Uncertainty analysis for industrial electrification systems

An Exploratory Modelling and Analysis (EMA) approach to mapping the effect of various uncertain factors on the performance of Power-to-X options for an integrated chemical cluster in the Port of Rotterdam

Rob Roos | MSc Thesis | Delft University of Technology | July 2020

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An Exploratory Modelling and Analysis (EMA) approach to mapping the effect of various uncertain factors on the performance of Power-to-X options for an integrated chemical cluster in the Port of Rotterdam

By

Rob Roos

In collaboration with

A thesis presented for the degree of

Master of Science

First Supervisor: Dr.ir. Rob Stikkelman
Chair & Second Supervisor: Dr.ir. Jan Kwakkel
Internship Company Supervisor: Dr.ir. Marit van Lieshout

Faculty of Technology Policy and Management
Delft University of Technology
The Netherlands
July 2020

Summary

Acknowledged by the United Nations as part of their sustainable development goals, reduction of greenhouse gas emissions is paramount in preserving our planet for future generations. Electrification in the industrial sector is considered one of the energy transition pathways that can contribute to meeting the emission reduction targets of the Paris Agreement. An important barrier that needs to be overcome in order to fully adopt its potential is uncertainty and its risk to the implementation of different electrification alternatives. The absence of information that illustrates the effect of uncertainty on the performance of these alternatives decreases the stability of business cases and hinders the decision-making process. To fill a part of this knowledge gap, this research performed a case-study revolving around a mixed integer linear programming (MILP) model of an integrated chemical cluster in the Port of Rotterdam. The following main research question was formulated:

"How does external uncertainty influence the Key Performance Indicators (KPIs) of (combinations of) alternatives that increase the decarbonization of the steam supply and the flexibility of an integrated chemical cluster in the Port of Rotterdam?"

During a study of the strategic and problem-specific objectives of the actors, two key performance indicators (KPIs) were identified: economic feasibility and decarbonization. The external uncertain factors were identified based on a literature review and by observation of uncertain modelling assumptions. For the generation of multiple plausible futures for these factors within the chosen time horizon, reference values and sampling ranges were identified (see Table 1).

Table 1: Overview of the identified uncertain factors

Uncertain factor	**Abbreviation**	**Reference Value**	**Lower Bound**	**Upper Bound**
Scaling factor day-ahead electricity price (-)	SF-DAE-P	0	0.7	1.3
Gas price in 2030 (€/Nm^3)	Gas-P-2030	0.28	0.16	0.32
CO_2 emission price in 2030 (€/ton)	CO2-P-2030	25	21	150
Hydrogen price in 2030 (€/Nm^3)	Hydro-P-2030	0.18	0.12	0.30
Cyclical frequency of NaOH 50% price (cycle/year)	CyFr-NaOH-P	0.2	0.1	0.3
Scaling factor up- and downward balancing electricity prices (-)	SF-(U/D)BE-P	0	0.7	1.3
Scaling factor electricity supply/demand on imbalance market (-)	SF-(S/D)IM	0	0.7	1.3
E-boiler CAPEX (€/MW)	Eb-CAPEX	$2*10^6$	$1.4*10^6$	$2*10^6$
E-boiler OPEX (€/MW/year)	Eb-OPEX	4000	2800	4000
Steam Pipe CAPEX (€)	SP-CAPEX	$12*10^6$	$6*10^6$	$12*10^6$

The effect of the uncertain factors on the KPIs was analyzed using an exploratory modelling and analysis (EMA) approach. In addition, a key opportunity of the MILP model was utilized by changing the objective function to look at individual and collective actor optimization perspectives. The results of a first global sensitivity analysis showed unexpected behaviour which deviated from valid expectations. Hence, the model was searched throughout and a number of problems were found. Unfortunately, not every problem could be resolved in the available time frame. This is potentially the reason why the next iteration of experiments showed similar behaviour during the global sensitivity analysis (see Figure 2).

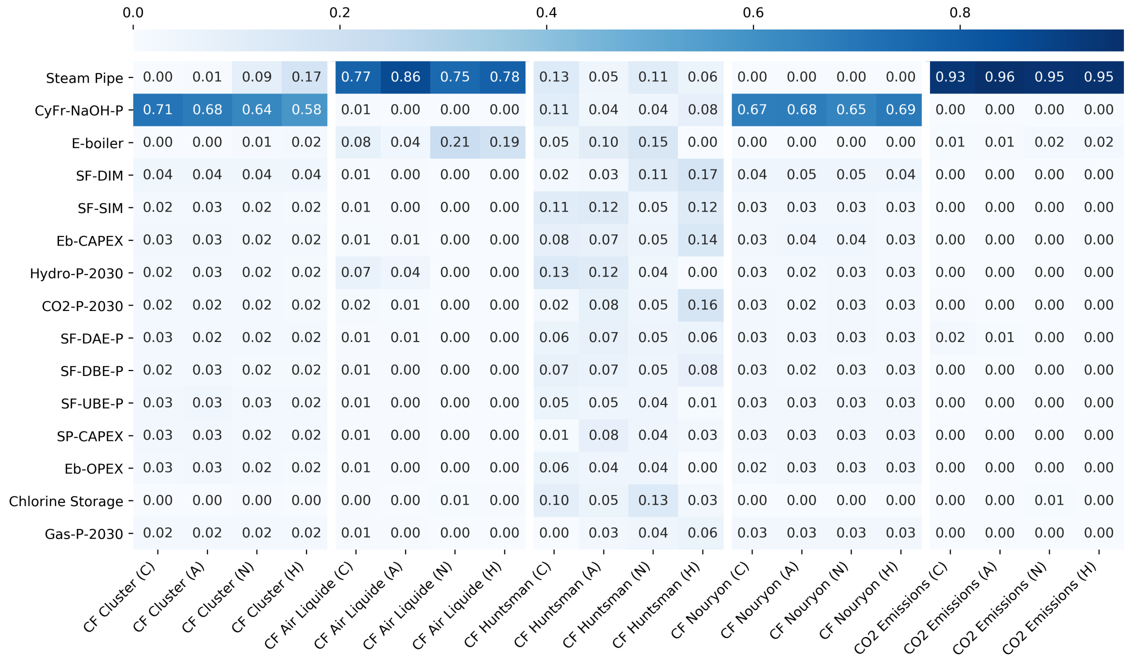

Figure 2: Results of the global sensitivity analysis

Within the uncertainty analysis, different methods were used to visualize the economic feasibility and decarbonization performance of the alternatives across the actor optimization perspectives. In addition, the trade-offs among these categories were visualized in parallel coordinate plots (see Figure 3).

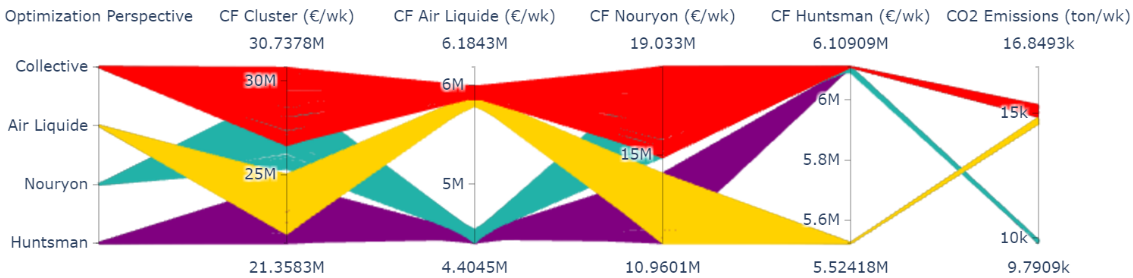

Figure 3: Trade-offs for the "Steam Pipe and E-boiler" alternative

This research implicates that EMA can be an effective approach to explore the effect of various uncertain factor on industrial systems undergoing electrification. Furthermore, when the goal is to perform a broad uncertainty analysis that allows for easy implementation of actor optimization perspectives while requiring only limited information about the uncertain factors in the form of sampling bandwidths, combining EMA and MILP might be a good idea. This depends, among other things, on the type of environment, the relative size of the feasible region and the extent to which the linear characteristics of the MILP model are able to validly represent the uncertainty of the real-world system.

Future research could focus on exploring the effect of linearity assumptions on the results of an uncertainty analysis. In addition, it would be interesting to study whether the optimization process in MILP models allows for a valid uncertainty analysis in a multi-actor environment with multiple conflicting interests.

Preface

This report is the result of my graduation internship at RoyalHaskoningDHV and it represents my thesis for the MSc Engineering and Policy Analysis at Delft University of Technology. It has been a challenging and wonderful experience.

I would like to express my deepest gratitude to my graduation committee members Rob Stikkelman and Jan Kwakkel for giving me the opportunity to perform this research. Their supervision and guidance throughout this adventure have been of great value to me.

In addition, I would like to thank my internship supervisor, Marit van Lieshout, for all the wisdom and support that she has given me. Her critical approach has helped me to stay focused and to pay attention to crucial details.

Last, but definitely not least, I would like to thank my family and friends for their constant source of inspiration and encouragement.

Rob Roos
Delft, July 2020

Contents

Abbreviations

aFRR	automatic Frequency Restoration Reserve
CAPEX	Capital Expenditure
DS	Dimensional Stacking
DSM	Demand Side Management
EACP	Economic Affairs and Climate Policy
EC	European Commission
EMA	Exploratory Modelling and Analysis
EU	European Union
ETS	Emission Trading System
GHG	Greenhouse Gas
KPI	Key Performance Indicator
LHS	Latin Hypercube Sampling
MILP	Mixed Integer Linear Programming
MOEA	Multi-Objective Evolutionary Algorithm
MORDM	Multi-Objective Robust Optimization Framework
OPEX	Operational Expenditure
PCP	Parallel Coordinate Plot
PRIM	Patient Rule Induction Method
RFD	Research Flow Diagram
RHS	Right Hand Sides
TSO	Transmission System Operator

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Awareness is the greatest agent for change.

– *Eckhart Tolle*

Chapter 1

Introduction

Global warming is becoming an increasingly relevant issue within modern society (Demeritt, 2001). Acknowledged by the United Nations as a part of their Sustainable Development goals, reduction of greenhouse gas (GHG) emissions is paramount in preserving our planet for future generations. Among their targets for 2030 are a substantial increase in the renewable energy share and a doubling of the global rate of improvement in energy efficiency (United Nations, 2019). However, studies have shown that decarbonized energy supply and technically feasible levels of energy efficiency alone are not sufficient; widespread electrification in different sectors is required (Williams, 2012).

1.1 Industrial electrification

The industry is one of the sectors where electrification is desirable, since it is responsible for a considerable part of the total GHG emissions. In 2010, the production of basic materials resulted in carbon dioxide emissions equivalent to 9% of total GHG emissions in EU28 (Lechtenböhmer et al., 2016). Therefore, the objective of the EU to reduce GHG emissions includes a suggested industry sector ambition of 83-87% reduction by 2050 relative to 1990 (European Commission, 2011). Furthermore, if the EU wants to meet the target of the Paris Agreement, this reduction needs to continue all the way down to zero emission in 2060-2070 (Åhman et al., 2017).

Electrification is considered as one possible energy transition pathway that can contribute to these targets (Deason et al., 2018). Note that electrification does not achieve neutral GHG emissions, unless the electricity comes from renewable sources. Apart from reducing emissions, electrification has many other benefits (Peng et al., 2018). For example, the implementation of flexible electrification alternatives allows for the integration of variable energy sources like wind and solar, because these alternatives are able to respond to their intermittent character of these energy sources by mitigating load imbalances on the grid (Den Ouden et al., 2017).

1.2 The knowledge gap

Studies regarding electrification in the industrial sector have identified various barriers that need to be overcome in order to fully adopt its potential (Brolin et al., 2017; Deason et al., 2018; Den Ouden et al., 2017). During a review of this literature, it was obvious that, although different approaches were used for the formulation and characterization of these barriers, they showed a considerable amount of overlap. More specifically, the notion of uncertainty seemed to be a common main barrier or a factor that caused other barriers to arise.

Within the study performed by Brolin et al. (2017), uncertainty is identified as a major barrier that is related not only to economic factors, but to technological futures as well. In addition, the lack of willingness to invest might also be explained by uncertainty, as it might hinder the stability of the business case.

