances the energy efficiency gains from the zero gap electrolyser are more attractive than the investment in a sustainable utility alternative. This is due to the low attractiveness of the sustainable assets in these scenario's, where electricity, hydrogen and biomass prices are high. While simultaneously the gas and CO_2 prices are low.

		Decision evaluation types								
		Baseline	Risk	Imperfect information	Hidden costs	Access to capital	All market barriers	Bounded rationality	Split incentives	Average
Nobian [Years installed 2022-2050]	CHP_1	10	20	28	28	20	20	28	28	16
	CHP_2	10	26	28	28	20	20	28	28	20.5
	CHP_3	10	0	8	0	6	12	1	1	6.5
	CHP_4	10	10	21	19	20	20	14	14	16
	Biomass_1	0	0	0	0	0	0	0	0	0
	Biomass_2	0	0	0	0	0	0	0	0	0
	Biomass_3	0	28	20	28	22	0	27	27	14
	Biomass_4	0	18	0	9	0	8	14	14	4.5
	E-boiler_1	19	8	0	0	8	8	0	0	12
	E-boiler_2	19	2	0	0	8	8	0	0	7.5
	E-boiler_3	19	0	0	0	0	16	0	0	7.5
	E-boiler_4	19	0	7	0	8	0	0	0	7.5
	MEV(3)_1	28	28	28	28	28	28	28	28	28
	MEV(3)_2	28	28	28	28	28	28	28	28	28
	MEV(3)_3	28	28	28	28	28	28	28	28	28
	MEV(3)_4	28	28	26	28	28	28	28	28	28
	MEV(5)_1	0	0	0	0	0	0	0	0	0
	MEV(5)_2	0	0	0	0	0	0	0	0	0
	MEV(5)_3	0	0	0	0	0	0	0	0	0
	MEV(5)_4	0	0	2	0	0	0	0	0	0
	Finite gap electrolysis_1	28	20	28	25	28	28	28	27	23.5
	Finite gap electrolysis_2	28	28	28	25	28	28	28	27	28
	Finite gap electrolysis_3	28	28	28	28	20	28	5	5	28
	Finite gap electrolysis_4	28	28	28	28	28	25	5	5	28
	Zero gap electrolysis_1	0	8	0	3	0	0	0	0	4.5
	Zero gap electrolysis_2	0	0	0	3	0	0	0	0	0
	Zero gap electrolysis_3	0	0	0	0	5	0	23	23	0
	Zero gap electrolysis_4	0	0	0	0	0	3	23	23	0
Shin-etsu [Years installed 2022-2050]	Gas-furnace_1	2	3	10	3	7	28	19	19	0
	Gas-furnace_2	2	28	28	28	28	28	27	27	1
	Gas-furnace_3	2	5	11	6	11	20	13	13	0
	Gas-furnace_4	2	20	20	24	13	15	20	20	2
	E-furnace_1	26	25	18	25	21	0	9	9	28
	E-furnace_2	26	0	0	0	0	0	1	1	28
	E-furnace_3	26	23	17	22	17	8	15	15	28
	E-furnace_4	26	8	8	4	15	13	8	8	28
	Hydrogen-furnace_1	1	0	0	0	0	0	0	0	0
	Hydrogen-furnace_2	1	0	0	0	0	0	0	0	0
	Hydrogen-furnace_3	1	0	0	0	0	0	0	0	0
	Hydrogen-furnace_4	1	0	0	0	0	0	0	0	0
Westlake [Years installed 2022-2050]	Natural gas boiler_1	1	1	13	15	13	15	15	15	5
	Natural gas boiler_2	14	16	15	15	15	15	15	15	11
	Natural gas boiler_3	14	1	13	13	13	2	17	17	3.5
	Natural gas boiler_4	14	5	18	18	15	15	15	15	10.5
	E-boiler_1	27	27	15	13	15	16	13	13	23
	E-boiler_2	27	12	13	13	13	13	13	13	17
	E-boiler_3	27	27	15	15	15	26	11	11	24.5
	E-boiler_4	27	23	10	10	13	13	13	13	17.5
Huntsman [Years installed 2022-2050]	E-boiler_1	15	0	0	0	0	0	0	0	0
	E-boiler_2	15	0	0	0	0	0	0	0	0
	E-boiler_3	15	0	0	0	0	23	0	0	0
	E-boiler_4	15	0	0	0	0	0	0	0	0
	Steam distribution_1	13	28	28	28	28	28	28	28	28
	Steam distribution_2	13	28	28	28	28	28	28	28	28
	Steam distribution_3	13	28	28	28	28	5	28	28	28
	Steam distribution_4	13	28	28	28	28	28	28	28	28
Shared [Years installed 2022-2050]	Brine recirculation_1	28	28	28	28	28	28	15	8	28
	Brine recirculation_2	28	28	28	28	28	28	14	2	28
	Brine recirculation_3	28	28	28	28	28	28	13	12	28
	Brine recirculation_4	28	28	28	28	28	28	14	11	28
	CCS_1	0	0	0	10	10	10	1	1	0
	CCS_2	0	0	0	0	0	10	0	0	0
	CCS_3	0	0	0	0	0	0	0	0	0
	CCS_4	0	10	0	0	0	10	0	0	0
Cashflows [Total CF 2022-2050 in billions]	NobianCF_1	€ 7.97	€ 2.96	€ 2.47	€ 2.34	€ -0.03	€ 2.30	€ 4.15	€ 4.15	€ 6.91
	NobianCF_2	€ 7.97	€ 5.97	€ 6.67	€ 6.54	€ 2.33	€ 2.30	€ 6.56	€ 6.56	€ 8.64
	NobianCF_3	€ 7.97	€ 21.28	€ 18.38	€ 21.00	€ 19.66	€ 8.24	€ 16.54	€ 16.54	€ 16.00
	NobianCF_4	€ 7.97	€ 21.34	€ 18.62	€ 21.10	€ 20.33	€ 21.59	€ 17.19	€ 17.19	€ 16.05
	Shin-etsuCF_1	€ 5.60	€ 3.52	€ 4.22	€ 4.11	€ 2.52	€ 4.46	€ 3.59	€ 3.59	€ 4.57
	Shin-etsuCF_2	€ 5.60	€ 5.38	€ 1.48	€ 0.44	€ 3.81	€ 4.46	€ 4.94	€ 4.94	€ 4.59
	Shin-etsuCF_3	€ 5.60	€ 10.82	€ 9.33	€ 9.43	€ 7.83	€ 5.68	€ 9.24	€ 9.24	€ 7.75
	Shin-etsuCF_4	€ 5.60	€ 11.13	€ 10.71	€ 9.80	€ 10.88	€ 9.86	€ 11.20	€ 11.20	€ 7.75
	WestlakeCF_1	€ 11.52	€ 11.24	€ 10.79	€ 10.81	€ 10.88	€ 10.18	€ 10.57	€ 10.57	€ 12.01
	WestlakeCF_2	€ 11.52	€ 9.69	€ 11.07	€ 11.01	€ 11.37	€ 10.18	€ 10.92	€ 10.92	€ 12.07
	WestlakeCF_3	€ 11.52	€ 45.46	€ 44.55	€ 44.62	€ 33.77	€ 11.93	€ 10.97	€ 10.97	€ 29.16
	WestlakeCF_4	€ 11.52	€ 45.41	€ 38.12	€ 43.22	€ 45.36	€ 44.10	€ 44.97	€ 44.97	€ 29.16
	HuntsmanCF_1	€ 8.09	€ 8.06	€ 8.06	€ 8.06	€ 8.06	€ 8.07	€ 8.06	€ 8.06	€ 7.91
	HuntsmanCF_2	€ 8.09	€ 8.07	€ 8.07	€ 8.07	€ 8.07	€ 8.07	€ 8.07	€ 8.07	€ 7.91
	HuntsmanCF_3	€ 8.09	€ 39.80	€ 39.80	€ 39.80	€ 39.80	€ 8.10	€ 39.80	€ 39.80	€ 23.70
	HuntsmanCF_4	€ 8.09	€ 39.80	€ 39.80	€ 39.80	€ 39.80	€ 39.80	€ 39.80	€ 39.80	€ 23.70
	TotalCF_1	€ 33.18	€ 25.78	€ 25.55	€ 25.32	€ 21.44	€ 25.01	€ 26.37	€ 26.37	€ 31.40
	TotalCF_2	€ 33.18	€ 29.11	€ 27.29	€ 26.06	€ 25.57	€ 25.01	€ 30.48	€ 30.48	€ 33.21
	TotalCF_3	€ 33.18	€ 117.37	€ 112.05	€ 114.84	€ 101.06	€ 33.95	€ 76.55	€ 76.55	€ 76.61
	TotalCF_4	€ 33.18	€ 117.68	€ 107.25	€ 113.92	€ 116.36	€ 115.35	€ 113.17	€ 113.17	€ 76.66
CO2 [Kton 2022-2050]	Total CO2_1	1666	3502	5923	5287	4357	6844	6913	6913	2716
	Total CO2_2	1666	7549	8132	7827	6769	6844	7929	7929	3751
	Total CO2_3	1666	551	1767	1139	2556	4005	6193	6193	1162
	Total CO2_4	1666	3802	5985	6151	5041	5319	7014	7014	2922

Figure 6.3: Model results. Colours are linked to the amount of years installed, green = high, white = average, red = low

Underneath, the difference between the baseline benchmark and the market & behavioural barriers is shown. We see a 32 Mton/288% increase in total CO_2 emission compared to the baseline benchmark. That is due to the lower amount of years that zero emission technology alternatives are installed. This shows that incorporation of the barriers does lead to significantly different transition pathways compared to the currently used optimisation models and verifies the claims made by Gerarden et al.[68]. Especially the market barriers Imperfect information and risk lead to a strong postponement of zero emission technology adoption. This suggests that the perceived uncertainty over time and the risk appetite of the companies is a strong influence on investment decision making at the PoR chlorine cluster.

Table 6.2: Difference between baseline benchmark and behavioural decision evaluation type

Alternative	Baseline	Average four scenario's Behavioural	Difference
NobianAssets | CHP	10	18	8
NobianAssets | Biomass	0	10	10
NobianAssets | E-boiler	19	0	-19
NobianAssets | MEV3	28	28	0
NobianAssets | MEV5	0	0	0
NobianAssets | Finite_gap	28	28	0
NobianAssets | Zero_gap	0	0	0
Shin-etsu_Assets | Gas-furnac	2	17.5	15.5
Shin-etsu_Assets | E-furnace	26	10.5	-15.5
Shin-etsu_Assets | Hydrogen-f	1	0	-1
Westlake_Assets | Gas-boiler	14	11.25	-2.75
Westlake_Assets | E-boiler	27	16.75	-10.25
Huntsman_assets | E-boiler	15	0	-15
Huntsman_assets | Steam_Dist	13	28	15
Westlake_Assets | Brine_reci	28	22.25	-5.75
Shared CCS (Nobian) | L	0	1.5	1.5
Total CO2 between 2022-2050	17	49	32

Furthermore, certain technologies are only adopted under very favourable external circumstances. In the case of Shin-etsu's hydrogen cracking furnace is only installed in scenario number three (see appendix F). This is due to the high fuel costs and relatively low efficiency. Allthough the Hydrogen furnace has a lot lower CAPEX and OPEX compared to the gas and e-furnace, it's efficiency is comparable to the gas furnace and the fuel costs are multiple times higher. Therefore, only under low hydrogen prices, high gas & electricity prices and technology preference, the hydrogen furnace is installed at Shin-etsu.