In respect to the research performed by Deason et al. (2018), uncertainty is not mentioned as a main barrier. However, uncertainty can explain the fact that the price of electrified operation relative to the price of combustion fuel operation is such a critical factor for the uptake of electrical technologies. For example, the price of natural gas might drop, while the cost of electricity might rise, making the relative cost of electrified operation unfavorable. In a similar way, uncertainty can also explain the notion of risk aversion and the effect of regulation on the relative attractiveness of electric vs. direct-fuel options.

The research conducted by Den Ouden et al. (2017) in the Netherlands shows that important regulatory barriers are an absence of a long-term view and financial incentives. Furthermore, they identified organizational barriers such as a difficult internal decision-making process and a lack of resources and knowledge. Uncertainty is intertwined with all of these barriers.

The knowledge gap identified in this review is the absence of information about the effect of uncertain factors on the performance of electrification alternatives in the industry. This lack of information hinders the decision-making process, as current knowledge about the future impact of alternatives is insufficient to allow a reasonable selection among them. Furthermore, it decreases the robustness of business cases, because it is unclear which alternatives perform well over a wide range of scenarios. Filling this knowledge gap will help to overcome these problems, thereby contributing to a full adoption of the potential of electrification and an acceleration of the energy transition.

1.3 The Botlek cluster

As a means of filling a part of this knowledge gap, this research conducts a case study that revolves around an off-the-shelf Mixed Integer Linear Programming (MILP) model of an integrated chemical cluster in the Botlek area in the Port of Rotterdam. This chemical cluster mainly consists of three companies: Nouryon (former AkzoNobel), Huntsman and Air Liquide. These companies are highly dependent on one another for carrying out their production processes.

The model was developed by TU Delft researchers Rob Stikkelman and Pieter Bots as a means for the FlexNet project. Within this project, the main objective was to analyze demand and supply of flexibility in the power system of the Netherlands (Sijm et al., 2018). The model was built to simulate and financially optimize several configurations of so-called “Power-to-X” options. Power-to-X can be defined as a number of electricity conversion, energy storage, and reconversion pathways that typically use surplus electric power originating from fluctuating renewable energy sources (Vázquez et al., 2018). The “X” in the terminology can refer to different energy carriers, for example: chemicals or heat. In other words, the Power-to-X notion divides electrification into different categories.

The Power-to-X options that are present in the model are an electrical steam generator (E-boiler), an expansion of the waste heat steam infrastructure (Steam Pipe) and Demand Side Management (DSM) using chlorine storage. These options can be implemented either individually or in different combinations. Using the E-boiler as a substitute for the current fossil fuel steam generator increases the decarbonization of the steam supply. Expanding the waste heat steam infrastructure realizes the same effect. DSM constitutes of a broad set of means to affect the patterns and magnitude of end-use consumption (Lund et al., 2015). In this case, storage of chlorine is used to reschedule respective demand, thereby increasing the flexibility of the production process.

1.4 Research questions

Based on the application of the knowledge gap within the context of the Botlek cluster, this research will try to answer the following main research question:

"How does external uncertainty influence the performance of (combinations of) Power-to-X alternatives that increase the decarbonization of the steam supply and the flexibility of an integrated chemical cluster in the Port of Rotterdam?"

In order to provide a proper answer to this question and to give an indication of the required steps, it is disaggregated into several sub questions:

1. *What are the interests and responsibilities of the interconnected stakeholders?*
2. *What are the external uncertain factors in this case?*
3. *To what extent do these factors affect the performance of the alternatives?*
4. *What strategies are optimal in terms of economic feasibility and decarbonization and what strategies are robust?*
5. *What are the key trade-offs among the strategies from individual and collective points of view?*
6. *What are the practical implications of this research for combining the yet to be determined uncertainty analysis methodology and MILP models?*

The main research question and its disaggregated sub questions will provide a clear path throughout the research and writing process.

1.5 Outline

Regarding the outline of this report, chapter two addresses the methodology used to answer the research questions. Chapter three presents a theoretical framework, where key concepts are defined and relevant theories are discussed. Chapter four entails a description of the case-study model. Chapter five contains a detailed stakeholder analysis and chapter six discusses the identification of the uncertain external factors. Within chapter seven, the experimental design and the results of the uncertainty analysis are discussed. Finally, a discussion and conclusion of the results are presented in chapters eight and nine respectively.

Chapter 2

Methodology

With the research questions in mind, it is time to consider the methodology. The first section consists of a brief introduction regarding the research approach. Afterwards, a research flow diagram is presented to illustrate the different steps of this research. In the final section, the research methods used in each step are discussed.

2.1 Research approach

To answer the main part of the research questions, a methodology called Exploratory Modeling and Analysis (EMA) is used. This methodology uses computational experiments to analyze complex and uncertain systems (Bankes, 1993). Therefore, it can be used as computational support for robust decision making under deep uncertainty.

More specifically, the case study model of the integrated chemical cluster is to be connected to an exploratory modelling package in Python called the "EMA Workbench". By means of this tool, a thorough analysis is performed that will contribute to understanding how regions in the uncertainty space map to the whole outcome space, or partitions thereof (Kwakkel, 2019).

The Workbench offers two approaches to investigate this mapping. The first approach is called 'open exploration', which uses systematic sampling through the uncertainty space. The second approach, often referred to as 'directed search', searches through the space in a directed manner by using some type of optimization method. By conducting this latter approach, best- and worst-case scenarios can be identified (Kwakkel, 2019). The intended result is able to contribute to the stability of electrification business cases in the industry, thereby enabling an acceleration of the energy transition.

2.2 Research flow diagram

In order to illustrate the design and the different steps of this research, a Research Flow Diagram (RFD) has been developed (see Figure 2.1). Within this diagram, the process is broken down into seven steps. Each step represents a specific chapter of this report and potentially answers certain research questions. Furthermore, each step consists of an input, a process and an output. Within each process, a specific research method is used in order to convert the input to the desired output. The underlying idea of this diagram is that it can structure and sharpen the project by getting a grip on the required research activities. In addition, it provides a useful overview of the backbone of the project during its execution.

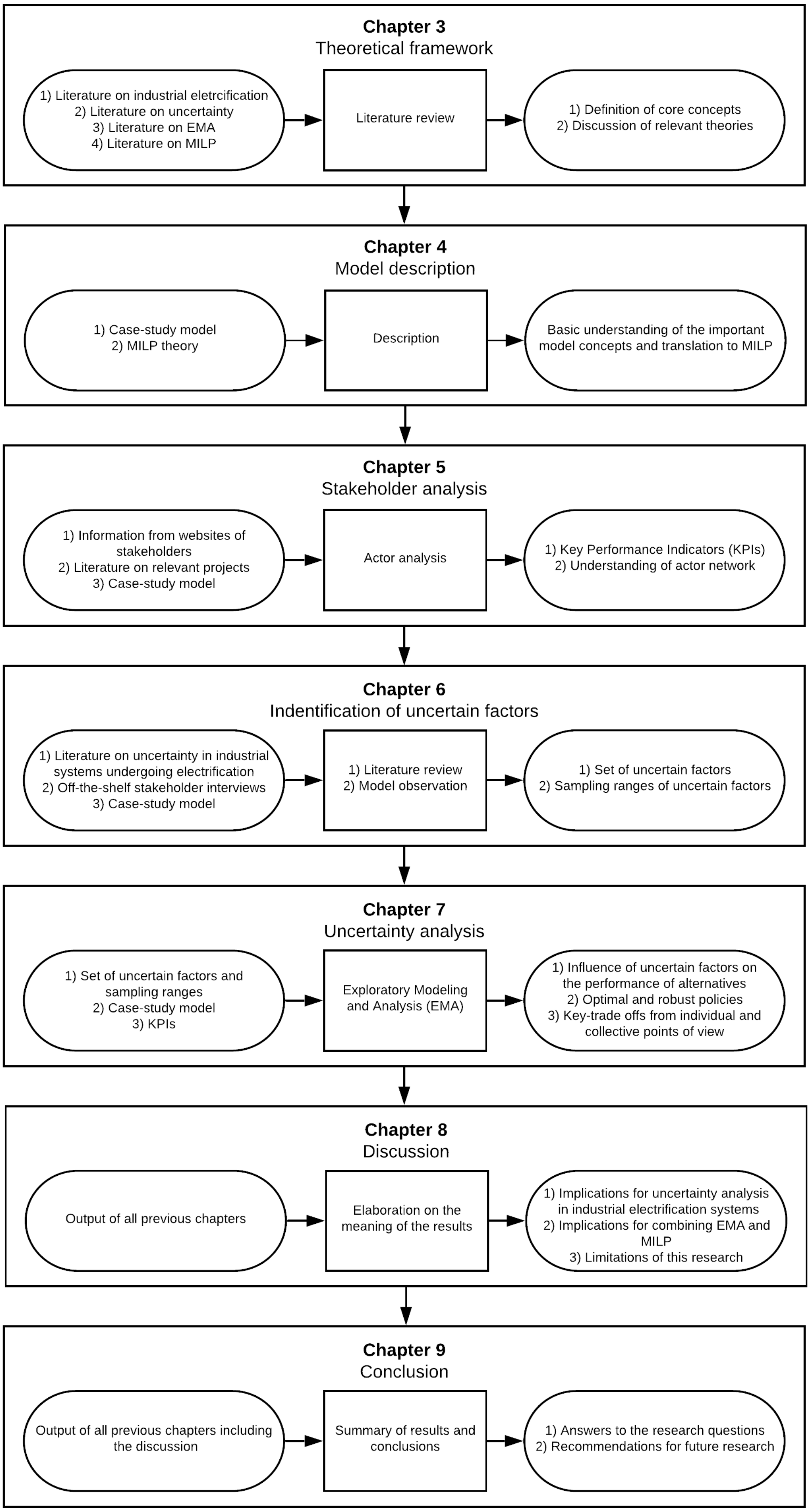


Figure 2.1: Research Flow Diagram

2.3 Research steps

The objective of this section is to explain the reasons for including each of the different steps in Figure 2.1 and to discuss their execution in more detail. To begin with, the theoretical framework is used to create a solid foundation of in terms of the theory required to perform and understand the rest of the steps. It is based on an extensive literature review, where the following sources are used: Scopus, ScienceDirect and Google Scholar. Furthermore, this literature review revolves around four main topics: industrial electrification, uncertainty, EMA and MILP. For each of these topics, various specific keywords are used to find the required literature.

In order to understand the decisions made within the subsequent research steps, it is crucial to create a basic understanding of the case-study model. Hence, the fourth chapter contains a description of the model to get a feel for its complexity, structure and how its different properties translate to MILP theory.

The stakeholder analysis is performed to identify the interests of the actors and thereby the Key Performance Indicators (KPIs) of the Power-to-X alternatives. This information will be used during the uncertainty analysis. In addition, this step is used to increase the understanding of the actor network by observing the interconnected responsibilities of the stakeholders. The combination of these results is the answer to the first research question. The data required to perform this step is mainly retrieved from the websites of stakeholders and by observation of the causal relationships within the case-study model.

The identification of the uncertain factors is a crucial step in this research. It provides an answer to the second research question and determines the scope of the uncertainty analysis. It is mainly based on existing literature and off-the-shelf stakeholder interviews. Furthermore, the case-study model is observed to find uncertain modelling assumptions. After the uncertain factors have been identified, their future development is modelled by identifying sampling ranges and techniques to translate this information into potential future trajectories.

Using the set of uncertain factors, the KPIs and the case-study model, an uncertainty analysis is performed by applying the EMA approach. This results in a large set of model experiments. The data contained in the results of these experiments is analyzed and visualized using various techniques. These visualizations provide answer to research questions three, four and five.

Within the discussion step of this research, the output of all previous chapters is used to elaborate on the meaning of the results. Within this elaboration, the implication and limitations of this research are addressed. More specifically, implications are discussed for analyzing uncertainty in industrial electrification systems and for combining EMA and MILP models. The latter category is an answer to research questions six. In other words, this step draws high level conclusions that contribute to an increased understanding of research that revolves around this topic.

The final and concluding step entails a summary of the results by answering each of the research questions. Furthermore, it provides recommendations based on the points of interest identified during the discussion of the implications and limitations of this research in the previous step.

Chapter 3

Theoretical framework

This chapter consists of a theoretical framework, which demonstrates an understanding of the concepts and theories relevant to the topic of this research. Following this line of reasoning, three main concepts need to be covered. The first section addresses electrification in the chemical industry by discussing the interconnectedness of industrial clusters and different electrification strategies. The second section contains a description of the mathematical approach that was used to model the chemical cluster in the Port of Rotterdam. The third section defines uncertainty and its dimensions, while also looking at the modelling of future development and exploring potential impacts of uncertainty. The final section discusses how the implications of the previously discussed theories can be applied in this research.

3.1 Electrification in the chemical industry

The companies in the integrated cluster mainly produce chemical products (Huntsman, 2020; Nouryon, 2020). In order to create a better understanding of the system at hand, it is key to dive into the background of this specific type of industry, specifically in relation to electrification.

The chemical industry is a large consumer of energy and a major contributor to global greenhouse gas emissions (Schiffer & Manthiram, 2017). More specifically, Global GHG emissions from chemical and petrochemical processes were roughly 1 gigatonne of carbon dioxide equivalent ($GtCO_2$-eq) in 2010, while total emissions were approximately 40 $GtCO_2$-eq in the same year (IEA et al., 2013). Hence, decarbonizing this industry by implementing electrification using renewable energy sources would be a great step towards reducing the global carbon footprint.

According to Schiffer & Manthiram (2017), there are two main sources of GHG emissions during the production process of chemicals, namely the combustion of fossil fuels and the production of feedstocks like hydrogen through the "water gas shift reaction". The energy released by the combustion of fossil fuels is used to increase temperatures, apply pressure or separate products. All of these processes can also use electricity as their source of energy.

3.1.1 The interconnectedness of industrial clusters

In order to realize the full potential of the decarbonization of the chemical industry, it is also important to apply a more holistic view across multiple product life-cycles (Jayal et al., 2010). By increasing the interconnectedness of energy and chemical industries, resource efficiency can be improved, thereby leading to an even greater impact on the reduction of CO_2 emissions.

These interconnected industries can form an industrial cluster. Porter (1998, p.81) describes an industrial cluster as "a host of linkages among cluster members" which "results in a whole greater than the sum of its parts". Apart from improving resource efficiency, there are several other benefits for the members of such a cluster. These include increased access to specialized employees, lower transaction costs and risk reduction (Thijsen, 2018).

Brown et al. (2007) conceptualized the industrial cluster as a value adding web consisting of direct and indirect links between vertical, horizontal and lateral actors. In this conceptualization, direct links are relationships between firms that act directly with one another. Indirect links imply that a third party functions as a connector between the firms. Furthermore, vertical actors are suppliers or buyers of products produced by horizontal actors. Lateral actors are institutions that facilitate improved performance for other actors. As means of illustrating the design of this conceptualization, it is visualized in Figure 3.1.

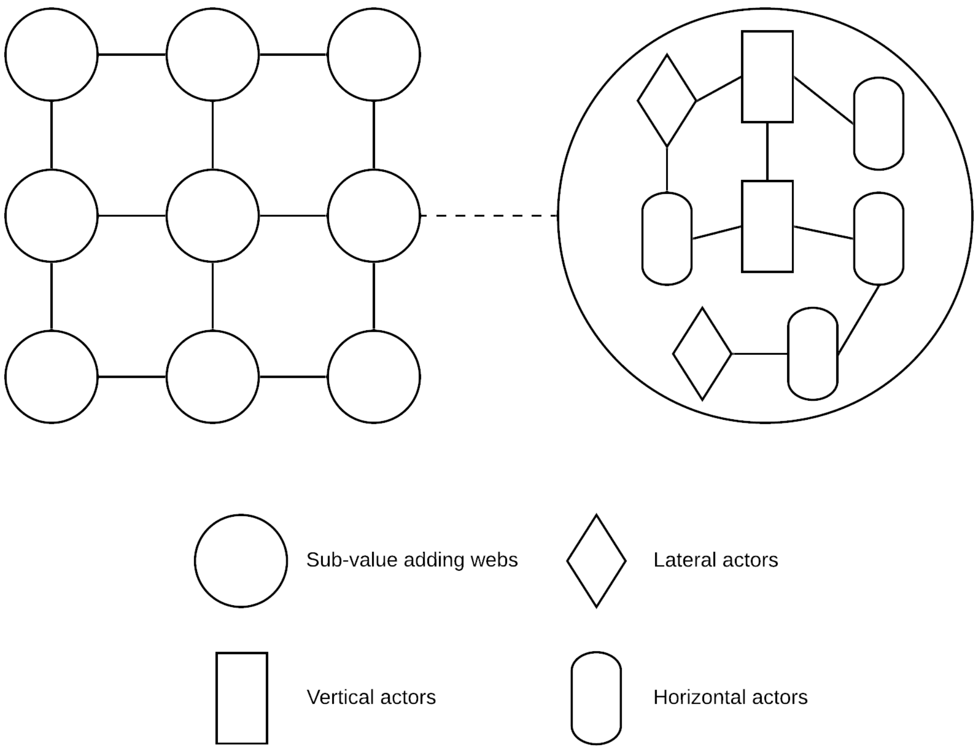


Figure 3.1: The cluster as a value adding web. Adapted from "Towards a new conceptualisation of clusters", by Brown et al., 2007, p.7.

When an industrial cluster is seen as a "value adding web", it is clear that actors do not only add value to their own firm, but also to the cluster as a whole. This is due to the fact that the industrial processes of the different actors are entwined, which implies that each actor has its own interests and objectives, but is dependent on other actors for achieving these interests and objectives (Thijsen, 2018). In the light of these observations, Porter (1990) argued that when an individual actor decides to change its system (actor level), it affects the whole cluster structure and therefore the processes of other actors (cluster level). Following this line of reasoning, it becomes obvious that it is key to consider both the actor and the cluster level during decision making.

3.1.2 Flexible and baseload electrification

According to Den Ouden et al. (2017), there are two distinct electrification strategies for the industry. The first strategy is *flexible electrification*, which is aimed at the part-time electrification of processes. Corresponding technologies are able to start and stop, ramp up and down, or have the ability to switch between electricity and other energy sources. Hence, these technologies are able to cope with the intermittent characteristics of current and future energy supply. They may poses the ability to change their electricity demand in response to fluctuating electricity prices. In times where electricity is scarce, the electricity price increases (Albadi & El-Saadany, 2008). In response, these flexible technologies can ramp down, stop or switch to a different energy source until the electricity price drops to a more feasible level. In this way, the industry can act as a balancing market for the electricity system (Schiffer & Manthiram, 2017).

The second strategy is *baseload electrification*, which entails constant electricity supply to processes, without the flexibility of the previous strategy. Therefore, this type of electrification is less suitable for the fluctuating energy supply of the future power grid. Renewable electricity can be used whenever available, but it is paramount that other (conventional) electricity generation technologies are present as back up. Furthermore, low operating costs are key to this strategy, since it cannot respond to economically infeasible electricity prices.

3.1.3 Characterizing the Power-to-X options

Each "Power-to-X" option present in the case-study model corresponds to one of the strategies discussed in the previous subsection and belongs to a certain electrification category. According to Den Ouden et al. (2017), the E-boiler is a flexible strategy in the "Power-to-Heat" category. They state that although this technology is commercially available, the economic feasibility in the Netherlands is poor due to grid connection costs, capacity tariffs and relatively high power prices.

The Steam Pipe option entails extending the waste steam infrastructure by connecting the local waste processing company (AVR) to the chemical cluster in the Botlek area. The production at AVR is characterized as a "Waste-to-Energy" process (Brunner & Rechberger, 2015). More specifically, since the resultant energy carrier of this process is steam, it is referred to as "Waste-to-Heat". Using this type of steam does not belong to any electrification category or strategy. However, since one of the companies in the chemical cluster (Air Liquide) would be able to feed electrically generated steam into the Steam Pipe as back up, this infrastructure would facilitate the usage of this "Power-to-Heat" option by other actors. Following this line of reasoning, it is considered a flexible electrification strategy.

The Demand Side Management (DSM) option using chlorine storage is obviously a strategy that increases the flexibility of the production process. Den Ouden et al. (2017) argue that in the "Power-to-Chemicals" category, flexible production of chlorine through electrolysis seems the most promising, due to its high power requirements. It is important to note that this strategy does not lead to an increase of electrification, but rather to a more flexible power consumption. Since this characteristic is a necessity in future power systems, it belongs to the total package of electrification solutions or "Power-to-X" options

3.2 Mixed integer linear programming

The model of the chemical cluster was built in "Linny-R", which is an executable graphical specification language for Mixed Integer Linear Programming (MILP) problems (Bots, 2020). As a means of understanding how this approach affects this research and its outcomes, it is paramount to define it properly and to discuss its advantages and limitations in relation to modelling industrial systems. Linear programming is a deterministic method to achieve the optimum outcome (such as maximum profit or lowest cost) in a given mathematical model for a set of constraints (Kosky et al., 2015, p.228). *Mixed integer* linear programming adds one condition to this definition, namely that at least one of the variables is constrained to be an integer, while other variables are allowed to be non-integers. The mathematical representation of a MILP problem is written as (NCSS, 2020, p.1):

Maximize or minimize

$$z = CX$$

Subject to

$$AX \leq b,\ X \geq 0,\ \text{some } x_i \text{ are restricted to integer values}$$

Where

$$X = (x_1, x_2, ..., x_n)'$$
$$C = (c_1, c_2, ..., c_n)$$
$$b = (b_1, b_2, ..., b_m)'$$
$$M = \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix}$$

The first function is called the "objective function". Furthermore, the x_i represent the "decision variables" (the unknowns) and the m inequalities (and equalities) are called "constraints". The bounds of these constraints (b_i) are often called Right Hand Sides (RHS). The set of all possible solutions that satisfy the problem's constraints is called the "feasible region" (Beavis & Dobbs, 1990).

Many MILP applications have been proposed for modelling problems originating in the process and other related industries (Pekny & Reklaitis, 1998; Pinto & Grossmann, 1996; Yee & Shah, 1998). The major advantage of this mathematical programming approach is that it provides a generic framework for modeling a large variety of problems. Its main limitation is the potentially large computational effort required to solve problems of practical size (Puigjaner et al., 2002). This might be a severe limitation for this research, as the proposed method for exploring the impact of uncertain factors often uses a large number of model runs. This matter will be discussed in more detail during the experimental design section in chapter six. Another limitation found by Puigjaner et al. (2002) is that linear models can lead to unsatisfactory or unfeasible solutions when they are used to describe the characteristics of a manufacturing environment. This is due to the fact that some objectives, constraints and policies are hard to capture in a linear representation. Hence, such models are always build upon certain simplifying assumptions. This limitation is very relevant for this research, since the case-study model also contains many of these assumptions. In order to cope with this limitation, the idea is to include some of the most crucial assumptions as uncertain factors. This will be addressed further during the identification of uncertain factors in chapter six and reflected upon during the final discussion in chapter eight.

3.3 Uncertainty

In model-based decision support, it is argued that uncertainty is not simply the absence of knowledge (Walker et al., 2003). Rather, uncertainty is described as a situation of information which is inadequate due to inexactness, unreliability or ignorance (Funtowicz & Ravetz, 1990). To further understand this complex notion and how to cope with it, three important topics are discussed within this section. To begin with, three different dimensions of uncertainty are described. Afterwards, the modelling of the future development of uncertainty is addressed. The last subsection explains how Exploratory Modelling and Analysis (EMA) can be used to explore the impact of uncertain factors on complex systems.

3.3.1 Dimensions of uncertainty

Many uncertainty typologies haven been developed for many purposes and few of them have claimed to be comprehensive. This research chooses to follow a framework developed by Walker et al. (2003), because it has model-based decision support as its point of departure. For the exploration, articulation and prioritisation of uncertain factors in multi-actor systems, Walker et al. (2003) defined three dimensions of uncertainty, namely location, level and nature (see Figure 3.2). They argue that using these dimensions leads to adequate acknowledgement and treatment of uncertainty in decision-making.