Next, as can be seen in the Model results file of appendix F, Westlake's E-boiler number of installed years is strongly dependent on the imperfect information barrier. In the normative benchmark and the NPV calculation by hand A, it is suggested that the Westlake E-boiler should be immediatly installed. However, the model results file suggests that the expected values for the efficiency of the alternative strongly influences the relative attractiveness with Westlake's gas-boiler. That is due to the fact that the CAPEX value for the E-boiler are high compared to the relative improvement in efficiency compared to the gas boiler. The CAPEX value is high because of the high perceived risk of the investment in the E-boiler. Furthermore when looking to the coloured cells in the model results file, we can see that the E-boiler is less installed under the configuration of the three year pay-back period. That is due to the low relative attractiveness to the currently installed steam distribution network. This results in a longer pay-back period than three years for the e-boiler compared to the steam network.

Lastly, we observe that the level of foresight and blocklenghts of the model settings lead to postponed adoption of zero emission technology. In figure 6.4, the optimizing settings are represented by the blue bars and the pay-back period by the orange bars. The reason for the postponed adoption of these technologies is due to the long pay-back period of the zero emission technologies compared to the non zero emission technologies. This longer pay-back period is based on the higher perceived risk for these technologies, the imperfect information regarding efficiency and relatively higher OPEX due to hidden costs. These result in lower attractiveness for the zero emission technologies and thus the shorter the period over which the alternatives should break-even is not achieved. The zero emission technologies are only adopted when the attractiveness is large enough due to energy prices and CO_2 prices.

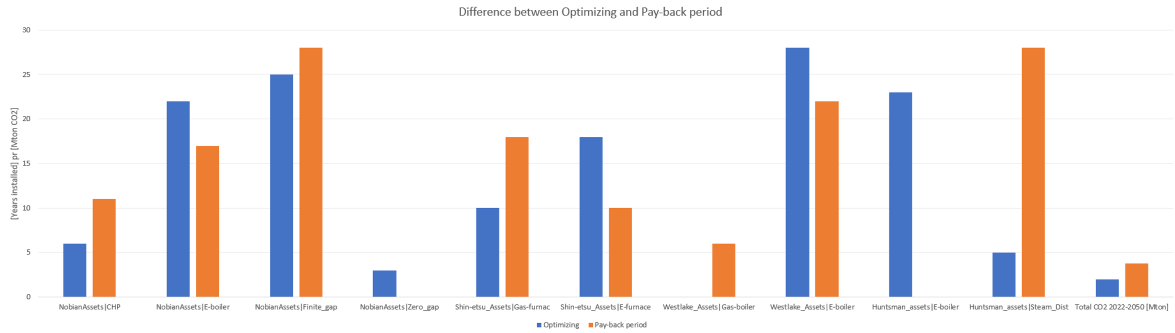

Figure 6.4: Difference Pay-back period and optimizing

The difference between the optimizing and pay-back period acceptance criteria is also reflected in figure 6.5. where the blue bars represent the optimizing decision criterium and the orange bars the pay-back period. The figures shows that the shorter the chosen pay-back period, the lower the amount of installed years for zero emission technology. Where a high amount of installed years reflect an early adoption of technology. This does imply that the level of risk appetite (the higher the level for the pay-back period is, the higher the risk appetite) of a decision maker strongly influences the adoption of technology.

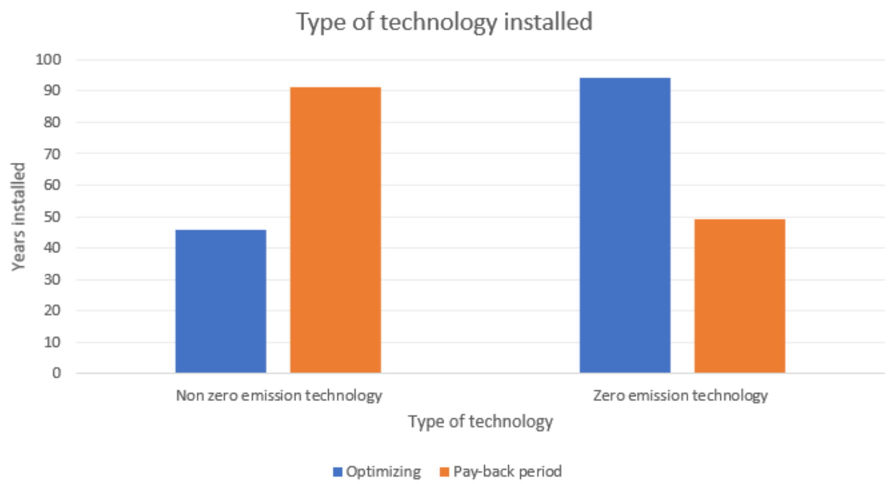

Figure 6.5: Types of technology installed under the condition of varying blocklengths

From these results we can conclude that the market & behavioural barriers do result postponed investment in zero emission technologies. Within the analysed scenario's, the difference between the normative benchmark resulted in an increase of 288% of CO_2 emissions between 2022 and 2050. Even though the used calibration of the parameters might not reflect 100% accurate values, they do show significant differences from the currently used optimisation approaches. So, with these model results we show the relevance of incorporating the market & behavioural barriers. This difference might explain why the investment gap exists. Where the normative models state that investments should be made, but they are not made because of the market & behavioural barriers that are not accounted for.

6.2.1. Conclusions

Following the model results shown above, we answer the third sub-question:

What is the effect of market and behavioural barriers on zero emission technology adoption at the PoR chlorine cluster?

The model results show that the incorporation of market and behavioural barriers lead to a lower adoption of zero emission technology adoption. This is reflected by the number of years that these alternatives are installed between 2022 and 2050. This lower adoption leads to significant higher CO_2 emission of 288% compared to the normative baseline benchmark. Underneath, the key findings from the model results are shown.

- The market & behavioural barriers lead to less zero emission technology adoption, compared to the normative baseline benchmark. Additionally, the barriers explain the existence of the perceived investment gap.
- Most of the direct CO_2 reduction can be achieved by decarbonising utility assets like steam boilers and cracking facilities.
- The pay-back period of three years, which represents a risk averse investor, leads to postponed zero emission technology investments.
- The build up of barriers is meaningful, because it makes it possible to identify interaction effects between barriers.

First off, the results clearly show that the incorporated barriers lead to a significant deviation from the normative baseline benchmark. This suggests that the incorporation of the theoretically sound barriers lead to very different results compared to the currently used normative optimisation models. The incorporation of the barriers show that the optimisation models overestimate the adoption of zero emission technology and might suggest why there is a perceived investment gap. As stated in the first chapter, according to the investment gap there should be made more investment than there are currently being made. But the results from this thesis suggest that it seems logical that these investments are not being made because of the mostly the perceived uncertainty and risk appetite of the companies at the cluster.

Secondly, the model results show that the quickest gains can be made by decarbonising the utility assets at the chlorine cluster. This is where the most direct CO_2 emissions are produced. In addition, the secondary emissions could be drastically reduced by the consumption of renewable electricity, due to the large consumption of electricity at the chlorine cluster's production processes. The placement of electric and biomass boilers to reduce the industry's direct emissions, as well as zero-gap membrane electrolyzers to tackle the industry's electricity consumption, and thus its indirect emissions.

Third, the used level for the pay-back period strongly influences the adoption for zero emission technology, as depicted by the results from decision evaluation type bounded rationality and split incentives. The companies at the PoR chlorine cluster use a pay-back period of three years in order to select their alternatives. Due to the large CAPEX of the zero emission technologies, the three years pay back period is too short to adopt new technology. So, the risk averseness of the investors leads to the postponement of technology adoption.

Lastly, the build-up used for the model experimentation is meaningful, as it identifies the interaction effects between barriers. This is best seen in decision evaluation types 'access to capital' and 'all market barriers'. Here, the limited access to capital results in lower total emissions as some of the high CAPEX polluting alternatives which have low OPEX are not adopted because it is not possible. There the somewhat lower CAPEX alternatives with high OPEX are adopted earlier. This is also due to the effect imperfect information and hidden costs have on the relative attractiveness of the technology alternatives. In a next study it would be interesting to conduct a full factorial experiment with the barriers to fully study the relative impact and interaction affect of the barriers on technology adoption.

7

Conclusion, Future Research and Recommendations

This chapter is dedicated to the conclusion 7.1, future research 7.2 and recommendations 7.3. The conclusion reflects back on the three sub-questions and main research questions and from chapter 1. In the following section, suggestions are given for future research. The last section gives recommendations for investment decision makers, based on the insights gained from this master thesis.

7.1. Conclusion

This section presents the final conclusions of this master thesis, by answering the main research question. Subsequently, the presented conclusions are used to address the scientific and social relevance.

Climate change has lead to one of the biggest societal challenges of this century. As environmental related risks caused by climate change in the form of, climate action failure, extreme weather and biodiversity loss, could lead to various devastating consequences to global society. The Netherlands faces one it's largest societal challenges that mankind has ever faced.

In order to limit the consequences of climate change, the Netherlands has to rapidly decarbonize its industrial sector to reach CO_2 neutrality by 2050. To achieve that goal large capital investments in zero emission technologies are needed. These investments would comprise out of renewable energy generation, energy conservation, higher production efficiency, electrification of end uses and many more. According to the 'Planbureau voor de Leefomgeving' (PBL), an estimated 350 billion euro investment is needed between 2020 and 2040 in order for the Netherlands to achieve net neutrality by 2050 [132].

Allthough there are various options for the decarbonisation of the industrial sector, the progress in the Dutch industrial sector has been seriously lagging. Possible explanations for the apparent lack of progress are market and behavioural barriers to zero emission technology adoption. Although these barriers seem to be theoretically sound, it is unclear to what extent both of these barriers contribute to the lack of investment. Therefore this thesis has focused on the following main research question:

What is the influence of market & behavioural barriers on investment decisions at the PoR chlorine cluster?

1. What are possible zero-emission technologies that can be implemented at the PoR chlorine cluster
To attain a overview of the current technological configuration of the PoR chlorine cluster, a comprehensive inventarisation was made of plants, processes, products and zero emission technology alternatives. This resulted in a detailed overview of the cluster's current technological configuration and a set of implementable zero-emission technologies like:

- Alternatives for fuel switching
- Technology that increases process efficiency

- Carbon Capture and storage technology
- Recirculation alternatives

For the PoR chlorine cluster, large gains regarding the reduction of CO_2 emission can be made by the decarbonisation of it's heat processes. This can be achieved mainly by means of electric or biomass steam boilers and electric cracking furnaces. Also the reduction of energy usage by implementing technology that increases process efficiency. For Nobian there would be an opportunity for the large-scale implementation of zero-gap membrane electrolyzers to largely reduce electricity consumption. Furthermore, a shared CCS system could reduce the direct CO_2 emissions of the cluster. Especially if the relative attractiveness of utility fuel switching turns out to be too low. Secondly, the brine recirculation alternative would reduce the waste streams of Westlake and the required salt production of Nobian's Delfzijl plant. So, this would lead in a reduction of indirect CO_2 costs for Nobian.

2. How can we represent market & behavioural barriers in an investment model at the PoR chlorine cluster?
In order to evaluate what the influence of the market & behavioural barriers is on the technology adoption of these alternatives, we conceptualised decision evaluation types. These decision evaluation types represent the risk, imperfect information, hidden costs, access to capital, bounded rationality and split incentives in the form of NPV formula's. In total, 7 different levels of representation of the barriers were conceptualised. This allows for the study of their relative relevance and interaction effects among them. These evaluation types were subsequently implemented in a modelling tool called Linny-R. The model incorporated the PoR chlorine cluster on a highly detailed technical level and was able to simulate technology adoption using the seven different types of decision evaluation.