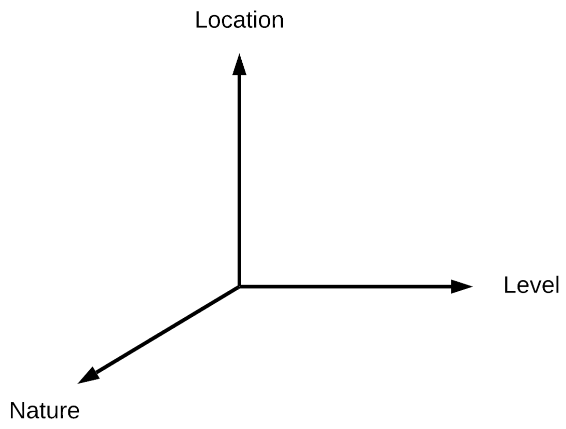


Figure 3.2: Uncertainty: a three-dimensional concept. Adapted from “Defining Uncertainty: A Conceptual Basis for Uncertainty Management in Model-Based Decision Support”, by Walker et al., 2003, p.5.

The *location* dimension describes where uncertainty is manifested, using model formulation logic. This creates the possibility to identify sources of uncertainty and their causal relationships with other system factors. Six distinct locations are identified with respect to the model (Kwakkel et al., 2010).

- System Boundary: Uncertainty regarding the choice of boundaries for the modelled system. This includes uncertainty about the external economic, environmental, political, social, and technological situation that forms the context for the problem being examined (Walker et al., 2003).
- Conceptual model: This uncertainty arises from a lack of understanding the behaviour and interrelationships among the variables within the system boundaries.
- Computer model: Uncertainty regarding the structure and parameters of the computer model. The latter can be divided into *fixed parameters inside the model* like the walking speed of pedestrians and *changeable parameters to the model* like policies (Walker et al., 2003).
- Input data uncertainty: Uncertainty associated with the determination of the values for both the parameters inside the model and as inputs to the model. These values are often based on empirical data or output of other models, both of which can be uncertain.
- Model implementation: Uncertainty arising from the implementation of the conceptual model into computer code. It is generated by software errors, hardware errors or other hidden flaws in the technical equipment or computer code.
- Processed output data: The uncertainty that is accumulated in all of the above locations within the model complex and which is expressed in the output data of the model.

The *level* dimension defines the severity of an uncertain factor along a spectrum ranging from deterministic knowledge to total ignorance. This knowledge is important during the development of effective coping strategies. Kwakkel et al. (2010, pp. 308-309) define four different levels of uncertainty:

1. Shallow uncertainty: Being able to enumerate multiple alternatives and provide probabilities (subjective or objective).
2. Medium uncertainty: Being able to enumerate multiple alternatives and rank order the alternatives in terms of perceived likelihood. However, how much more likely or unlikely one alternative is compared to another cannot be specified.
3. Deep uncertainty: Being able to enumerate multiple alternatives without being able to rank order the alternatives in terms of how likely or plausible they are judged to be.
4. Recognised ignorance: Being unable to enumerate multiple alternatives, while admitting the possibility of being surprised.

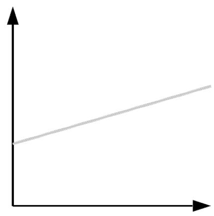
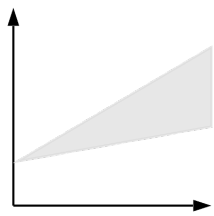
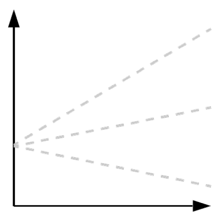
The *nature* dimension describes what causes the uncertainty. Assessing this dimension may help to understand how uncertain factors can be addressed. Three different natures of uncertainty are defined (Kwakkel et al., 2010; Walker et al., 2003):

- Epistemological uncertainty: Uncertainty due to the imperfection of knowledge. New knowledge or information by research may reduce the level of uncertain factors of this nature.
- Ontological uncertainty: Uncertainty due to the inherent variability of a certain system factor. Inherent variability is typically found in factors regarding the randomness of nature, human behaviour, social dynamics, etc.
- Ambiguity: Uncertainty due to the same data being interpreted differently by various actors based on their individual frames and perspectives. Uncertain factors of this nature can be coped with by implementing strategies that aim at integrating different frames and support joint sense making.

3.3.2 Modelling the future development of uncertainty

To be able to explore the potential impact of uncertain factors, it is paramount to model their future development. Thijsen (2018) has developed an overview (see Table 3.1) with guidelines for modelling the future development of uncertainty. This overview combines various paradigms for modelling the future by Maier et al. (2016) with different levels of uncertainty as defined by Kwakkel et al. (2010).

Table 3.1: Guidelines for modelling the future development of uncertain factors. Adapted from "Uncertainty in electrified industrial systems", by Thijsen, 2018, p.39.

Level of uncertainty	**Paradigm**	**Development function**
Clear enough future	Use of best available knowledge	
Shallow uncertainty	Quantification of future uncertainty	
Medium uncertainty Deep uncertainty Recognized ignorance	Exploring multiple plausible futures	

For each level of uncertainty, Thijsen (2018) proposes a different paradigm to model the future development of uncertain factors. Each paradigm corresponds to a development graph where an uncertain system state (vertical axis) is displayed as a function of time (horizontal axis).

In a clear enough future, current knowledge of the system and its processes can be used to anticipate the future behaviour of the system (Bankes, 1993). A limitation of this paradigm is that knowledge will not always to lead to more insights Thijsen (2018). Therefore, it is only appropriate for factors that are not noticeable uncertain or considered not very important (Walker et al., 2013).

In cases of shallow uncertainty, future uncertainty can be treated as quantifiable. Following this paradigm, predictions can be made for parameters and structure by using probability distribution functions to develop an estimated bandwidth of output uncertainty (Beyer & Sendhoff, 2007; Schoups & Vrugt, 2010). This allows the modeller to develop multiple forecasts within this bandwidth, each having its own probability of occurrence (Walker et al., 2013). An important limitation here is that the statistical properties of the uncertain factors are assumed to be constant, while this kind of uncertainty often increases over time (Mahmoud et al., 2009). In other words, the performance of this paradigm is very vulnerable to future changes.

Under circumstances of medium and deep uncertainty or recognized ignorance, which are often associated with climate, technological, socio-economic and political change (Maier et al., 2016), Thijsen (2018) argues that the dynamics and the impact of processes over time of the system are not well understood. Hence, developing single possible futures based on probabilities is not sufficient. Instead, exploratory modelling can be used to explore the impact of multiple plausible futures on various system states.

3.3.3 Exploratory modelling and analysis

As introduced in the second chapter, Exploratory Modelling and Analysis (EMA) can be used to explore the impact of uncertain factors on complex systems. More specifically, through the EMA Workbench (Kwakkel, 2019), two different approaches are available: "open exploration" and "directed search".

Open exploration is mainly based on sensitivity analysis, which generally measures the output behaviour of a model across the input space of uncertain factors (Q. Liu & Homma, 2009). Instead of using a "one-at-a-time" sensitivity analysis for this purpose, Jaxa-Rozen & Kwakkel (2018) argue to perform a global sensitivity analysis by evaluating the full distribution of each uncertain factor across the domain of all other parameters. This type of analysis entails a broader measurement of a system's sensitivity to uncertainty. In addition, it can deal with nonlinear responses and explores the non-additive effects between model parameters (Saltelli & Annoni, 2010). A specific type of global sensitivity analysis offered by the EMA Workbench is called *variance-based* and is often referred to as the "Sobol method" (Thijsen, 2018). This technique "provides first-order and total indices, which respectively describe the fraction of output variance contributed by each factor on its own, and by the sum of first-order and all higher-order interaction for each factor" (Jaxa-Rozen & Kwakkel, 2018, p.246).

The directed search approach is based on various optimization algorithms. With these algorithms, the uncertainty space can be searched to find the best- and worst-case scenarios for the alternatives. Furthermore, a robust many objective optimization problem can be formulated, where one searches for alternatives with robust performance over a set of scenarios (Kwakkel, 2019). This type of optimization requires a robustness metric, which takes as input the performance of a candidate alternative over a set of scenarios and returns a single robustness score.

Using Multi-objective Evolutionary Algorithms (MOEAs) to discover solutions that show decision makers critical trade-offs between their performance measures is one step of the Multi-Objective Robust Optimization Framework (MORDM) presented by Kasprzyk et al. (2013). Figure 3.3 shows that other steps of this process focus on problem formulation, scenario discovery and trade-off analysis. Noticeable are the double headed arrows and constant stakeholder collaboration along every step. These observations point out that exploratory modelling processes can be subject to many iterations and that it is paramount to continuously collaborate with stakeholders. This framework provides a decent foundation for many objective robust decision making in complex uncertain systems. Hence, it can be used in the experimental design of the uncertainty analysis.

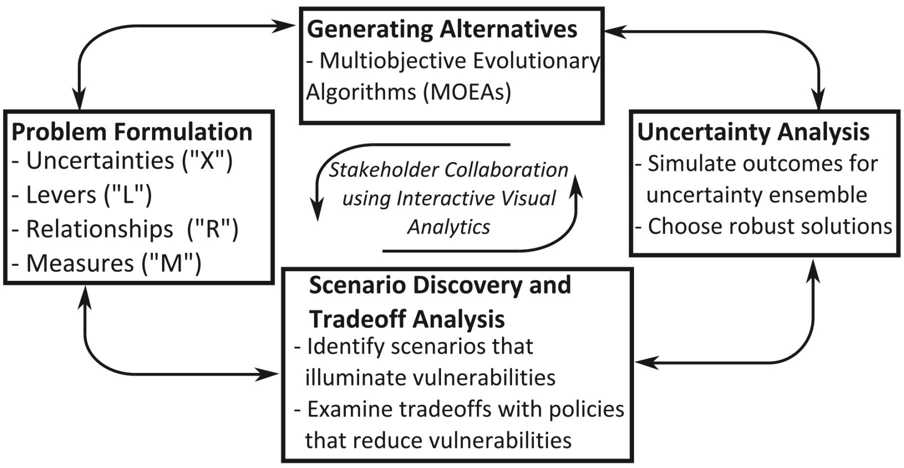


Figure 3.3: The four steps of the many objective robust decision making (MORDM) framework. Copied from "Many objective robust decision making for complex environmental systems undergoing change", by Kasprzyk et al., 2012, p.58.

To understand the implications of using EMA for this specific research, it is paramount to discuss its main advantages and limitations. A key advantage is that it is not focused narrowly on optimizing a system to accomplish a particular goal or answer a specific question. Rather, it can be used to address 'beyond what if' questions, such as "under what circumstances would this policy do well and under what circumstances would it fail?". This specific focus ensures that EMA stimulates 'out of the box' thinking. Therefore, it has the ability support the development of adaptive plans or policies (Kwakkel & Pruyt, 2013). Furthermore, in cases where multiple data sets are available, EMA can be used to identify the extent to which the choice of data influences the model outcomes. This encourages the development of policies that produce satisfying results across different sets of data, instead of long-lasting discussions regarding data selection (Kwakkel & Pruyt, 2013).

Something that can arguably be considered either an advantage or limitation to EMA, is that it provides “foresight” and not “forecasting”. There is an important difference between these two concepts. Forecasting attempts to predict the future as accurately as possible, whereas foresight places several realizable or desirable futures side by side (Mietzner & Reger, 2005). On the one hand, this introduces limitations in the sense that the results can never be used as if they provide certain knowledge about the future. On the other hand, it incentivizes the development of robust solutions that perform well over a wide range of scenarios.

3.4 Application of theory

The goal of this final section is to summarize the implications of the previously discussed theories for this research and to demonstrate how these theories can be applied. During the discussion of the interconnectedness of industrial clusters in Section 3.1.1, it was clear that it is paramount to consider both the actor and the cluster level during decision-making. Hence, it is important to explore the possibilities of the model to look at these different perspectives. Furthermore, the characterization of the three Power-to-X alternatives in Section 3.1.3 showed that it is not immediately obvious how the Steam Pipe and chlorine storage options relate to an electrification strategy. Therefore, it is key to explain these relationships carefully whenever they are used in this context. The discussion of the mathematical representation of a MILP problem in Section 3.2 resulted in an understanding that can be used during the model description in the next chapter. In addition, two important limitations of MILP applications were addressed in this section. More specifically, the potentially large computational effort required to solve MILP problems of practical size is something that has to be considered carefully during the experimental design of the uncertainty analysis. The other limitation regarding the extent to which the linear characteristics of MILP influence the validity of modelling a manufacturing environment is an important topic for the discussion section of this research. In Section 3.3.1, three dimensions of uncertainty were explored. This information allows for a more precise identification and classification of the uncertain factors influencing the performance of the Power-to-X alternatives. Within Section 3.3.2 was discussed how the future development of these factors can be modelled by using various paradigms corresponding to their level of uncertainty. This will help to create proper future trajectories for the identified uncertain factors. Finally, the discussion of EMA in section 3.3.3 contributed to understanding the benefits and limitations of this approach, which is a crucial subject to reflect on during the discussion.

Chapter 4

Model description

The goal of this chapter is to create a basic understanding of the case-study model. This is crucial for the comprehension of the subsequent steps within this research. To begin with, an overview is presented of the model to give an impression of its complexity and size. Afterwards, the model structure is explained by considering its different object types. Finally, this information is translated to the specification of the MILP problem.

4.1 Overview

The MILP model of the integrated chemical cluster developed by TU Delft researchers Rob Stikkelman and Pieter Bots is relatively large in size and therefore quite complex. Figure 4.1 shows an overview of the first layer of this model within the Linny-R software in which it was developed. Due to confidentiality reasons, it is not allowed to zoom in further or to show any numerical information. Nevertheless, when baring in mind this model consists of multiple layers, this overview gives a decent impression of its size and complexity.

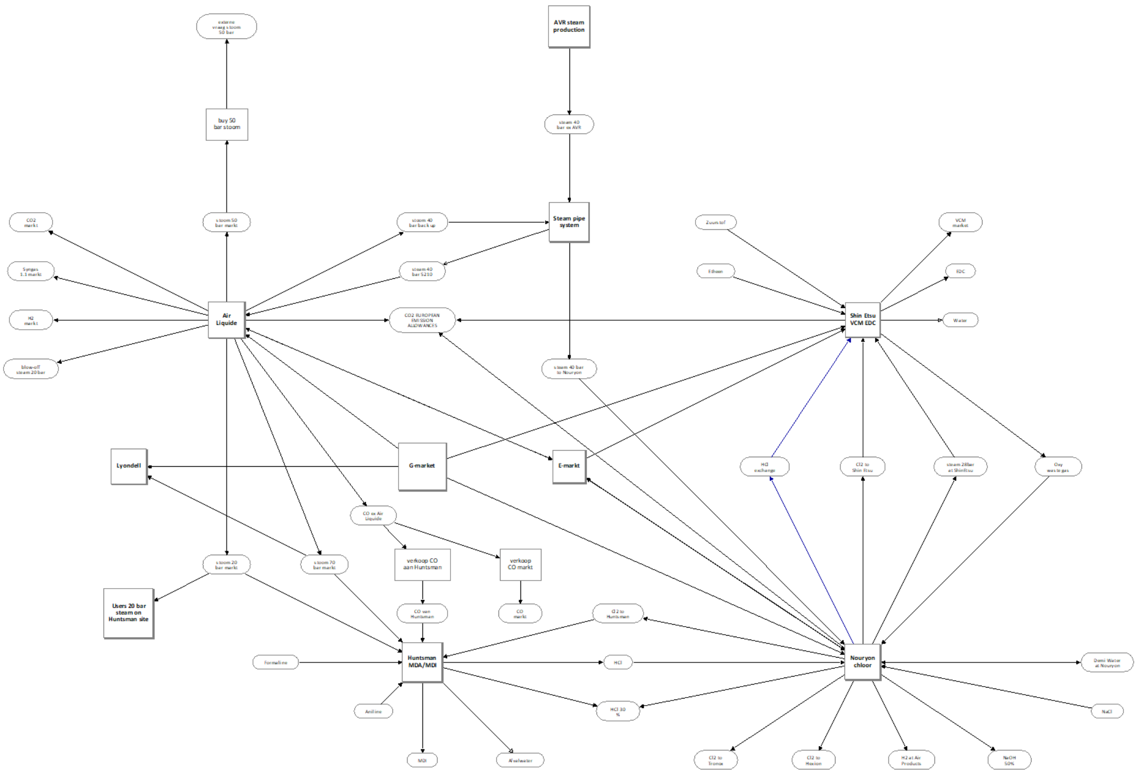


Figure 4.1: Overview of first model layer within Linny-R

4.2 Structure

To understand the structure of the model layer displayed in Figure 4.1, it is paramount to discuss the different object types. Figure 4.2 shows that there are four object types: clusters, products, processes and links. Each of these will be discussed in the following subsections.

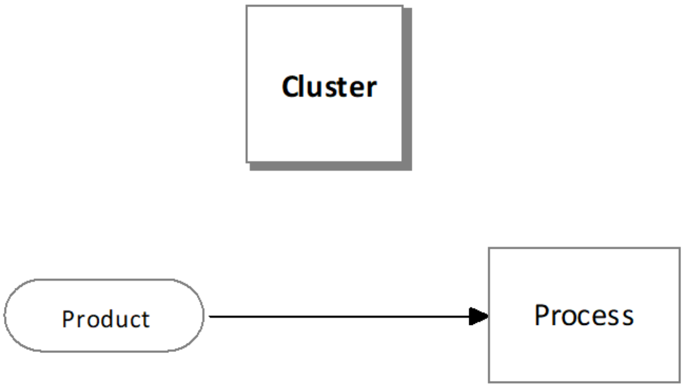


Figure 4.2: Overview of object types within Linny-R

4.2.1 Clusters

The cluster object allows for what is referred to as hierarchical modular modelling (Pidd & Castro, 1998). This functionality is used in the Linny-R software to keep models organized by creating different layers. Both products and processes can be "tucked away" in a cluster so that they are no longer visible on the parent layer.

4.2.2 Products

Products are used to represent the in- and output materials of the production processes that take place within the modelled system. These products have a number of customizable properties (see Figure 4.3).

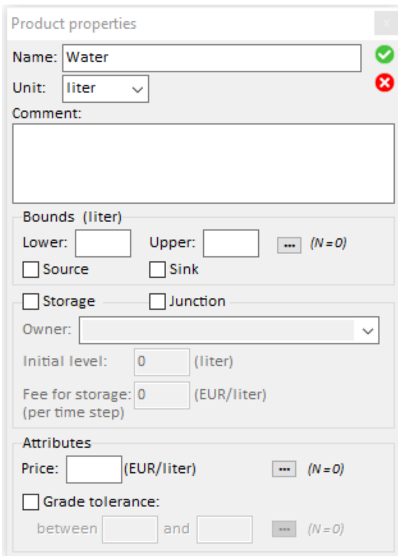


Figure 4.3: Product properties within Linny-R

To begin with, products can be given a name and a unit. Furthermore, a lower and upper bound can be specified. In this case, these bounds determine what value the product can take. There are different types of products: sources, sinks, junctions and storage systems. Sources are objects where products enter the system by depletion (negative values), while sinks are objects where products accumulate and leave the system (positive values). Junctions always take a value of zero, since the input flow must be equal to the output flow. Storage systems can be seen as sinks which can also be depleted until they are empty. Hence, they are always represented by a positive value. A last important attribute of products is their price. If no price is specified, the software will use the so called "cost price" for this product, based on its production costs. In contrast, when a product is given a certain price based on a fixed value or a function, the difference between this price and its "cost price" entails the profit/loss margin for the actor producing it.

4.2.3 Processes

Processes are used to convert input products into output products at a certain "production level". The properties of processes can be altered (see Figure 4.4). To begin with, processes can be owned be a certain actor. This property allows the model to optimize for an individual actor or group of multiple actors. Furthermore, the production level of processes can be constrained by a lower and upper bound. For example, a lower bound can entail the minimal production level that a company has to apply to cover the costs. A typical upper bound for a process is the maximum production capacity of a certain machine. Another important customizable property of processes is the ratio in which products are consumed or produced. There are more properties of processes, but these are the most important for now.

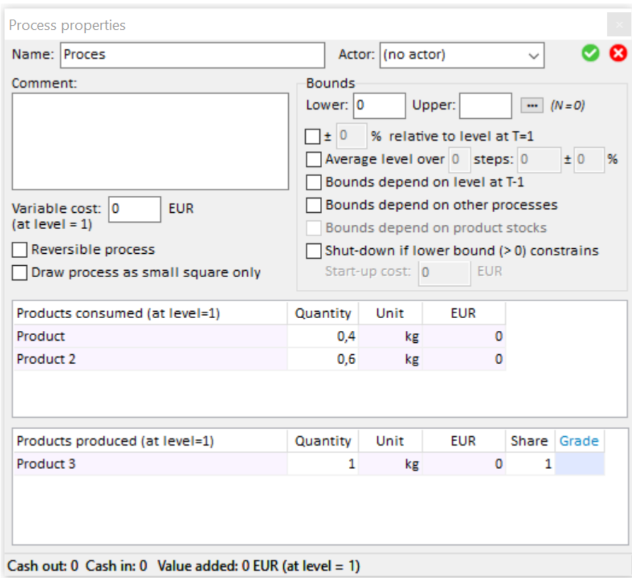


Figure 4.4: Process properties within Linny-R

4.2.4 Links

Links form the connection between products and processes. They represent the amount of flow of a certain product.

4.3 Translation to MILP problem

Now that there is a proper understanding of the object types and their properties, it is key to translate this to the specification of a MILP problem. The following subsections will explain how the previously mentioned components translate to constraints, decision variables and an objective function.

4.3.1 Constraints

The model contains 248 constraints for every time step part of the simulation time horizon. These constraints were created through the properties of the products and processes (see Figure 4.4 and 4.3). Among other things, the bounds of these constraints can entail the lower and upper bounds products and processes, the ratios between products used in a certain process and a minimum or maximum storage capacity.

4.3.2 Decision variables

Subject to these constraints, the model contains 382 decision variables for every time step. There two main types of decision variables: the production level of processes and slack variables. The latter category is used by the software to allow for the violation of certain constraints to ensure that the solver is able to find a solution.

4.3.3 Objective function

The objective function constructed by the Linny-R software is the same for every model: minimize the costs for the selected actors. Following this line of reasoning, the objective function takes the follow form:

$$MIN\ TC_a = c_{a1} * x_1 + c_{a2} * x_2 + ... + c_{an} * x_n$$

Within this function, TC_a represents the total amount of costs for the selection of actors (a). Furthermore, the c_{ai} represent the costs for the selected actor(s) associated with the decision variables (x_i). According to the properties of the products and processes, these decision variables can be constrained by certain bounds (b_i) in various ways. For example:

$$x_1 \geq b_1$$
$$x_1 + x_2 = b_2$$

A different selection of actors for the optimization results in different costs per decision variable. When optimizing for an individual actor, the costs associated with the decision variables of other actors can potentially be zero, because the production processes of these other actors might not influence the costs of the selected actor. This means that these decision variables are allowed to take any value within the boundaries of their constraints. In other words, the actors not included in the optimization perspective will do anything in their power to ensure the lowest possible costs for the selected actor(s).

Chapter 5

Stakeholder analysis

The production processes of the integrated chemical cluster in the Botlek area form an industrial complex. An industrial complex comprises processes that are heavily interconnected via utility infrastructure networks and product chains, where the product of plant X is the feedstock of plant Y. Since these production processes are owned by different companies, each having their own objectives, this can incentivize either cooperation or conflict.

As a means of understanding these dynamics, it is paramount to perform a stakeholder analysis. This method entails scanning the existing actor network and is used by many different actors, as it serves a wide range of purposes (Hermans & Cunningham, 2018). In project design and management, stakeholder analysis is used identify sources of opposition and support or to find out what actors need to be involved to ensure that the project meets the requirements of its stakeholders (MacArthur, 1997). Public policy makers use the method to assess the implementation feasibility of different policy alternatives by observing the motivations and abilities of the stakeholders in relation to these alternatives (Phi et al., 2015).

There are many techniques available that can help scan an existing actor network. This research applies some of the crucial steps for actor network scanning as defined by Hermans & Cunningham (2018). The first step entails problem formulation. The second step consists of the identification of involved actors, other than the three industrial companies. The third step identifies key actor characteristics that contribute to understanding their strategic behavior. The fourth step illustrates the network context in which they operate. The final step discusses the implications of the results from the previous steps for this research.