3. What is the effect of market and behavioural barriers on zero emission technology adoption at the PoR chlorine cluster?
The model was subsequently used with a scenario analysis to simulate the technology adoption under varying uncertain contexts. These contexts were mainly determined by the variation of energy prices, commodity prices and government policy. Thereafter, simulation of technology adoption was carried out per decision evaluation type under varying contexts.

The results from the scenario analysis gave insights into the effect of market & behavioural barriers. The barriers resulted in a significant difference in zero emission technology adoption, compared to an earlier normative benchmark baseline run. Due to the lower adoption of zero emission technology we observed a 288% increase of total expected CO_2 emissions between 2022 and 2050, compared to the baseline.

Answering the main research question
To conclude, by combining a thorough inventarisation of the current and possible future configurations of the PoR chlorine cluster, the representation of market & behavioural barriers in the form of decision evaluation types and combining these in a model that simulates technology adoption, we were able to answer the main research question. The inventorization, conceptualization, experimentation and analysis of the influence of market & behavioural barriers on investment decision at the PoR chlorine cluster has helped to understand the opportunities and threats to decarbonizing the production chain. The findings of this investigation further underscore the relevance of incorporating these barriers in quantitative decision support models. Only with a complete and realistic representation of reality, industry actors and policymakers are able to both act and cooperate faster and better.

7.1.1. Scientific and Societal relevance

Both the scientific an societal relevance of this master thesis are depicted in the bullet points below.

Scientific relevance
During this research, scientific knowledge and expert elicitation were combined to conceptualize the current and possible future technical configuration of the PoR chlorine cluster. This was achieved through a series of scientific structures, calculation frameworks, interviews with stakeholders. Together, these approaches resulted in a clear and concise methodology to conceptualize and analyze an industrial production processes.

The plant-process-product analysis from Bartel et al. [11] made it possible to gain a total overview of the PoR chlorine cluster's current state which was needed for 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 cluster works from the bottom up.Followed by the zero-emission technology inventarisation, which made it possible to allow possible future configurations of the cluster.

Secondly, by studying the influence of market & behavioural barriers, we have further contributed to the understanding of the investment gap. Furthermore, the used approach might prove interesting for other decarbonisation studies focusing on the industrial sector.

Thirdly, The more qualitative STEEP framework [18] [164] allowed the author to identify the key driving forces at play in the chlorine cluster's production chain as a whole, and analyze the industry from the top down. This approach helped 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 cluster, and for the experimentation in Linny-R and analysis of possible transition pathways.

- Added research to the understanding of the investment gap.
- Relevant for decarbonisation studies focusing on the industrial sector.

Societal relevance
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 to give insight into possible transition pathways and the effect barriers have on development. The research shows stakeholders about strategies to decarbonize the PoR chlorine cluster and enables 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.

From a more broad perspective, this study provides insights about possible transition pathways for the PoR chlorine cluster. Apart from the model results, also the inventarisation of the entire technical system of the chlorine cluster and integrated links might be relevant. Furthermore, the influence of market & behavioural barriers on technology adoption does not limit itself solely to the industrial sector. Therefore, this study might prove insightful for the Dutch energy transition as a whole. Where other sectors like the electricity, built environment and agriculture might face similar key challenges to investment.

- This study discusses key challenges that are experienced in the Dutch energy transition as a whole.
- Provides insights to possible transition pathways for the PoR chlorine cluster.

7.2. Future Research

This section gives suggestions to researchers for future research within the scientific field of investment modeling, based on the insights gained from this master thesis. These future research suggestions should in turn cover the limitations of this research. The key suggestions for future research are:

1. Further develop the representation of market & behavioural barriers and interaction effects between them.
2. Broaden the scope of the investment evaluation further, besides solely decarbonisation alternatives.
3. Further analyze the technologies that lie on the horizon for the PoR chlorine cluster.
4. Expand the current model with the integration of other industrial plants at the Rotterdam harbour industrial cluster.
5. Further investigate the interaction between key uncertainties.
6. Deploy exploratory analysis techniques to explore the investment decision making under deep uncertainty.

For this thesis, a deliberate choice was made to use the same decision protocol for every level of decision making and only differentiate in the decision evaluation part. As earlier mentioned in chapter 4, investment heuristics could be used to capture the cognitive limitations and biases of decision makers and their behavioural aspects in more detail and therefore more accurately represent behavioural barriers. Examples like the recognition heuristic, take-the-best heuristic and fast-and-frugal trees. Besides that these heuristics capture a variety of decision evaluation types, they also differentiate in their decision protocols and acceptance criteria. Nevertheless, we acknowledge that parameterisation is a simplification of truly capturing bounded rationality and behavioural aspects in quantitative models. However, there are also various strengths to the chosen representation of market & behavioural barriers:

- The representation in the form of evaluation types is interchangeable and can be used in various heuristics that contain an evaluation process.
- Can be easily expanded with other/more parameters to represent the barriers.
- Can identify whether it is necessary to conduct a more detailed investment analysis.

Especially the last point is of interest. The used methodology is implementable in quantitative models and can determine whether barriers are of a large interest for a investment project. If for example a large discrepancy is identified concerning a certain barrier, compared to the normative benchmark, the investor could decide for a more detailed study. If not, the investor is informed that the barriers probably do not play a large role in that specific investment project. However, we do acknowledge that currently conceptualised parameterisation of the decision evaluation types is simplified way of representing market & behavioural barriers. Therefore, we argue to further develop decision evaluation types with more parameterisation of the evaluation types.

The second suggestion is based on observations from the access to capital evaluation type and insights gained from conversations with experts at Nobian & Westlake. The model results showed that the access to capital type did not have a significant influence on the technology adoption at the PoR chlorine cluster. Even though the experts from Nobian & Westlake mentioned that the access to capital one of the largest barrier is to zero emission technology adoption. They mentioned that they have to make various investments to ensure the continuity of their companies. Although they find the decarbonisation of their production process very important, their main concern is to most effectively allocate capital. Therefore, other investments, that might not concern the reduction of emissions are favoured above the zero emission technologies. As the expert at Westlake noticed, they investment projects are prioritised by their expected return on investment. Therefore, we argue that the investment evaluation for technology adoption should be broadened to all possible investment projects and not solely the decarbonisation alternatives. This leads to a more holistic overview of how investment projects are addressed on company level.

Thirdly, it is recommended to further analyze the technologies that lie on the horizon for the chlorine cluster's industries. A set of zero emission technologies were identified and discussed in chapter 3. However, this is a set of technologies which is currently available. To keep the model relevant, the modeled stock of technology should be periodically be updated. As, these technologies will, can 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.

Next, the STEEP analysis has shed 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 represent the factors of importance to the decarbonisation of the cluster.

The fifth suggestions states that the current model should be expanded, by representing the rest of the Rotterdam harbour industrial complex. As mentioned in the first chapter, the industrial cluster of Rotterdam is a very interconnected site with various interdependencies. Therefore, we suggest to broaden the scope of the model and also consider the rest of the industrial complex. This might prove to be beneficial as chain effects between certain industries can be further investigated. The CCS alternative for example did not achieve the levels of installment that were expected beforehand. In reality the Dutch industrial sector and government are very much invested in CCS for the PoR. Given the limited scope, alternatives like the CCS could be better represented with a broadened scope where we take in to account the other polluting plants at the PoR industrial sector.

The last point aims to solve the shortcomings of a scenario analysis. The conducted scenario analysis is a very quick and easy method to explore likely possible futures. However, to further understand the effects the exogenous environment can have on technology adoption we suggest to deploy analysis techniques that explore investment decision making under deep uncertainty. This would result in a higher resolution of the solution space and give better insights about possible & likely futures.

7.3. Recommendations

This section gives recommendations to investment decision makers, based on the insights gained from this master thesis. The insights from this master thesis result in the following key recommendations for investment decision makers:

1. Consider the incorporation of market & behavioural barriers in investment models for the industrial sector.
2. The companies at the chlorine cluster should adjust their currently used decision acceptance criteria to further decarbonize the cluster.
3. Policy should be made to increase the relative attractiveness of sustainable utility assets at the cluster to achieve large CO_2 reductions.
4. Proceed with the Brine recirculation alternative, as it seems to be profitable in all the scenario's.
5. WEI should dedicate to the expansion of the model and create a support base among the Harbour Industrial Complex Rotterdam-Moerdijk.

First off, investment decision makers should become more aware that zero emission technology investment is subjected to various market & behavioural barriers. As the model results show a discrepancies between normative benchmark optimizing and non normative optimisation, in case of the PoR chlorine cluster. This result is juxtaposed from the perceptions of the experts at Nobian and Westlake. They did acknowledge that the considered barriers are theoretically sound, but did not perceive them as thus impactful to consider in their investment models. Therefore, the recommendation to incorporate market & behavioural barriers in investment models to more incorporate more of the possible costs and benefits. This leads to a far more accurate representation of technology adoption and might prove insightful for possible paths of decarbonisation. Also, the industrial sector should alter their decision acceptance criteria to a less risk averse ones. As is clearly seen for some of the alternatives in the model results file, the pay-back period of three years strongly impacts the adoption of zero emission technologies. Eventually, we will probably achieve a situation where the zero emission technology alternatives are within the margin of a three year pay-back period. A situation with a extreme surplus of cheap renewable electricity, more proven technology and higher CO_2 prices. However, the time that we lose with the postponement of adopting zero emission technology might lead to irreversible negative consequences for society.

Secondly, as shown in the results from 6, the pay-back period chosen by the companies strongly influences the postponement for the adoption of zero emission technology. This in turn leads to lower profits for the companies over time and an increase in total CO_2 emissions. Therefore, it is recommended for the companies to use less risk averse decision acceptance criteria.

Thirdly, a recommendation to policy makers. As explained earlier, the large and cost-effective gains regarding (CO2) emission reduction can be made in the utility alternatives for the chlorine cluster. These are mainly the utility technologies responsible for heat and steam production. Financial stimulation of these specific technology alternatives could make quick gains in CO_2 reduction by the subsidation of these technologies and higher taxation on gas use & CO_2 costs.

Fourthly, the model results show that the brine recirculation alternative between Nobian and Westlake is profitable under almost every circumstance. Therefore, it is suggested to proceed with the alternative and scale the project up from the demonstration site to full scale recirculation. Of course, this recommendation is only based on the financial profitability of the project and the companies should consider the desirability of further interconnection & interdependence.

Lastly, WEI should dedicate to the expansion of the model with more of the PoR industrial cluster and simultaneously create a support base among these companies for the use of the model. This thesis has proven the functionality of Linny-R by being able to present possible transition pathways on an asset level, in combination with CO_2 reduction. Especially the ease of modelling in combination with the graphically appealing representation of technical systems, should be reasons to adopt the Linny-R modelling method. In light of the IMPETUS project the model could be expanded with the rest of the industry in Rotterdam-Moerdijk and result in a model that would give insight to all the relevant parties. At the same time a strong support base for the model should be created among the potential users, in order for the model to be accepted and actually be used in the future. To achieve that, WEI could opt for a more cooperative modelling approach with the potential users and create a easily accessible version of the model in the form of a online decision support system. A lot of inspiration could be drawn from the ETM from Quintel.

Bibliography

[1] National Academies. *Is it possible to achieve net-zero emissions?* 2021. URL: https://www.nationalacademies.org/based-on-science/is-it-possible-to-achieve-net-zero-emissions.

[2] Varun Advani. *Finding robust transition paths for industrial ecosystems*. Nov. 2020. URL: https://repository.tudelft.nl/islandora/object/uuid%3A72c4aa12-16cc-41c9-b15f-67bb06a12754.

[3] Ministerie van Algemene Zaken. *CO2-Heffing voor Industrie*. Jan. 2021. URL: https://www.rijksoverheid.nl/onderwerpen/milieubelastingen/co2-heffing-voor-industrie#:~:text=CO2%5C%2Dheffing%5C%20industrie%5C%20vanaf%5C%201,uitstoot%5C%20voor%5C%20mens%5C%20en%5C%20milieu..

[4] Maurice Allais. "Le comportement de l'homme rationnel devant le risque: critique des postulats et axiomes de l'école américaine". In: *Econometrica: Journal of the Econometric Society* (1953), pp. 503–546.

[5] Corey Allan, Adam B Jaffe, and Isabelle Sin. "Diffusion of green technology: a survey". In: (2014).

[6] Soren T Anderson and Richard G Newell. "Information programs for technology adoption: the case of energy-efficiency audits". In: *Resource and Energy Economics* 26.1 (2004), pp. 27–50.

[7] Eeonora Laura Avram et al. "INVESTMENT DECISION AND ITS APPRAISAL." In: *Annals of DAAAM & Proceedings* (2009).

[8] Catherine SE Bale, Liz Varga, and Timothy J Foxon. "Energy and complexity: New ways forward". In: *Applied Energy* 138 (2015), pp. 150–159.

[9] Steven C Bankes. "Agent-based modeling: A revolution?" In: *Proceedings of the National Academy of Sciences* 99.suppl 3 (2002), pp. 7199–7200.

[10] Elsa Barazza and Neil Strachan. "The impact of heterogeneous market players with bounded-rationality on the electricity sector low-carbon transition". In: *Energy Policy* 138 (2020), p. 111274.

[11] Ann Bartel, Casey Ichniowski, and Kathryn Shaw. "How does information technology affect productivity? Plant-level comparisons of product innovation, process improvement, and worker skills". In: *The quarterly journal of Economics* 122.4 (2007), pp. 1721–1758.

[12] Barus. *Ethylene dichloride (EDC)*. June 2022. URL: https://barusgolden.com/ethylene-dichloride-edc/.

[13] Aqeel Ahmed Bazmi and Gholamreza Zahedi. "Sustainable energy systems: Role of optimization modeling techniques in power generation and supply—A review". In: *Renewable and sustainable energy reviews* 15.8 (2011), pp. 3480–3500.

[14] Pedro Belli et al. "Handbook on economic analysis of investment operations". In: *World Bank* (1998), pp. 17–28.

[15] Pieter Bots. 2021. URL: https://sysmod.tbm.tudelft.nl/linny-r.html.

[16] Pieter Bots. *Products*. 2021. URL: https://sysmod.tbm.tudelft.nl/linny-r/docs/.

[17] Bouma. *Interview with Westlake*. 2022.

[18] Ron Bradfield et al. "The origins and evolution of scenario techniques in long range business planning". In: *Futures* 37.8 (2005), pp. 795–812.

[19] Thomas Brinkmann et al. *Best Available Techniques (BAT) Reference Document for the Production of Chlor-alkali*. 2014.

[20] Georg Buchner, Johannes Wunderlich, and Reinhard Schomacker. *Technology readiness levels guiding cost estimation in the chemical ...* 2018. URL: https://www.researchgate.net/publication/326211036_Technology_Readiness_Levels_Guiding_Cost_Estimation_in_the_Chemical_Industry.

[21] Sergio Mario Camporeale et al. "Part load performance and operating strategies of a natural gas—biomass dual fueled microturbine for combined heat and power generation". In: *Journal of Engineering for Gas Turbines and Power* 137.12 (2015).

[22] Jaworski C Capricho, Bronwyn Fox, and Nishar Hameed. "Multifunctionality in epoxy resins". In: *Polymer Reviews* 60.1 (2020), pp. 1–41.

[23] Claudio Carnevale et al. "An integrated assessment tool to define effective air quality policies at regional scale". In: *Environmental Modelling & Software* 38 (2012), pp. 306–315.

[24] CBS. *Aardgas en elektriciteit, gemiddelde prijzen van eindverbruikers*. 2022. URL: https://opendata.cbs.nl/statline/#/CBS/nl/dataset/81309NED/table?fromstatweb.

[25] Emile Chappin and Gerard PJ Dijkema. "Modeling for transition management". In: *Available at SSRN 2618413* (2015).

[26] Emile JL Chappin et al. "Simulating climate and energy policy with agent-based modelling: The Energy Modelling Laboratory (EMLab)". In: *Environmental modelling & software* 96 (2017), pp. 421–431.

[27] Chemanalyst. *Ethylene dichloride (EDC) price trend and forecast*. 2022. URL: https://www.chemanalyst.com/Pricing-data/ethylene-dichloride-44.

[28] Chemanalyst. *Hydrochloric acid price trend and forecast*. 2022. URL: https://www.chemanalyst.com/Pricing-data/hydrochloric-acid-61.

[29] Chemanalyst. *Hydrochloric acid price trend and forecast*. 2022. URL: https://www.chemanalyst.com/Pricing-data/hydrochloric-acid-61.

[30] Marian R Chertow. "Industrial symbiosis: literature and taxonomy". In: *Annual review of energy and the environment* 25.1 (2000), pp. 313–337.

[31] Damiana Chinese and Antonella Meneghetti. "Optimisation models for decision support in the development of biomass-based industrial district-heating networks in Italy". In: *Applied energy* 82.3 (2005), pp. 228–254.

[32] John Conlisk. "Why bounded rationality?" In: *Journal of economic literature* 34.2 (1996), pp. 669–700.

[33] Aswath Damodaran. *Strategic risk taking: a framework for risk management*. Pearson Prentice Hall, 2007.

[34] BW Daniëls and AWN Van Dril. "Save production: A bottom-up energy model for Dutch industry and agriculture". In: *Energy economics* 29.4 (2007), pp. 847–867.

[35] Klundert J.J van de. *Supply chain management en technologie: Onder Druk Wordt alles vloeibaar*. METEOR, Maastricht research school of Economics of TEchnology and ORganizations, 2003.

[36] Anne De Bruin and Susan Flint-Hartle. "A bounded rationality framework for property investment behaviour". In: *Journal of Property Investment & Finance* (2003).

[37] Henri LF De Groot, Erik T Verhoef, and Peter Nijkamp. "Energy saving by firms: decision-making, barriers and policies". In: *Energy Economics* 23.6 (2001), pp. 717–740.

[38] Stephen J DeCanio. "Barriers within firms to energy-efficient investments". In: *Energy policy* 21.9 (1993), pp. 906–914.

[39] Stephen J DeCanio. "The efficiency paradox: bureaucratic and organizational barriers to profitable energy-saving investments". In: *Energy policy* 26.5 (1998), pp. 441–454.

[40] CE Delft. *Potential for power-to-heat in the netherlands - CE delft*. 2015. URL: https://cedelft.eu/wp-content/uploads/sites/2/2021/04/CE_Delft_3E04_Potential_for_P2H_in_Netherlands_DEF.pdf.

[41] Mercedes Delgado, Michael E Porter, and Scott Stern. "Clusters and entrepreneurship". In: *Journal of economic geography* 10.4 (2010), pp. 495–518.

[42] Michael J Dempsey. "A multidisciplinary perspective on the evolution of corporate investment decision making". In: *Accounting, Accountability & Performance* 9.1 (2003), pp. 1–33.

[43] Derwent. *Derwent Top 100 global innovators 2018-19 report*. Feb. 2020. URL: https://clarivate.com/derwent/campaigns/derwent-top-100-global-innovators-2018-19-report/.

[44] Michela Desideri Perea. *A MILP-based approach for the analysis of cooperative relationships in the transition of the energy-intensive industry*. Aug. 2021. URL: https://repository.tudelft.nl/islandora/object/uuid%3Ad657e933-7c81-4757-9e55-ef9616769c0d.

[45] Alexandra C Dimian and CS Bildea. "Phenol hydrogenation to cyclohexanone". In: *Chemical Process Design: Computer-Aided Case Studies* (2008), pp. 129–172.

[46] Mark Dowson et al. "Domestic UK retrofit challenge: Barriers, incentives and current performance leading into the Green Deal". In: *Energy Policy* 50 (2012), pp. 294–305.

[47] Wolfgang Drobetz et al. "Policy uncertainty, investment, and the cost of capital". In: *Journal of Financial Stability* 39 (2018), pp. 28–45.

[48] L Drouet and J Thénié. *An Energy-Technology-Environment Model to Assess Urban Sustainable Development Policies-Reference Manual*. Tech. rep. Technical report, Ordecsys Technical Reports, 2009.

[49] Peter N Duinker and Lorne A Greig. "Scenario analysis in environmental impact assessment: Improving explorations of the future". In: *Environmental impact assessment review* 27.3 (2007), pp. 206–219.

[50] Earle. 2003. URL: https://web.archive.org/web/20081008030448/http://www.nzifst.org.nz/unitoperations/evaporation2.htm.

[51] Echemi. *Vinyl chloride price list in global market - echemi*. 2022. URL: https://www.echemi.com/pip/vinylchloride-pid_Rock16631.html.

[52] Ministerie van Economische Zaken en Klimaat. *Daling CO2-Uitstoot Grote Bedrijven Tot stilstand*. Apr. 2022. URL: https://www.klimaatakkoord.nl/actueel/nieuws/2022/04/14/nea-uitstootcijfers.

[53] EEA. *Climate change is one of the biggest challenges of our Times*. Nov. 2021. URL: https://www.eea.europa.eu/themes/climate/climate-change-is-one-of.

[54] EIA. *U.S. Energy Information Administration - EIA - independent statistics and analysis*. 2022. URL: https://www.eia.gov/energyexplained/natural-gas/factors-affecting-natural-gas-prices.php.

[55] Wolfgang Eichhammer et al. "Study on the energy savings potentials in EU member states, candidate countries and EEA countries". In: (2011).

[56] Barbara Elvers et al. *Ullmann's encyclopedia of industrial chemistry*. Verlag Chemie, 1991.

[57] Energy and Climate change directorate. *Deep decarbonisation pathways for Scottish Industries: Research Report*. 2020. URL: https://www.gov.scot/publications/deep-decarbonisation-pathways-scottish-industries/pages/5/#:~:text=8%5C%20Appendix-,4%5C%20Decarbonisation%5C%20options,%5C%2C%5C%20and%5C%20storage%5C%20(%5C%20CCUS%5C%20)..

[58] ESC. *6.8 cost of CHP: Engineering and installation costs*. Sept. 2018. URL: https://understandingchp.com/chp-applications-guide/6-8-rules-of-thumb-for-chp-engineering-and-installation-costs/.

[59] Edward J Farragher, Robert T Kleiman, and Anandi P Sahu. "Current capital investment practices". In: *The Engineering Economist* 44.2 (1999), pp. 137–150.

[60] R Ian Faulconbridge and Michael J Ryan. *Systems engineering practice*. Argos Press Canberra, 2014.

[61] Lucía Fernández. *PVC prices globally 2022*. Aug. 2021. URL: https://www.statista.com/statistics/1171131/price-polyvinyl-chloride-forecast-globally/.

[62] Domenico Ferrero et al. "Power-to-Gas Hydrogen: techno-economic assessment of processes towards a multi-purpose energy carrier". In: *Energy Procedia* 101 (2016), pp. 50–57.