5.1 Problem formulation

During the introductory chapter of this report, the problem was already formulated: the uncertainty surrounding industrial electrification decreases the stability of business cases and hinders the decision-making process. Problems, challenges and opportunities are perceived differently by different actors and are also socially constructed (Enserink et al., 2010). Hence, to sharpen this problem formulation, it is key to determine who owns the problem.

In this case, the problem is owned not only by the companies from the chemical cluster, but also by the Dutch government. More specifically, the Ministry of Economic Affairs and Climate Policy (Ministry of EACP). This is due to the fact that they need to meet certain targets like the ones part of the Paris Agreement (Åhman et al., 2017). In order to sharpen this problem formulation even further, it is useful to define the gap between the desired situation and the observed situation, followed by the determination of the main dilemma faced by the problem owners (De Haan & De Heer, 2012; Enserink et al., 2010). The observed situation follows logically from the knowledge gap identified in section 1.2, namely that information regarding the effect of uncertainty on the KPIs of different electrification alternatives is missing. In the desired situation, there would be a clear map or other source of information that illustrates both short- and long-term effects. This would improve the stability of business cases and incentivize continuity in decision making, thereby contributing to a full adoption of the potential of electrification.

This information gap translates into dilemmas for both problem owners. The main dilemma that presents itself to the industrial companies is the following:

"How can we invest in sustainable alternatives, without carrying the risk that they turn out to be economically infeasible or otherwise ineffective?"

The main dilemma faced by the Ministry of EACP is:

"How can we ensure that industrial actors choose a decarbonization strategy, without disturbing our international competitive position and business climate?"

5.2 Actor identification

At first sight, the system of analysis seems to consist of three actors, namely the companies of the chemical cluster: Nouryon, Huntsman and Air Liquide. The previous section added one important actor to this list, namely the Ministry of EACP. However, since the objective is to analyze the role of external uncertainty in this system, it is paramount to consider other actors that are either able to create a certain form of external uncertainty or are able to directly influence one. Research performed by Thijsen (2018) shows that uncertainty in electrified industrial systems can be divided into four different categories: policy, market, technology and process. An attempt will be made to identify actors in each category.

An important actor in the policy category is obviously the Ministry of EACP itself. It is able to create or adapt policies that directly affect the chemical cluster. For example, it can charge a national CO_2 tax or promise subsidies on electricity saving investments and tools (Sijm & Van Dril, 2003). Another influential player in this field is the European Commission (EC). It has a number of ways to control the European Union Emission Trading System (EU ETS). For example, it can decrease the amount of emission allowances that are allocated freely to the industry. Furthermore, it can lower the emission cap, resulting in higher prices for the remainder of the allowances that are auctioned (Ellerman & Joskow, 2008).

Due to globalization, the market and technology categories have grown very complex (Thoumrungroje & Tansuhaj, 2007), meaning countless actors have the ability to partly or indirectly influence uncertain factors that belong to these categories. Trying to include all of these actors would be an impossible task. Moreover, it will be hard to estimate the exact influence of these individual actors, resulting in a very assumption-based stakeholder analysis. However, since there is a lot of uncertainty regarding the prices of both in- and output products, the applied solution is to include a generic "markets" actor. Another essential actor in this category is the local waste processing company called AVR. It can potentially feed a great amount of steam into the Steam Pipe alternative. However, since AVR has other contractual obligations and is also profit oriented, its behaviour is considered uncertain.

According to Thijsen (2018), process uncertainty in electrified systems consists solely of the impact that potential flexible characteristics of such a system might have on the delivery of products to other actors in the cluster. This is due to uncertainty regarding the way the chain of processes is affected by electrification over time. This uncertainty is not clearly influenced by a certain actor.

5.3 Actor characteristics

In this third step, key characteristics are identified that contribute to understanding the strategic behaviour of the identified actors. More specifically, their level of interest in the current situation is assessed based on two different types of objectives (Keeney, 1996): strategic and problem-specific. Strategic objectives are relatively stable and ultimate objectives of an actor, regardless of the specific situation. Problem-specific objectives indicate what actors desire to achieve in a certain situation (Hermans & Cunningham, 2018). If there is a direct link between the two types of objectives for a certain actor, it is expected to have a high level of interest in the problem situation. For the identification of the objectives, both company websites and relevant literature were used. The results are shown in table 5.1.

Table 5.1: Actor Characteristics

Actor	**Strategic objective**	**Problem-specific objective**	**Interest**
European Comission	Striving to be the first climate-neutral continent, by empowering people with a new generation of technologies (European Commission, 2020).	Decarbonizing Europe's power production and, at the same time, increasingly electrifying our energy use (ten Berge, 2016).	Medium
Dutch Government (Ministry of EACP)	Promoting the Netherlands as a country of enterprise with a strong international competitive position and an eye for sustainability. Creating an excellent entrepreneurial business climate, by creating the right conditions and giving entrepreneurs room to innovate and grow. (Ministry of EACP, 2020).	Decreasing carbon emissions to reach climate goals and agreements (Den Ouden et al., 2017).	Medium
Nouryon	Capturing profitable growth through collaboration with customers and continuing to meet or exceed targets through operational excellence (Nouryon, 2020).	Reducing carbon emissions through a combination of improved energy efficiency and increased use of renewable energy (Nouryon, 2020)	High
Huntsman	Striving towards an aggressive growth philosophy that reflects the spirit of free enterprise and maximization of long- term profits (Huntsman, 2020).	Operating safe, clean and efficient facilities in an environmentally and socially responsible manner (Huntsman, 2020).	Medium
Air Liquide	Delivering long-term performance and profitable growth, while contributing to sustainability (Air Liquide, 2020).	Reduce the carbon intensity of its activities, but also to work with its customers toward a sustainable industry and to contribute to the development of a low-carbon society (Air Liquide, 2020).	High
AVR	Creating a cleaner world in which nothing is wasted (AVR, 2020).	AVR can expand its steam supply in the port and connect other companies in the Botlek area. Here it is imperative to assure maximum availability (AVR, 2020).	High
Markets	Trade based on profit-maximization (Mendelson, 1987) and good price-quality relationship (Yan & Sengupta, 2011).	Some consumers are concerned about the environment and want to translate this into purchases (Young et al., 2010).	Low

5.4 Network structure

In order to understand how the actors depend on each others resources and products, it is important to look at the structure of the network. The resulting network diagram does not have to contain all relationships between the actors, but just those deemed most important for the problem analysis (Hermans & Cunningham, 2018). Figure 5.1 shows the network diagram that has been developed for this analysis. In this diagram, relationships are illustrated by arrows, where the direction of the arrow displays either hierarchy or flow direction of materials. The relationships between companies of the chemical cluster and markets are based on the contents of the optimization model. The formal relationships between governmental actors and companies are based on research performed by Sijm & Van Dril (2003). The relationship between the EC and the Ministry of EACP is based on information from the website of the European Union (2020).

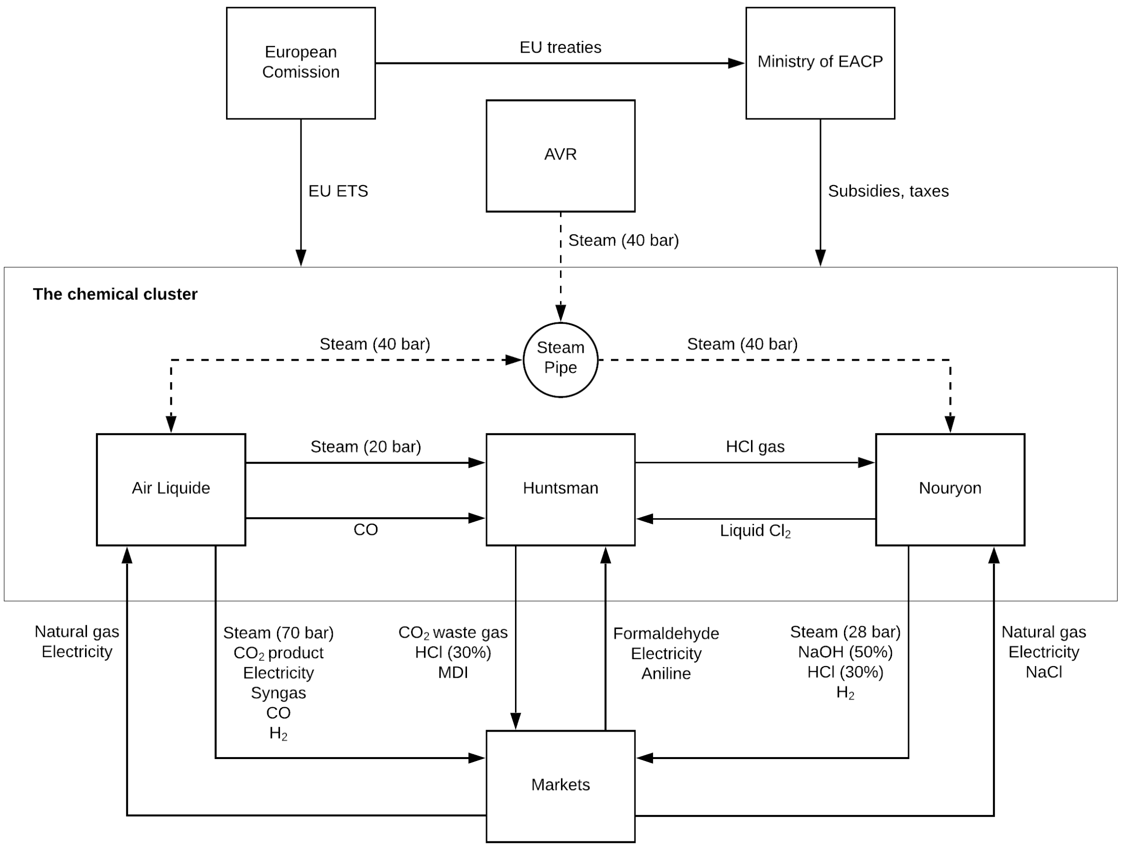


Figure 5.1: Actor Network Diagram

The dotted lines in Figure 5.1 represent a deviation from the current situation, namely the steam-based relationships that are born when the Steam Pipe option is implemented. In this new situation, the Steam Pipe is mainly fed steam at a pressure of forty bar produced by AVR. In order to improve security of supply, similarly pressurized steam produced by Air Liquide can be used as back up. Air Liquide and Nouryon are directly connected to the Steam Pipe, while Huntsman is connected via the steam balancing system of Air Liquide, as it requires steam at a pressure of twenty bar.

5.5 Implications

With the results of the previous steps in mind, it is time to think about their implications for the remainder of this research. During the problem formulation step, dilemmas were formulated for both problem owners. It is interesting that the dilemma faced by the members of the chemical cluster does not conflict in any way with the dilemma faced by the Ministry of EACP. This means that there are great incentives for collaboration, where both parties can benefit from each others resources.

During the identification of the actors in the second step of this analysis, it was discussed that there are countless actors involved in the markets. The uncertain factors within this category can therefore be considered extra unpredictable. This must be taken into account during the identification of the possible future development trajectories of these factors in the next chapter.

The actor characteristics in Table 5.1 allow for the identification of Key Performance Indicators (KPIs) that can be used to assess the performance of the Power-to-X options during the uncertainty analysis. Based on the combination of the strategic and problem-specific objectives of the actors, three KPIs are identified: economic feasibility, decarbonization and security of supply. These KPIs will be worked out in more detail later on in this report. Furthermore, Table 5.1 shows a fascinating difference in the level of interest among the companies in the chemical cluster. When comparing the strategic objective of Huntsman to its problem-specific objective, less overlap is found compared to other two members of the cluster. Therefore, its interest in the problem situation was assessed to be medium, whereas the others were given a high level of interest. This means that Air Liquide and Nouryon can expect Huntsman to be less interested in finding a solution to the problem. This can be valuable information during the decision making process.

The network diagram in Figure 5.1 contains a number of interesting observations. First of all, it shows that the members of the chemical cluster heavily depend on trade with the markets. This means that the price uncertainty of the in- and output products deserves extra attention during the identification of the uncertain factors and their future development. Furthermore, it is clear that the Steam Pipe option introduces a new actor into the arena, namely AVR. As discussed earlier, the behaviour of this actor is considered uncertain. In spite of the fact that its problem-specific objective in Table 5.1 shows its determination to assure a maximum availability of steam, the production is still dependent on certain waste resources. Therefore, the amount of steam that they feed into the Steam Pipe remains an important uncertain factor. Another key observation from the network diagram is that the Steam Pipe option further increases the interconnectedness of the chemical cluster. The latter might not be favored by all actors, because it decreases the level of independence. On the other hand, it creates new sustainable possibilities. This is an important dilemma for these actors, which should be taking into account during the discussion of the feasibility of the Steam Pipe.