[63] Finra. *The reality of investment risk*. 2022. URL: https://www.finra.org/investors/learn-to-invest/key-investing-concepts/reality-investment-risk.

[64] Stylianos Flegkas et al. "Profitability analysis and capital cost estimation of a thermochemical energy storage system utilizing fluidized bed reactors and the reaction system MgO/Mg (OH) 2". In: *Energies* 12.24 (2019), p. 4788.

[65] Tobias Fleiter, Joachim Schleich, and Ploypleam Ravivanpong. "Adoption of energy-efficiency measures in SMEs—An empirical analysis based on energy audit data from Germany". In: *Energy Policy* 51 (2012), pp. 863–875.

[66] Tobias Fleiter, Ernst Worrell, and Wolfgang Eichhammer. "Barriers to energy efficiency in industrial bottom-up energy demand models—A review". In: *Renewable and sustainable energy reviews* 15.6 (2011), pp. 3099–3111.

[67] George W Gallinger. "Capital expenditure administration". In: *Sloan Management Review (pre-1986)* 22.1 (1980), p. 13.

[68] Todd D Gerarden, Richard G Newell, and Robert N Stavins. "Assessing the energy-efficiency gap". In: *Journal of Economic Literature* 55.4 (2017), pp. 1486–1525.

[69] Dolf Gielen and Michael Taylor. "Modelling industrial energy use: the IEAs energy technology perspectives". In: *Energy Economics* 29.4 (2007), pp. 889–912.

[70] Gerd Gigerenzer and Wolfgang Gaissmaier. "Heuristic decision making". In: *Annual review of psychology* 62.1 (2011), pp. 451–482.

[71] Bruce Gilley and David Kinsella. "Coercing climate action". In: *Survival* 57.2 (2015), pp. 7–28.

[72] Kenneth Gillingham and Karen Palmer. "Bridging the energy efficiency gap: Policy insights from economic theory and empirical evidence". In: *Review of Environmental Economics and Policy* (2020).

[73] Daniel G Goldstein and Gerd Gigerenzer. "Models of ecological rationality: the recognition heuristic." In: *Psychological review* 109.1 (2002), p. 75.

[74] Uwe Götze, Deryl Northcott, Peter Schuster, et al. "Investment appraisal". In: *Methods and models* 2 (2008).

[75] John R Graham and Campbell R Harvey. "The theory and practice of corporate finance: Evidence from the field". In: *Journal of financial economics* 60.2-3 (2001), pp. 187–243.

[76] David L Greene. "Uncertainty, loss aversion, and markets for energy efficiency". In: *Energy Economics* 33.4 (2011), pp. 608–616.

[77] Michael Grubb. *Planetary economics: energy, climate change and the three domains of sustainable development*. Routledge, 2014.

[78] Päivi Haapasaari, Samu Mäntyniemi, and Sakari Kuikka. "Baltic herring fisheries management: stakeholder views to frame the problem". In: *Ecology and Society* 17.3 (2012).

[79] Yusriadi HALA et al. "The financial behavior of investment decision making between real and financial assets sectors". In: *The Journal of Asian Finance, Economics, and Business* 7.12 (2020), pp. 635–645.

[80] Chemical Economics Handbook. *Ethylene Dichloride*. 2020. URL: https://ihsmarkit.com/products/ethylene-dichloride-chemical-economics-handbook.html.

[81] Geoffrey Colin Harcourt, Peter Henry Karmel, Robert Henry Wallace, et al. "Economic activity". In: *Cambridge Books* (1967).

[82] Eric Hirst and Marilyn Brown. "Closing the efficiency gap: barriers to the efficient use of energy". In: *Resources, Conservation and Recycling* 3.4 (1990), pp. 267–281.

[83] Provincie Zuid Holland. *€2,7 Miljoen Subsidie voor Botlek Stoomnetwerk*. 2022. URL: https://www.zuid-holland.nl/actueel/nieuws/april-2022/e2-7-miljoen-subsidie-botlek-stoomnetwerk/.

[84] Provincie Zuid Holland. *Kennisgeving aanvraag Huntsman Holland B.V (9999231505)*. 2021. URL: https://zoek.officielebekendmakingen.nl/prb-2021-5275.pdf.

[85] Bongghi Hong et al. "An integrated monitoring/modeling framework for assessing human–nature interactions in urbanizing watersheds: Wappinger and Onondaga Creek watersheds, New York, USA". In: *Environmental Modelling & Software* 32 (2012), pp. 1–15.

[86] Mark Howells et al. "OSeMOSYS: the open source energy modeling system: an introduction to its ethos, structure and development". In: *Energy Policy* 39.10 (2011), pp. 5850–5870.

[87] IMPETUS. *Impetus - turning climate commitments into action*. Mar. 2022. URL: https://climate-impetus.eu/.

[88] Kaveri K Iychettira et al. "Towards a comprehensive policy for electricity from renewable energy: Designing for social welfare". In: *Applied Energy* 187 (2017), pp. 228–242.

[89] Anthony J Jakeman and Rebecca A Letcher. "Integrated assessment and modelling: features, principles and examples for catchment management". In: *Environmental Modelling & Software* 18.6 (2003), pp. 491–501.

[90] Daniel Kahneman and Amos Tversky. "Prospect theory: An analysis of decision under risk". In: *Handbook of the fundamentals of financial decision making: Part I*. World Scientific, 2013, pp. 99–127.

[91] Mikiko Kainuma, Yuzuru Matsuoka, and Tsuneyuki Morita. "The AIM/end-use model and its application to forecast Japanese carbon dioxide emissions". In: *European Journal of Operational Research* 122.2 (2000), pp. 416–425.

[92] Ivan Kantor et al. "A mixed-integer linear programming formulation for optimizing multi-scale material and energy integration". In: *Frontiers in Energy Research* 8 (2020), p. 49.

[93] Ralph L Keeney. "Decision analysis: an overview". In: *Operations research* 30.5 (1982), pp. 803–838.

[94] Rebecca A Kelly et al. "Selecting among five common modelling approaches for integrated environmental assessment and management". In: *Environmental modelling & software* 47 (2013), pp. 159–181.

[95] Ilkka Keppo and Manfred Strubegger. "Short term decisions for long term problems–The effect of foresight on model based energy systems analysis". In: *Energy* 35.5 (2010), pp. 2033–2042.

[96] Klimaattafel Haven en Industrie Rotterdam-Moerdijk. *Clusterplan industriecluster Rotterdam-Moerdijk*. 2020. URL: https://www.klimaatakkoord.nl/documenten/publicaties/2020/10/22/koplopersprogramma-cluster-rotterdam_moerdijk.

[97] Florian Knobloch and Jean-Francois Mercure. "The behavioural aspect of green technology investments: A general positive model in the context of heterogeneous agents". In: *Environmental Innovation and Societal Transitions* 21 (2016), pp. 39–55.

[98] Jan H Kwakkel, Warren E Walker, and Vincent AWJ Marchau. "Classifying and communicating uncertainties in model-based policy analysis". In: *International journal of technology, policy and management* 10.4 (2010), pp. 299–315.

[99] Howard A Latin. *Climate change policy failures: why conventional mitigation approaches cannot succeed*. World Scientific, 2012.

[100] PBL Planbureau voor de Leefomgeving. "DECARBONISATION OPTIONS FOR THE DUTCH POLYCARBONATE INDUSTRY-D. Mooij, MA Muller". In: (2021).

[101] Gregory Lenoir and Nils S Tuchschmid. "Investment time horizon and asset allocation models". In: *Financial Markets and Portfolio Management* 15.1 (2001), p. 76.

[102] Francis GN Li. "Actors behaving badly: Exploring the modelling of non-optimal behaviour in energy transitions". In: *Energy Strategy Reviews* 15 (2017), pp. 57–71.

[103] Tom CW Lin. "A behavioral framework for securities risk". In: *Seattle UL Rev.* 34 (2010), p. 325.

[104] Richard Loulou, Gary Goldstein, Ken Noble, et al. "Documentation for the MARKAL Family of Models". In: *Energy Technology Systems Analysis Programme* (2004), pp. 65–73.

[105] Richard Loulou et al. "Documentation for the times model, part i: Energy technology systems analysis programme". In: *International Energy Agency Paris* (2005).

[106] Henrik Lund and J Thellufsen. "Advanced Energy Systems Analysis Computer Model Documentation Version 11.4". In: *Aalborg University: Aalborg, Denmark* (2014), pp. 1–188.

[107] Yizheng Lyu et al. "Exploring the cost of wastewater treatment in a chemical industrial Park: Model development and application". In: *Resources, Conservation and Recycling* 155 (2020), p. 104663.

[108] Coen Makker. *Kansen en bedreigingen in het PVC-cluster*. 2013.

[109] Vincent AWJ Marchau et al. *Decision making under deep uncertainty: from theory to practice*. Springer Nature, 2019.

[110] David C Mauer and Steven H Ott. "Investment under uncertainty: The case of replacement investment decisions". In: *Journal of Financial and Quantitative Analysis* 30.4 (1995), pp. 581–605.

[111] Jean-Francois Mercure et al. "Modelling complex systems of heterogeneous agents to better design sustainability transitions policy". In: *Global environmental change* 37 (2016), pp. 102–115.

[112] Marc J Metzger et al. "How personal judgment influences scenario development: an example for future rural development in Europe". In: *Ecology and Society* 15.2 (2010).

[113] Mathias Mier and Valeriya Azarova. *Investor type heterogeneity in bottom-up optimization models*. Tech. rep. ifo Working Paper, 2021.

[114] Ministerie van Economische Zaken en Klimaat. *Industrie*. Mar. 2021b. URL: https://www.klimaatakkoord.nl/industrie.

[115] Ministerie van Economische Zaken en Klimaat. *Kabinetsinzet voor het Klimaatakkoord*. 2018.

[116] Enayat A Moallemi and Shirin Malekpour. "A participatory exploratory modelling approach for long-term planning in energy transitions". In: *Energy research & social science* 35 (2018), pp. 205–216.

[117] Global Energy Monitor. *Oil and gas pipeline construction costs*. May 2021. URL: https://www.gem.wiki/Oil_and_Gas_Pipeline_Construction_Costs#:~:text=A%5C%20survey%5C%20by%5C%20BTU%5C%20analytics,built%5C%20from%5C%202017%5C%20to%5C%202020..

[118] Luis Mundaca et al. "Evaluating energy efficiency policies with energy-economy models". In: *Annual review of environment and resources* LBNL-3862E (2010).

[119] Stewart C Myers. "Capital structure". In: *Journal of Economic perspectives* 15.2 (2001), pp. 81–102.

[120] Tomas Nauclér and Per-Anders Enkvist. "Pathways to a low-carbon economy: Version 2 of the global greenhouse gas abatement cost curve". In: *McKinsey & Company* 192.3 (2009).

[121] NEA. *Verdeling van heffingsplichtige inrichten per industriecluster 2019 - Nederland*. 2021. URL: https://dashboardklimaatbeleid.nl/jive?workspace_guid=9d8941f7-62e6-4041-abb2-7f5ea6d8cbcf.

[122] nea. *Emissiecijfers over 2021*. 2022. URL: https://www.emissieautoriteit.nl/onderwerpen/rapportages-en-cijfers-eu-ets/documenten/publicatie/2022/04/14/emissiecijfers-2021.

[123] Francesco Fuso Nerini, Ilkka Keppo, and Neil Strachan. "Myopic decision making in energy system decarbonisation pathways. A UK case study". In: *Energy strategy reviews* 17 (2017), pp. 19–26.