Chapter 6

Identification of uncertain factors

To be able to explore how external uncertainty affects the performance of the Power-to-X options in the chemical cluster, the uncertain factors must first be identified. Within the first section, these factors are identified based on a literature review. Since the model is built upon uncertain assumptions, the second section discusses which of these assumptions should be included as uncertain factors as well. The third section provides an overview of the uncertain factors identified in the previous steps. Finally, section four addresses the future development of these factors by identifying sampling ranges.

6.1 Literature review

This literature review is based on research performed by Thijsen (2018), where a method was developed to identify and explore uncertain factors in electrified industrial systems. Table 6.1 shows a content taxonomy of uncertainty in electrified industrial systems that has been developed during this research.

Table 6.1: Content taxonomy of uncertainty in electrified industrial systems. Adapted from "Uncertainty in electrified industrial systems", by Thijsen, 2018, p.29.

Category	**Uncertain factor**
Policy	Subsidies
	Taxes
	Product restrictions
Market	Fuel prices
	Market prices of in- and output products
	Costumer perceptions
Technology	OPEX
	CAPEX
	System failures
	Energy capacity management
	Availability of new technologies
Process	Cluster product delivery

Thijsen (2018) used this taxonomy to identify uncertain factors during interviews with various companies in the industrial sector. Fortunately, interviews were conducted with two stakeholders present in the cluster industrial central to this research, namely Nouryon and Huntsman. Table 6.2 shows the results. Each factor is quantified using a certain unit, in this case either euros (€) or volume (V). Furthermore, the factors are classified according to the three dimensions of uncertainty as defined by Walker et al. (2003) (see Section 3.3.1).

Table 6.2: Uncertain factors identified by Thijsen through interviews with Nouryon and Huntsman. Adapted from "Uncertainty in electrified industrial systems", by Thijsen, 2018, pp. 57-58.

Uncertain factor	**Category**	**Location**	**Nature**	**Level**
Renewable energy subsidy (€)	Policy	Context	Ambiguity	1
CO_2 emission price (€)	Policy/Market	Context	Ambiguity	2
Electricity and gas fuel tax (€)	Policy	Context	Ambiguity	1
Electricity price (€)	Market	Context	Ambiguity/Ontology	4
Gas price (€)	Market	Context	Ambiguity	4
Electrified steam contract price (€)	Market	Cluster	Ambiguity	4
Chlorine price (€)	Market	Cluster	Ambiguity	3
NaOH price (€)	Market	Context	Ambiguity	4
MDI price (€)	Market	Context	Ambiguity	4
Steam by-product hydrogen price (€)	Market/Process	Cluster	Ambiguity	2
Steam by-product hydrogen supply (V)	Market/Process	Cluster	Ambiguity	2
Chlorine demand by partners (V)	Market/Process	Cluster	Ambiguity	2
Balance of steam and chlorine supply (V)	Process	Cluster	Ambiguity/Epistemology	2
Steam demand (V)	Market/Process	Internal	Ambiguity	2
Chlorine storage (V)	Process/Technology	Internal	Epistemology	1

The results from the interviews show that some uncertain factors have more than one corresponding category. This is due the fact that a factor can be influenced by actors or equipment from different categories. For example, the CO_2 price is influenced by both the government (policy) and private actors (market). Regarding the three dimensions, Thijsen (2018) used specific notions to assess the *location* dimension of the uncertain factors: "context" for outside the cluster system, "cluster" for between cluster partners and "internal" for within the actor's own system. The *nature* dimension was assigned by asking the respondents how the uncertainty was caused. Most policy, market and cluster categorised factors induce uncertainty due to differences in human perceptions of the same phenomena. Hence, these factors were assessed as "ambiguous". In addition, the electricity price was considered "ontological", because it is increasingly affected by the inherent variability of weather conditions. The supply balance and chlorine storage factors were assigned an "epistemic" nature, as there is a lack of knowledge with respect to the flexible capacity of cluster partners. The *level* dimension is based on stakeholder expectations regarding the future development of uncertain factors. If they expect specific development with some variability, uncertainty was assessed as "shallow" (level 1). If one was able to both enumerate and rank multiple development paths, the uncertainty was assessed as "medium" (level 2). If a respondent was only able to enumerate multiple developments paths without ranking them, the uncertainty was assessed as "deep" (level 3). Lastly, if a stakeholder had no clue about the future development of a certain factor, its uncertainty was assessed as "recognised ignorance" (level 4).

6.1.1 Exclusion of uninfluential factors

In this research, the goal is to explore how *external* uncertainty influences the performance of Power-to-X alternatives in the chemical cluster. The external character of this research goal allows for the exclusion of certain factors that Thijsen (2018) identified during the interviews with Nouryon and Huntsman. More specifically, all the uncertain factors in Table 6.2 that are located either in the cluster or internally can be excluded from further analysis. This leaves only factors whose uncertainty is located in the 'context' or in other words, outside of the cluster.

Furthermore, the second part of the research goal entails uncertain factors that influence the performance of the Power-to-X alternatives. Some of the external factors identified during the interviews might be uncertain, while their impact on the performance of the Power-to-X alternatives is very low or non-existing. This can be checked by following the causal relationships within the model and by conducting simple experiments where single factors are varied to explore sensitivity.

To begin with, the factor “renewable energy subsidy” is currently to broad in its definition. Hence, it is paramount to analyze this factor in greater detail to find out whether it can influence the economic feasibility of the alternatives. Generally speaking, there two types of subsidies: ones decreasing capital expenditure (CAPEX) and ones decreasing operational expenditure (OPEX). In terms of the E-boiler, its CAPEX can be decreased by an investment subsidy. Likewise, its OPEX can be lowered through the means of a feed-in tariff. Therefore, both the CAPEX and the OPEX of the E-boiler are included as uncertain factors. Regarding the Steam Pipe alternative, an investment subsidy is relevant in respect with its CAPEX. A subsidy lowering its maintenance costs (OPEX) seems less likely in this case. Hence, only the CAPEX of the Steam Pipe is included for further analysis. As discussed during the characterization of the chlorine storage alternative in the theoretical framework, this option belongs to the electrification package. However, this link is rather indirect and therefore it is unlikely to qualify for any subsidy.

Regarding the electricity and gas fuel tax, the model does not account for these factors in the sense that they are not specifically defined on the factor level. Instead, they are already included within the comprehensive electricity and gas prices. Hence, these taxes can be excluded from the analysis.

The prices for CO_2 emission, gas and (day-ahead) electricity all directly affect the economic feasibility of the E-boiler. If the electricity price is low while the prices for gas and CO_2 emission are high, this alternative becomes more affordable for Air Liquide compared to conventional steam production. The other way around, when the price for electricity is high and the gas and CO_2 emission prices are low, the E-boilers becomes less attractive.

In respect to the price of caustic hydroxide (NaOH), simple exploring experiments with the model revealed that this factor plays an important role in the optimal storage behaviour of chlorine at Nouryon. At high NaOH prices the tendency is to fill the storage tank close to its limit, while at low prices it is only filled to its lower bound. In other words, the NaOH price greatly influences the Demand Side Management (DSM) alternative through determination of the chlorine storage level and must therefore be included in the uncertainty analysis.

A changing market price for methylene diphenyl diisocyanate (MDI) could influence the production level of MDI at Huntsman. Since steam is used during this production process, this might affect the amount of 'green' steam used from the Steam Pipe alternative. However, the model shows that the amount of MDI that Huntsman is obliged to supply through market contracts lies very close the amount of their maximum production capacity. Therefore, a change in the MDI price would not result in significantly a different production level, which means it would not affect the performance of the Steam Pipe alternative. Hence, the MDI price is excluded from the analysis.

In summary, Table 6.3 shows the uncertain factors derived from the interviews and included for further analysis. The uncertainty nature of the CAPEX and OPEX factors is assessed ambiguous, because the allocation of a subsidy depends on different perspectives of various actors. Their respective uncertainty level is 'medium' (level 2), as one is able to rank different alternatives based on their likelihood.

Table 6.3: Overview of included uncertain factors from the interviews

Uncertain factor	**Category**	**Location**	**Nature**	**Level**
Day-ahead electricity price (€)	Market	Context	Ambiguity/Ontology	4
Gas price (€)	Market	Context	Ambiguity	4
CO_2 emission price (€)	Policy/Market	Context	Ambiguity	2
NaOH 50% price (€)	Market	Context	Ambiguity	4
E-boiler CAPEX and OPEX (€)	Policy	Context	Ambiguity	1
Steam Pipe CAPEX (€)	Policy	Context	Ambiguity	1

6.1.2 Uncertain factors for Air Liquide

Since Air Liquide has not been interviewed by Thijsen (2018), it is essential to take another look at their production process as a means of capturing all external uncertainty affecting the Power-to-X alternatives. Looking back at the network diagram in figure 5.1, one can observe that Air Liquide buys natural gas and electricity from the market and sells steam, carbon dioxide, electricity, syngas, carbon monoxide and hydrogen (its main output product) to the market. Furthermore, they sell steam and carbon monoxide to their cluster partner Huntsman. Comparing this information with that in Table 6.2, it is clear that most uncertainty regarding these in- and output products is already covered by the uncertain factors identified during the interviews with Nouryon and Huntsman. However, the market prices of hydrogen, syngas and carbon monoxide are not yet accounted for. Syngas and carbon monoxide are often intermediate products for captive use. Hence, there is a lack of information regarding the price development of these products, making it very difficult to estimate their respective uncertainty.

In contrast, a lot of information is available about the future economics of hydrogen, due to its many applications. The latest report by the Hydrogen Council (2020), a global initiative of leading energy, transport and industry companies with a united ambition for hydrogen, shows that significant cost reductions are expected across different hydrogen applications, making the hydrogen route the decarbonization option of choice. Benoît Potier, Chairman and CEO of Air Liquide and Co-chair of the Hydrogen Council has even announced "the decade of hydrogen". More specifically, Patel (2020) concludes that in the short term (through 2025), hydrogen could become competitive in large vehicle transportation. Moreover, if the costs of its production and distribution continue to fall, hydrogen solutions could compete with other low-carbon alternatives by 2030. In other words, the price of hydrogen is expected to decrease, but the speed and trajectory of this process are uncertain.

The next step is to explore whether this factor also has a significant impact on one of the Power-to-X alternatives. In this case, this can be determined by considering the factors and causal relationships in the model. Hydrogen is the main output product of Air Liquide and they are relatively flexible in terms of its production level. This means that there is a significant difference between the minimum amount they are obliged to supply to the market and the maximum amount that they can produce. Hence, changes in the hydrogen price allows Air Liquide to change its production level. At a low hydrogen price, Air Liquide will ramp down their production, which decreases the amount of steam generated by this process. In this case, the E-boiler can be used to meet the contractual steam demand by their cluster partners and the market. In summary, the hydrogen price influences the need for the E-boiler at Air Liquide and therefore it is paramount to include it within the uncertainty analysis (see Table 6.4). Based on the aforementioned report, its uncertainty level is estimated as 'deep' (level 3).

Table 6.4: Uncertain factors identified for Air Liquide

Uncertain factor	**Category**	**Location**	**Nature**	**Level**
Hydrogen price (€)	Market	Context	Ambiguity	3

6.2 Uncertain model assumptions

As discussed in the theoretical framework, some objectives, constraints and policies are hard to capture in a Mixed Integer Linear Optimization (MILP) problem. Furthermore, since it is impossible to model the whole system, the modellers had to decide on certain model boundaries. Both of these problems result in the fact that certain simplifying assumption were made during the modelling process. Some of these assumptions may be both uncertain and influential in terms of evaluating the performance of the Power-to-X alternatives. Hence, the idea is to include these kind of assumptions as uncertain factors within the analysis. As means of identifying the most influential uncertain assumptions within the model, the factors surrounding the Power-to-X alternatives are carefully observed and compared to the uncertainty taxonomy found by Thijsen (2018).