[124] Junichiro Oda et al. "Diffusion of energy efficient technologies and CO2 emission reductions in iron and steel sector". In: *Energy Economics* 29.4 (2007), pp. 868–888.

[125] Akomeno Omu, Ruchi Choudhary, and Adam Boies. "Distributed energy resource system optimisation using mixed integer linear programming". In: *Energy Policy* 61 (2013), pp. 249–266.

[126] Scott E Page. "Agent-based models". In: *The new Palgrave dictionary of economics* 1 (2008), p. 8.

[127] Francesca Palazzi et al. *Osmose-User Manual version 2.0*. Tech. rep. Laboratoire d'Energétique Industrielle (LENI-EPFL), 2010.

[128] Argyris Panagopoulos, Katherine-Joanne Haralambous, and Maria Loizidou. "Desalination brine disposal methods and treatment technologies-A review". In: *Science of the Total Environment* 693 (2019), p. 133545.

[129] *Paris Agreement*. UNTC XXVII 7.d. 2015.

[130] PBL. *Decarbonisation options for the industry cluster Botlek/Pernis Rotterdam*. Aug. 2022.

[131] PBL. *Financiering van Energietransitie Versnellen en Opschalen*. 2020. URL: https://www.tno.nl/nl/aandachtsgebieden/energietransitie/roadmaps/systeemtransitie/de-sociale-aspecten-van-de-energietransitie/financiering-van-de-energietransitie/.

[132] PBL. *Investeringen Energietransitie en financierbaarheid*. May 2017. URL: https://www.pbl.nl/publicaties/investeringen-energietransitie-en-financierbaarheid.

[133] PBL. *The database - manufacturing industry Decarbonisation Data Exchange Network*. 2022. URL: https://www.pbl.nl/en/middenweb/the-database.

[134] PBL and TNO. *Manufacturing Industry Decarbonisation Data Exchange Network - PBL.NL*. 2021. URL: https://www.pbl.nl/sites/default/files/downloads/pbl-2021-manufacturing-industry-decarbonisation-data-exchange-network-the-database-4841.pdf.

[135] PlasticsEurope. *ISOPA Eco Profile*. 2012. URL: https://www.isopa.org/media/1101/isopa-eco-profile-mdi-tdi-2012-04.pdf.

[136] PlasticsofEurope. *Process Data set: Methylenediphenyl diisocyanate ((p)MDI*. 2010. URL: https://plasticseurope.lca-data.com/datasetdetail/process.xhtml?lang=en&uuid=d7679212-da86-4656-b9d7-24423e64a68d&version=00.00.000#:~:text=The%5C%20production%5C%20of%5C%20MDI%5C%20involves,of%5C%20a%5C%20hydrochloric%5C%20acid%5C%20catalyst..

[137] Michael G Pollitt and Irina Shaorshadze. "The role of behavioural economics in energy and climate policy". In: *Handbook on energy and climate change*. Edward Elgar Publishing, 2013.

[138] Kris Poncelet et al. "Myopic optimization models for simulation of investment decisions in the electric power sector". In: *2016 13th International Conference on the European Energy Market (EEM)*. IEEE. 2016, pp. 1–9.

[139] PoR. *Flood Risk Management*. 2017. URL: https://www.portofrotterdam.com/en/building-port/safe-port/flood-risk-management.

[140] Ulrich Poth. "Drying oils and related products". In: *Ullmann's Encyclopedia of Industrial Chemistry* (2000).

[141] Xavier Ragot. "Heterogeneous agents in the macroeconomy: reduced-heterogeneity representations". In: *Handbook of Computational Economics* 4 (2018), pp. 215–253.

[142] Karthik Rajendran et al. "Impacts of retrofitting analysis on first generation ethanol production: process design and techno-economics". In: *Bioprocess and biosystems engineering* 38.2 (2015), pp. 389–397.

[143] MH Ross et al. *Long-term industrial energy forecasting (LIEF) model (18-sector version)*. Tech. rep. Argonne National Lab., IL (United States), 1993.

[144] Port of Rotterdam. *Grootste Nederlandse project voor CO2-reductie, Porthos, ligt op schema*. 2021. URL: https://www.portofrotterdam.com/nl/nieuws-en-persberichten/grootste-nederlandse-project-voor-co2-reductie-porthos-ligt-op-schema.

[145] Port of Rotterdam. *Voortgangsrapportage herijkte havenvisie*. 2020.

[146] SA. *Liquid alkaline electrolysis techno-economic review - energy*. 2021. URL: https://www.energy.gov/sites/default/files/2022-02/7-TEA-Liquid%5C%20Alkaline%5C%20Workshop.pdf.

[147] Julia Sachs et al. "An agent-based model for energy investment decisions in the residential sector". In: *Energy* 172 (2019), pp. 752–768.

[148] Karolina Safarzyńska and Jeroen CJM van den Bergh. "An evolutionary model of energy transitions with interactive innovation-selection dynamics". In: *Journal of Evolutionary Economics* 23.2 (2013), pp. 271–293.

[149] Yasin Sagdur. "A proof of concept for simulating long-term energy system development in a myopic investment detailed operational model". PhD thesis. 2021.

[150] Olivier Sassi et al. "IMACLIM-R: a modelling framework to simulate sustainable development pathways". In: *International Journal of Global Environmental Issues* 10.1-2 (2010), pp. 5–24.

[151] Edzard Scherpbier. "The energy transition in the Dutch chemical industry – Worth its salt?" 2018.

[152] Edzard Scherpbier and H Eerens. *Decarbonisation options for the Dutch Chlor-Alkali Industry*. 2021.

[153] H Schweiger, C Brunner, and A Bertrand. "Guide for EINSTEIN thermal energy audits". In: *Barcelona, Spain* (2012).

[154] V P Semeijn and K M Schure. *Decarbonisation options for the Dutch PVC industry*. 2020.

[155] Frank Sensfuß and Mario Ragwitz. "An agent-based simulation platform as support tool for the analysis of the interactions of renewable electricity generation with the electricity and CO2 market". In: *New methods for energy market modelling* (2008), p. 63.

[156] Keefe Environmental Service. *1,4-dioxane remedial alternative evaluation - semspub.epa.gov*. 2004. URL: https://semspub.epa.gov/work/01/232799.pdf.

[157] Jason F Shogren and Laura O Taylor. "On behavioral-environmental economics". In: *Review of Environmental Economics and Policy* (2020).

[158] Herbert A Simon. "Bounded rationality". In: *Utility and probability*. Springer, 1990, pp. 15–18.

[159] Steve Sorrell, Alexandra Mallett, and Sheridan Nye. *Barriers to industrial energy efficiency: A literature review*. United Nations Industrial Development Organization (UNIDO), 2011.

[160] Meir Statman and James F Sepe. "Managerial incentive plans and the use of the payback method". In: *Journal of Business Finance & Accounting* 11.1 (1984), pp. 61–65.

[161] Rob Stikkelman. *TB341E Procesoptimalisatie*. 2022.

[162] Sunsirs. *China commodity spot price provided by SunSirs, China Commodity Data Group*. 2022. URL: http://www.sunsirs.com/commodity-price.html.

[163] Ronald J Sutherland. "Market barriers to energy-efficiency investments". In: *The Energy Journal* 12.3 (1991).

[164] Hadrien Szigeti et al. "STEEP analysis as a tool for building technology roadmaps". In: *Proceedings of the Conference: eChallenges e-2011, Florence, Italy*. Vol. 28. 2011.

[165] Ben H Thacker et al. "Concepts of model verification and validation". In: (2004).

[166] LECOMTE Thierry et al. "Best Available Techniques (BAT) Reference Document for Large Combustion Plants. Industrial Emissions Directive 2010/75/EU (Integrated Pollution Prevention and Control)". In: (2017).

[167] David Thorpe et al. *Why the UK green deal failed*. Apr. 2016. URL: https://energypost.eu/uk-green-deal-failed-needs-replacement/.

[168] Jonas Timmerman, Lieven Vandevelde, and Greet Van Eetvelde. "Towards low carbon business park energy systems: Classification of techno-economic energy models". In: *Energy* 75 (2014), pp. 68–80.

[169] TNO. *Een chloorbalans voor Nederland*. 1995.

[170] Kenneth Train. "Discount rates in consumers' energy-related decisions: a review of the literature". In: *Energy* 10.12 (1985), pp. 1243–1253.

[171] Andrea Trianni and Enrico Cagno. "Dealing with barriers to energy efficiency and SMEs: Some empirical evidences". In: *Energy* 37.1 (2012), pp. 494–504.

[172] Evelina Trutnevyte. "Does cost optimization approximate the real-world energy transition?" In: *Energy* 106 (2016), pp. 182–193.

[173] KC Tseng. "Behavioral finance, bounded rationality, neuro-finance, and traditional finance". In: *Investment Management and Financial Innovations* 3, Iss. 4 (2006), pp. 7–18.

[174] UNEP. *Conversion from Mercury to alternative technology in the chlor-alkali ...* 2012. URL: https://www.worldchlorine.org/wp-content/uploads/2015/08/Partnership-Document-on-the-Conversion-from-Mercury-to-Alternative-Technology-in-the-Chlor-Alkali-Industry.pdf.

[175] unfccc. *Climate Tops 2022 WEF Global Risks Report*. 2022. URL: https://unfccc.int/news/climate-tops-2022-wef-global-risks-report.

[176] Jeroen Vetter. *A Safer route to MDI*. 2010.

[177] Agnes Virlics. "Investment decision making and risk". In: *Procedia Economics and Finance* 6 (2013), pp. 169–177.

[178] J Voerman. *Inventarisatie en vergelijking jaaremissies*. 2020.

[179] Alexey Voinov and Francois Bousquet. "Modelling with stakeholders". In: *Environmental modelling & software* 25.11 (2010), pp. 1268–1281.

[180] Detlef P van Vuuren et al. *Wat betekent het Parijsakkoord voor het Nederlandse langetermijn-klimaatbeleid*. Planbureau voor de Leefomgeving, 2016.

[181] water-mining. *About Us*. June 2022. URL: https://watermining.eu/.

[182] F G.H Wees and W G van Arkel. *Terugblik op 8 Jaar Grijze Data-ontsluiting - PDF free download*. 1998. URL: https://adoc.pub/terugblik-op-8-jaar-grijze-data-ontsluiting.html.

[183] WEF. *Global risks report 2022*. 2022. URL: https://www.weforum.org/reports/global-risks-report-2022.

[184] Tobias Wittmann, Robbie Ian Morrison, and Thomas Bruckner. "A bounded rationality model of private energy investment decisions". In: *Available at SSRN 922020* (2006).

[185] Julie Young. *Metrics-what they are, how they're used*. July 2022. URL: https://www.investopedia.com/terms/m/metrics.asp.

A

NPV calculation PoR chlorine cluster as a case

In table A.1, the data that is used to calculate the cost savings of the E-boiler compared to the natural gas boiler at Westlake. In total this would lead to a total cost savings of 112 million euros over the 15 year life time. The NPV formula, shown in A.1 was used to calculate the NPV of both the investment options.

$$NPV = \sum_{i=1}^{n} \frac{Cash\ Flow_i}{(1+r)^i} - Initial\ Investment$$

Figure A.1: NPV-formula

Table A.1: Data used for NPV calculation

Variable	Natural gas boiler	E-boiler
CAPEX [MEUR]	16.3	15
ELT [Year]	15	15
Efficiency [%]	69	99
Electricity price [EUR\MWh]	-	7.3
Gas price [EUR/GJ]	14.6	-
Yearly energy use	2700000 [GJ/year]	525.6 GWh/year
Yearly energy costs	39.42 MEUR/year	38.3 MEUR/year
CO2 costs	50 euro/ton	-
Yearly CO2 payments	7.56 MEUR/year	-
Discount rate	0.03	0.03

B

Overview of asset sets and individual assets

This appendix gives an overview of all the asset sets and individual assets that are considered in this thesis

Asset list Nobian					
Heat	**Electrolysis**	**Recirculation N&W**		**Vaporisation**	**CCS**
CHP	Standard membrane	No recirculation		Multiple effect (3) vaporisation	No CCS
E-Boiler	Zero gap membrane	Brine recirculation		Multiple effect (5) vaporisation	CCS
Biomass-Boiler				Vaporisation with MVR	
Asset list Shin-Etsu					
Heat					**CCS**
Natural gas furnace EDC cracking					No CCS
Hydrogen furnace EDC cracking					CCS
E-furnace EDC cracking					
Asset list Westlake					
Heat		**Recirculation N&W**			**CCS**
Natural gas steam boiler		No recirculation			No CCS
E-boiler steam		Brine recirculation			CCS
Asset list Huntsman					
Heat					**CCS**
Natural gas steam boiler					No CCS
E-boiler steam					CCS

Individual assets Nobian					
Heat	**Electrolysis**	**Recirculation N&W**		**Vaporisation**	**CCS**
CHP_1	Standard membrane_1	No recirculation		Multiple effect (3) vaporisation_1	No CCS
CHP_2	Standard membrane_2	N&W Brine recirculation_1		Multiple effect (3) vaporisation_2	CCS_1
	Standard membrane_3			Multiple effect (5) vaporisation_1	
E-Boiler_1	Standard membrane_4			Multiple effect (5) vaporisation_2	
E-Boiler_2	Standard membrane_5				
Biomass-Boiler_1	Standard membrane_6				
Biomass-Boiler_2	Standard membrane_7				
Biomass-Boiler_3	Zero gap membrane_1				
Biomass-Boiler_4	Zero gap membrane_2				
	Zero gap membrane_3				
	Zero gap membrane_4				
	Zero gap membrane_5				
	Zero gap membrane_6				
Individual assets Shin-Etsu					
Heat					**CCS**
Natural gas furnace EDC cracking_1					No CCS
Natural gas furnace EDC cracking_2					CCS_1
Hydrogen furnace EDC cracking_1					
E-furnace EDC cracking_1					
Individual assets Westlake					
Heat		**Recirculation N&W**			**CCS**
Natural gas steam boiler_1		No recirculation			No CCS
Natural gas steam boiler_2		N&W Brine recirculation_1			CCS_1
Natural gas steam boiler_3					
E-boiler steam_1					
E-boiler steam_2					
Individual assets Huntsman					
Heat					**CCS**
Natural gas steam boiler_1					No CCS
Natural gas steam boiler_2					CCS_1
Natural gas steam boiler_3					
E-boiler steam_1					
E-boiler steam_2					

C

Expert elicitation

C.1. Nobian

On the 11th of july 2022, an interview was held with the progam lead renewable & circular and open innovation at Nobian. He mainly focuses on three key areas, being CO2 capture use, Energy storage (incl batteries) and Circular Economy (incl recycling of salty waste streams). Managing portfolio, initiating new projects, developing business cases and models and leading projects. All of his projects are done in close collaboration with external parties, a lot of which are start-ups. Hence the focus on Open Innovation. For Open Innovation, he is developing a strategy, defining company challenges and collaborating with solvers.

C.1.1. Interview questions and answers

1. *What are barriers to investment that you encounter?*

   The main barrier we currently have, is to find economically viable decarbonisation alternatives for our production processes. The large upfront capital investment costs and uncertainty about energy prices & government policy makes it difficult to find viable alternatives. I do recognize the barriers you mention, like imperfect information, hidden costs, etc. However, we do not see them as major barriers at this moment.

2. How do you make investment decisions?

   (a) *What does the decision making process look like*
   At Nobian we use a investment process called front end loading (FEL). The FEL process is a method is used for conceptual development of projects in industries such as upstream oil and gas, petrochemical And pharmaceuticals. It is a flexible method that works as a sort of filter for the selection of projects. With this process we can early on identify if the investment project is to be considered in more detail. That is the process where more the technical aspects are considered.

   (b) *What kind of evaluation metrics do you use?*
   We currently use two evaluation metrics, which are pay-back period and internal rate of return (IRR). For an investment to be accepted the payback period has to be 3 years and IRR value 30%. Allthough these values are not hard decision values. Depending on the situation we might variate a bit from these values.

   (c) *What is your budget for CAPEX investments per year?*
   I am sorry, I cannot disclose that to you. You could try to get it from our decarbonisation outlook for 2040. Or look at the financial reports of Nobian.

   (d) *What are the role of models for your investments decision making process?*
   Models play a central role in our decision making process and are taken very seriously. For

every investment we consider a model study is performed. The eventual decisions are strongly influenced by the values obtained from the investment models.

3. *What are your decarbonisation alternatives*
   We search for alternatives via analyzing our technical systems, imitating competitors and attaining alternatives via startups and universities. I have not looked specifically at the MIDDEN-database. But the alternatives you mention like the electrification of our energy supply and energy efficiency alternatives are certainly considered.

4. *How do you cooperate with other companies?*
   We currently work together with competitors and cluster neighbours via consortia. When it comes to the cost division, that is a long negotiating process. Especially because of information asymmetry between mutually dependent plants.

   (a) *What does the process look like?* When we or others see opportunities for cooperation, a cooperation is initiated. Afterwards multiple rounds of negotiating and conceptualising starts.

   (b) *How do you allocate costs?* That is very dependent on the type of project and business case. We allocate the costs by comparing the relative benefits per cooperating company.

C.1.2. Key-Takeaways Nobian interview

This subsection describes the key-take ways regarding sub questions one and two. In the first subsection, the key takeaways regarding the decision evaluation metrics are given. The second subsection, describes the key takeaways of the plant-process-product inventarisation and zero-emission evaluation alternatives.

Decision evaluation metrics

Nobian's expert mentioned that Nobian conducts the decision making process, following the FEL method. Furthermore, he mentioned that he recognizes the market & behavioural barriers, but does not take them into account in his investment models. Lastly, Nobian uses either a pay-back period of three years or a IRR of 30% as acceptance criteria.

The plant-product-process and zero-emission evaluation alternatives

Regarding a validation of the plant-process-product inventarisation, additional mail-contact was required. He later on sended an overview of the brine recirculation project between Nobian and Westlake. This was used to validate the earlier found specifications for both the Nobian and Westlake plants. Regarding the zero-emission evaluation alternatives, the expert referred to the Nobian sustainability approach: Carbon neutral by 2040. This document describes an outlook for the decarbonisation of Nobian by 2040, including the proposed zero emission technology alternatives.

C.2. Westlake

For this expert elicitation, we were able to speak with the process technology director at Westlake. The process technology director is closely involved with the current production operations at Westlake. He also is closely involved with the investment decision making investment process at Westlake, where also decarbonisation alternatives are assessed.

C.2.1. Interview questions and answers

1. *What are barriers to investment that you encounter?*
   The main barriers that we perceive are based on access of capital and uncertainty. Because we have a limited amount of capital to spend on capital investments, the projects with the highest rate of return are prioritised. A lot of the time, the decarbonisation alternatives turn out to not make the cut because the ROI is not high enough. Furthermore, the high uncertainty related to our operations and investment makes it difficult for us to make large capital investments like e-boilers etc. Uncertainty that is mostly related to the price development of electricity, because electrification is our most probable decarbonisation alternative. Also, how is the relative attractability of decarbonisation options going to be affected by CO_2 pricing. We have got a bit more certainty with the new Dutch emission tax for the industry, but we still regard policy measures to be uncertain.

   Regarding the barriers you mention like imperfect information and hidden costs, we don't really see them as large barriers. I have not experienced projects where either the efficiency gains were much lower than expected or that the OPEX costs were significantly higher than expected. It probably happens, but we don't take it into account during our investment process.

   Split incentives plays a large role in potential cooperative investment projects. When the incentives are to far apart from two companies we will not engage in a cooperation. It might occur that we have missed possibly attractive projects because of that. But it is rather an exception than rule.

2. How do you make investment decisions?

   (a) *What does the decision making process look like*
   We start of with our main strategy, which is largely profit driven. Besides that we also have a sustainability strategy, which is a starting point for decarbonisation investments. We make our investments during the engineering phase, when the capital expenses are clear and the benefits aswell.

   (b) *What kind of evaluation metrics do you use?*
   We make our investments based on an IRR and pay-back period. I cannot disclose to you which specific values that are, but they are comparable to other companies in our industry. .

   (c) *What is your budget for CAPEX investments per year?*
   I cannot disclose that to you. You might look at out financial reports and retract a value from there.

   (d) *What are the role of models for your investments decision making process?*
   Models are crucial in our decision making process. Every significant investment decision is backed up with a model study. Especially sensitivity is important to us, that plays a large role in the larger projects.

3. *What are your decarbonisation alternatives*
   We focus on the lowering of energy use, efficiency alternatives and energy source replacement. Also in that order, as in the past we have seen that these options are the most likely to be successful.

   But the largest gain can be made by dismantling our gas boilers. We currently receive refinery gas from Shell, which is a rest product of their production process. It is a mixture of hydrocarbons and a bit of hydrogen. The refinery gas that we burn in our boilers directly contributes to our scope 1 emissions. So replacing that with a sustainable energy source would be a large step in the good direction.

4. *What is the price paid for brine water treatment*
   I cannot disclose the specific price we pay for our brine waste water treatment at Shell. However, the prices are relatively comparable to common prices for general waste water treatment.

5. *How do you cooperate with other companies?*
   Our main strategy is to come to a total net plus for both companies. This is a long and difficult process, especially because of we don't want to share important corporate sensitive information with our competitors. For example the brine re circulation project with Nobian is not so much about that we don't think the project is not going to be profitable, but takes a long time to find common ground during cooperative investment projects.

C.2.2. Key takeaways Westlake interview

Decision evaluation metrics

Regarding the decision evaluation metrics, the key take aways are based on the perception of Westlake regarding the barriers in general and the values that they use for their decision acceptance. The expert at Westlake states that the most important barriers to him are risk due to uncertainty, access to capital and to some degree split incentives. The other barriers are not considered to be large barriers to zero technology adoption. Next, the expert stated that Westlake uses comparable decision acceptance criteria as other companies within their sector. So, an IRR of 30% and/or pay back period of 3 years is close.

The plant-process-product inventarisation and zero-emission technologies

Some additions were made to the model regarding the used refinery gas from Shell. Earlier it was assumed that the boilers at Westlake operated on natural gas. Now the Linny-R model has included refinery gas from shell as the fuel used in their steam boilers. Next, the zero-emission technologies align with what is modeled. The expert stated that the largest gain could be made by installing a e-boiler at Westlake. Also the brine recirculation project was mentioned as an alternative to the current waste water treatment at Shell.

C.3. Project manager MIDDEN database - PBL

The project manager of the MIDDEN database was contacted to attain additional information about technology alternatives. He is one of the main contributors to the MIDDEN project provided additional information about zero-emission technologies for Westlake and Huntsman. He mentioned that Westlake can implement an E-boiler to replace their natural gas boiler. As for Huntsman, all though they do not emit a lot of CO_2 directly they could install an E-boiler. Huntsman currently receives it's heat from the chlorine cluster's steam distribution network. Huntsman could locally install an E-boiler to suffice it's own steam demand and could so decarbonize it's steam use.

D

Scenario analysis configurations

D.1. Scenario 1: High priority at unfavourable circumstances

Decision evalution type	Paremeter configuration	Price scenario
Risk	Risk	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High
Imperfection	Risk Imperfect info	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High
Hidden costs	Risk Imperfect info Hidden costs	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High
Access to capital	Risk Imperfect info Access to capital	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High
Market barriers	Risk Imperfect info Hidden costs Access to capital	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High
Satisficing	Risk Imperfect info Hidden costs Access to capital Pay back period: 3 years Tech pref	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High
Behavioural	Risk Imperfect info Hidden costs Access to capital Pay back period: 3 years Tech pref Cooperation	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High

D.2. Scenario 2: Slow decarbonisation

Decision evalution type	Paremeter configuration	Price scenario
Risk	Risk	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low
Imperfection	Risk Imperfect info	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low
Hidden costs	Risk Imperfect info Hidden costs	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low
Access to capital	Risk Imperfect info Access to capital	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low
Market barriers	Risk Imperfect info Hidden costs Access to capital	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low
Satisficing	Risk Imperfect info Hidden costs Access to capital Pay back period: 3 years Tech pref	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low
Behavioural	Risk Imperfect info Hidden costs Access to capital Pay back period: 3 years Tech pref Cooperation	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low

D.3. Scenario 3: High priority and favourable circumstances

Decision evalution type	Paremeter configuration	Price scenario
Risk	Risk	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High
Imperfection	Risk Imperfect info	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High
Hidden costs	Risk Imperfect info Hidden costs	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High
Access to capital	Risk Imperfect info Access to capital	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High
Market barriers	Risk Imperfect info Hidden costs Access to capital	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High
Satisficing	Risk Imperfect info Hidden costs Access to capital Pay back period: 3 years Tech pref	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High
Behavioural	Risk Imperfect info Hidden costs Access to capital Pay back period: 3 years Tech pref Cooperation	Electricity_Low Hydrogen_Low Biomass_Low Gas_High Commodity_High CO2_High

D.4. Scenario 4: Slow decarbonisation with barriers

Give the industry more incentives	Paremeter configuration	Price scenario
Risk	Risk	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low
Imperfection	Risk Imperfect info	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low
Hidden costs	Risk Imperfect info Hidden costs	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low
Access to capital	Risk Imperfect info Access to capital	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low
Market barriers	Risk Imperfect info Hidden costs Access to capital	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low
Satisficing	Risk Imperfect info Hidden costs Access to capital Pay back period: 3 years Tech pref	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low
Behavioural	Risk Imperfect info Hidden costs Access to capital Pay back period: 3 years Tech pref Cooperation	Electricity_High Hydrogen_High Biomass_High Gas_Low Commodity_Low CO2_Low

E

STEEP analysis

Society and the PoR chlorine cluster

For this aspect, the history of the chlorine cluster, it's relation to society is explained and how it is still affecting society today. From that analysis the most uncertain and highly impactful drivers are identified. The PoR chlorine cluster is largely situated at the Botlek area, apart from Westlake and PVC production plant of Shin-etsu who are place in Pernis. The first plans for the industrialisation of the Botlek were drawn up in 1947 after the American DoW Chemical and shipbuilder Cornelis Verolme decided to settle their operations in the Botlek area. Almost fifteen years later, the chlorine cluster started to take form when in 1961 AkzoNobel (now Nobian) opened an electrolysis plant in the Botlek area. This plant would eventually form the heart of the chlorine cluster in the port of Rotterdam and by the 1970s Akzonobel was the largest producer of chlorine in the Netherlands. Where the Akzo transported around 300 kton of chlorine every year [35]. Not much later the rest of the chlorine cluster's plants were established, which changed ownership various times over the last fifty years. As of late in the beginning of 2022, Westlake bought the Hexion epoxy manufacturing plant. The chlorine cluster plays a sizeable role for local society as it employs approximately 1,000 people [133]. For this part no drivers were found that influence the technology adoption at the PoR chlorine cluster.

Technical developments and the Chemical industry

As of late, a large amount of technologies have become viable alternatives to the current configuration of the cluster. The zero-emission technology inventarisation has given a large set of options for the achievement of higher efficiency, circularity or substitution of fuel.

Substitution of fuel
Electricity, steam and heat generation are the core source of CO_2 emissions at the chlorine cluster.

Efficiency and electrification
Also the increased efficiency and electrification of production processes are promising technical developments for the chlorine cluster.

In 2005, the zero gap electrolyzer 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, but due to the high investment costs, chlorine producing plants that had switched to the conventional membrane electrolysis before 2005 are struggling to catch up [151]. 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 . 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[151]. 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 [151].

Circularity and recycling
Lastly, there are developments in the increased use of circularity among cluster players. The hydrogen that is generated from at Nobian's production process is sold within the cluster 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 [151]. Nobianaims 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.

These developments have a high impact on the ability for the decarbonisation of the cluster. However, it is somewhat uncertain what the future technological developments will bring and even what the future prices will be. What we do know is that the price of technology will go down over time, with the progression of it's technology readiness level [20]. Therefore, two drivers were identified related to technological developments in the chemical sector:

- Future technical developments
- Future technology prices

Economic

The costs side of a chemical manufacturing plant is mostly energy- and commodity dependent. According to Scherpbier [151], around 41% of the total production costs is spend on energy needs. So, both the energy and commodity prices have a large impact on the total financial costs. Besides, as earlier mentioned both of these factors are highly uncertainty.

Next, the level of cooperation is an important factor when it comes to alternatives where multiple companies are involved. This was also mentioned by the experts from Westlake and Nobian. They stated that if not all the contributing companies are dedicated to cooperate, no cooperation will be achieved. Therefore the key drivers are:

- Energy prices
- Commodity prices
- Level of cooperation

Environment

More and more environmental organizations developed increasing concerns regarding chlorine transportation via railway to neighboring countries in the 1990s. This resulted in a significant switch in public opinion regarding chlorine transport [35]. This shift in public opinion lead to tighter regulation on chlorine production and transport. This eventually lead to many Dutch chlorine plants being closed. The Solvay Chemie closed in 199 and Akzonobel's other facilities in Hengelo and Delfzijl closed in 2002. Currently, almost all of the chlorine that is produced is shared with companies within the chlorine cluster. The other plants did not suffer such public denouncement and therefore were less affected by societal pressure. Also because the products produced at the other plants are less hazardous to transport.

Besides environmental societal pressure as an impactful driver, natural disasters might prove to be a factor to consider. With rising sea levels, the PoR becomes more prone to flooding. This is also realised by the PoR company [139]. They state that the risk of flooding will rise in the PoR and surrounding areas over the coming decades as a result of climate change. Particularly the sea level rise poses a threat to the PoR. According to current climate models, a sea level rise of between 35 cm and 85 cm is expected by the end of this century [139]. Although this can be impactful for the PoR, it is not so much an uncertain driver. This is an expected development in the coming decades and can be anticipated upon. Therefore we both deem societal pressure as natural disasters in the form of sea level rise, not key drivers.

- Societal pressure
- Natural disasters

Political

Despite the fact that chlorine trains were largely banned in the Netherlands as of 2006, Nobian and the Dutch government signed a covenant in which it was determined that incidental transport for the maintenance of factories would still be possible [151]. Nobian 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 [151]. If Nobian were allowed to store chlorine on its chlor-alkali plant site, it could build up reserves to reduce the dependence of transports from Germany.

As earlier mentioned by both the experts from Nobian and Westlake, political policy strongly influences the attractiveness of sustainable technology adoption. They both mentioned that the current EU ETS + Dutch emission tax for the industrial sector are a giving them more incentives to decarbonise. However, they perceive the development of the pricing as very uncertain. The combination of these policy mechanisms being very impactful and uncertain makes this a key driver.

- Uncertainty of governmental policy

To conclude, all of the drivers have been placed in the uncertainty X impact matrix which resulted in three key drivers. See the top right square for the identified key drivers.

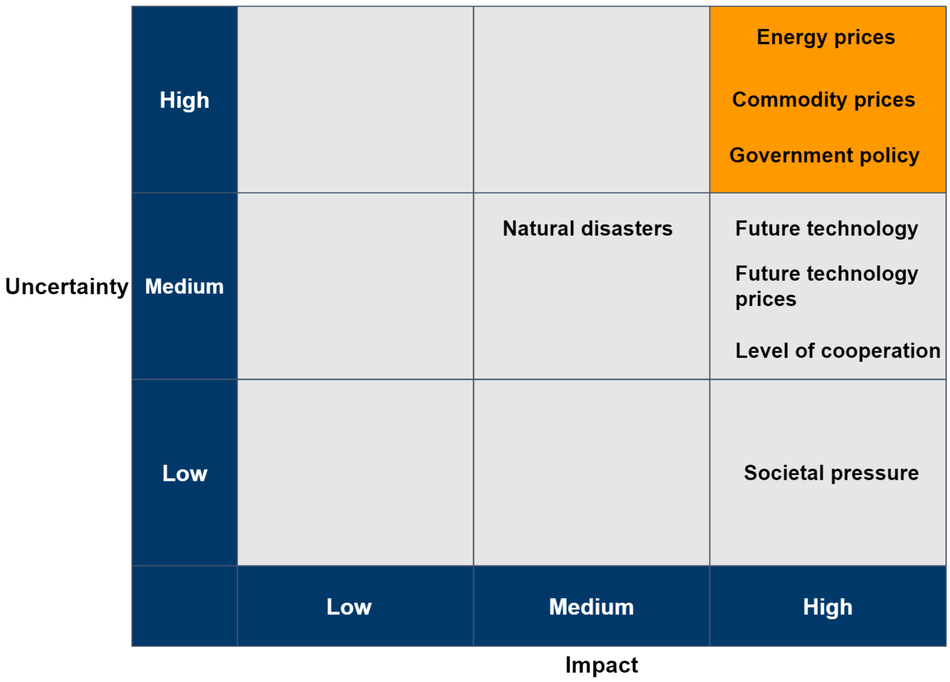

Figure E.1: STEEP analysis Key drivers

F

Model input data and Results

This appendix is dedicated to the model input data for the model validation & results.

Model validation input data

Table F.1: Input data model validation test 1

Parameter	Value	Unit
Electricity price	8194	EUR/TJ
Natural gas price	2490	EUR/TJ
Biomass price	21600	EUR/TJ
Hydrogen price	20000000	EUR/Kton
CO_2 price	83190	EUR/Kton
CAPEX, OPEX and ELT	See table 3.29	-
Block length	28	Year
Look-ahead	28	Year

Table F.2: Input data model validation test 2

Parameter	Value	Unit
Electricity price	0	EUR/TJ
Natural gas price	$2 * 10^{10}$	EUR/TJ
Biomass price	0	EUR/TJ
Hydrogen price	0	EUR/Kton
CO_2 price	$2 * 10^{10}$	EUR/Kton
CAPEX, OPEX and ELT	See table 3.29	-
Block length	28	Year
Look-ahead	28	Year

Table F.3: Input data model validation test 3

Parameter	Value	Unit
Discount rate normal sustainables	0.1	[0-1]
Discount rate high sustainables	0.5	[0-1]
No Access to capital	0	EUR
Tech pref high sustainables	0.5	Rate
Tech pref normal sustainables	1	Rate
CAPEX, OPEX and ELT	See table 3.29	-
Block length	28	Year
Look-ahead	28	Year

Scenario analysis Input data & Model results

- Time series input data Linny-R
- Model results