To begin with, various uncertain assumptions were made for the E-boiler alternative at Air Liquide. In the current model, the values for its OPEX and CAPEX are fixed, based on certain assumptions made by the modellers. In the previous section, both these factors were already included in the uncertainty analysis, due to the potential effect of renewable energy subsidies. As Thijsen (2018) shows in Table 6.1, this inclusion is also justified through the uncertainty caused by external technological innovations.

Furthermore, the implementation of the E-boiler entails that Air Liquide has an automatic Frequency Restoration Reserve (aFRR) contract with the Transmission System Operator (TSO) to obligatory use surplus power as a means of maintaining balance on the electric grid. Figure 6.1 shows that the price for this downward balancing electricity can be either negative (receive) or positive (pay), depending on the *lowest* downward bid (TenneT & DTe, 2014). In the current model, the downward balancing price is fixed based on a certain average. However, due to potential changes in the merit order of the downward bids, this factor is considered uncertain and will be included for further analysis.

The final uncertain assumptions surrounding the E-boiler also revolve around the dynamics of the imbalance market shown in Figure 6.1. More specifically, Air Liquide buys a certain amount of electricity on the day-ahead market, based on the

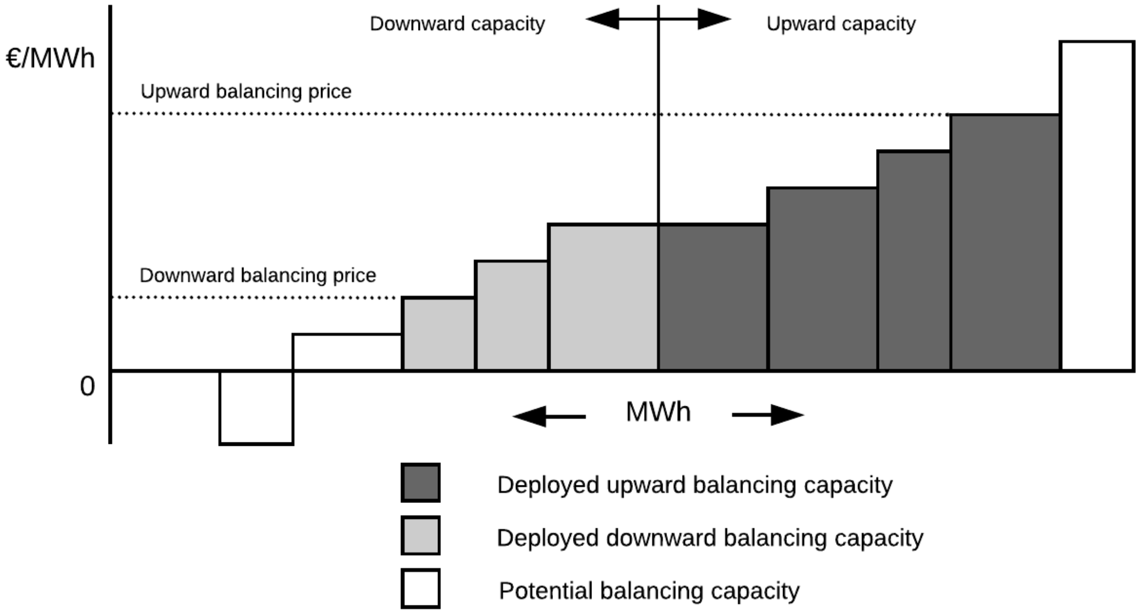


Figure 6.1: Identification of imbalance prices. Adapted from "Transparency for imbalance system", by Tennet and DTe, 2004, p.9.

requirements of their production process. If the *upward* balancing electricity price rises beyond a certain level, it might be more profitable to sell this electricity to the imbalance market than to use it for their own production process. Likewise, if the *downward* balancing electricity price drops, they can buy electricity from the imbalance market and use it to ramp-up their production. However, this system is fully dependent on the amount of electricity supply/demand on the imbalance market and the values of the up- and downward balancing prices. The current model assumes a fixed time series for these factors, while there is a lot of uncertainty surrounding the future development of this market (Conejo et al., 2010). Hence, in addition to the *downward* balancing electricity price, the *upward* balancing electricity price must be included for further analysis as well. The same applies to the amount of electricity supply/demand on the imbalance market.

Considering the Steam Pipe alternative, there is uncertainty regarding the amount of steam that is being injected into the Steam Pipe by the waste processing company AVR. As discussed during the stakeholder analysis, AVR has other contractual obligations and is also profit oriented. More specifically, it can/must use its generated heat for three purposes: electricity generation, district heating and steam delivery. Depending on the electricity price, seasonal temperature and contractual obligations, AVR will change the production ratio of these end products. Furthermore, the current model assumes that, apart from the back-up plan with Air Liquide, AVR is the only steam source in this alternative. However, a report by AVR (2017) shows that they have signed a contract for joint steam delivery with a chemical company named Cabot. In other words, there is a lot of uncertainty surrounding the steam supply for the Steam Pipe alternative. However, the model currently implements this factor as an optimization variable. This means that the solver finds a optimal value for the steam supply in the Steam Pipe, depending on its production costs and the demand of its users. Hence, it cannot be included as an uncertain factor. Instead, during the discussion and interpretation of the results, its feasibility will be assessed based on the identified uncertainty.

In respect to the third Power-to-X alternative, which entails Demand Side Management (DSM) using increased chlorine storage at Nouryon, there are two uncertain factors. The first factor is already covered by the interview results in Table 6.2 and concerns the required volume of storage capacity. The current model assumes certain upper and lower bounds for this factor and finds an optimal solution accordingly. Since the model was developed in consultation with Nouryon and potential storage capacity can be estimated without uncertainty, one can assume that these values are correct. Hence, this factor will be excluded from further analysis. Furthermore, the model assumes certain values for the chlorine demand by market actors. Since this market consists of only two actors and this assumption is not considered uncertain by the modellers, this factor will not be included in the analysis.

Table 6.5 shows the uncertain factors identified in this section. Since their source of uncertainty is located outside the chemical cluster, the location dimension of these factors is assessed as contextual. Similarly to the electricity price, their nature is considered to be part ontological due to the inherent variability of weather conditions that affects the renewable energy supply. The level dimensions are estimated based on previously mentioned reports and modeller consultation.

Table 6.5: Uncertain factors identified in the model assumptions

Uncertain factor	**Category**	**Location**	**Nature**	**Level**
Up- and downward balancing electricity prices (€)	Market	Context	Ambiguity/Ontology	2
Electricity supply/demand on imbalance market (MWh)	Market	Context	Ambiguity/Ontology	2

6.3 Overview of included uncertain factors

In summary, Table 6.6 presents an overview of the uncertain factors that were identified in the previous sections. The units are now specified in more detail, based on model properties. Furthermore, an explanation is provided per factor to indicate the reason for its inclusion and the source of its identification.

Table 6.6: Overview of included uncertain factors

Uncertain factor	**Explanation**	**Level**
Day-ahead electricity price (€/MWh)	Directly affects the economic feasibility of the E-boiler alternative. Identified by Thijsen (2018).	4
Gas price (€/Nm^3)	Affects the economic feasibility of the E-boiler alternative compared to gas combustion. Identified by Thijsen (2018).	4
CO_2 emission price (€/ton)	Affects the economic feasibility of the E-boiler alternative compared to gas combustion. Identified by Thijsen (2018).	2
Hydrogen price (€/Nm^3)	Affects the need for the E-boiler alternative to meet steam demand. Identified in Section 6.1.2 using model causalities.	3
NaOH 50% price (€/ton)	Plays an important role in the behaviour of the chlorine storage alternative. Identified in Section 6.1.1 using research by Thijsen (2018).	4
Up- and downward balancing electricity prices (€/MWh)	Affects the economic feasibility of the E-boiler alternative, also through aFRR contracts. Identified in Section 6.2 using information provided by TenneT & DTe (2014).	2
Electricity supply/demand on imbalance market (MWh)	Determines the potential production level of the E-boiler alternative. Identified in Section 6.2 using information provided by TenneT & DTe (2014).	2
E-boiler CAPEX (€/MW)	Affects the economic feasibility of the E-boiler alternative. Identified in Section 6.1.1 using research by Thijsen (2018).	2
E-boiler OPEX (€/MW/year)	Affects the economic feasibility of the E-boiler alternative. Identified in Section 6.1.1 using research by Thijsen (2018).	2
Steam Pipe CAPEX (€)	Affects economic feasibility of the Steam Pipe alternative. Identified in Section 6.1.1 using research by Thijsen (2018).	2

6.4 Modelling future development

To determine how the future development of the included uncertain factors should be modelled, it is important to take another look at the guidelines in Table 3.1 of the theoretical framework. All of the included factors are of medium uncertainty (level 2) or higher. Hence, to explore their potential impact, it is paramount to model their future development by looking at multiple plausible futures.To be able to generate and analyze these plausible futures, this research uses a methodology called Exploratory Modeling and Analysis (EMA). This methodology requires data regarding current (reference) values and sampling ranges of the uncertain factors. A sampling range entails a lower and upper bound of a factor at a certain point in future time. This fixed point in time is called the time horizon and defines the duration of time for outcome assessment. In this case, it also represents the run-time of the model. Since economic feasibility is an important KPI in this analysis, the time horizon must be carefully considered (Basu & Maciejewski, 2019). One the one hand, it must be long enough to capture the intended and unintended benefits and harms of the alternatives. On the other hand, if the time horizon is too long, it may add unnecessary costs and complexity to the analysis. Kim et al. (2017) recommend the use of *lifetime* horizon for this type of analysis. Following this line reasoning, the time horizon should be based on the lifetime of the Power-to-X alternatives. The lifetimes of the Steam Pipe and the chlorine storage alternatives are very long and would cause unnecessary costs and complexity. Hence, the minimal lifetime of the E-boiler is used for the time horizon, which entails a period of 10 years (Navigant, 2019). Since the current year is 2020, this means that the lower and upper bound of the uncertain factors will be based on forecasts for 2030.

Furthermore, for some of the uncertain factors, the reference value and future bandwidth cannot be based on single values. This is due to the fact that these factors are characterized by heavy fluctuations on a very small time scale. For example, the balancing electricity prices change every quarter of an hour. Incorporating these fluctuations is crucial for modelling the dynamic workings of the electricity market. Hence, for these kinds of uncertain factors, historical or forecast *time series* are used. These entire time series can then by multiplied by a scaling factor to create multiple futures. The lower and upper bound of such a scaling factor determine the sampling ranges. Its current value represents the reference scenario and is therefore zero. In contrast, other uncertain factors like the CAPEX and OPEX of the E-boiler, entail certain investment decisions that take place at time step zero and are not repeated afterwards. This means that the value of such a factor stays *constant* over time based on the sampled value between its lower and upper bound.

Appendix A contains a detailed description of the identification of the reference values and sampling ranges for every uncertain factor. As discussed previously, some of the uncertain factors use a scaling factor to generate multiple future trajectories. In these cases, uncertainty is often located in that specific factor. Hence, some of the names of the uncertain factors are altered. In summary, Table 6.7 provides an overview of the results from Appendix A. Apart from the constant data, there are various types of time series representing the future development of the uncertain factors. To provide a decent understanding of the characteristics of these different types and how they are generated, they are explained in the following subsections.

Table 6.7: Sampling ranges of the uncertain factors

Uncertain factor	**Reference Value**	**Lower Bound**	**Upper Bound**	**Resultant data**
Scaling factor day-ahead electricity price (-)	0	0.7	1.3	Scaling time series
Gas price in 2030 (€/Nm^3)	0.28	0.16	0.32	Linear time series
CO_2 emission price in 2030 (€/ton)	25	21	150	Linear time series
Hydrogen price in 2030 (€/Nm^3)	0.18	0.12	0.30	Linear time series
Cyclical frequency of NaOH 50% price (cycle/year)	0.2	0.1	0.3	Cyclical time series
Scaling factor up- and downward balancing electricity prices (-)	0	0.7	1.3	Scaling time series
Scaling factor electricity supply/demand on imbalance market (-)	0	0.7	1.3	Scaling time series
E-boiler CAPEX (€/MW)	$2*10^6$	$1.4*10^6$	$2*10^6$	Constant
E-boiler OPEX (€/MW/year)	4000	2800	4000	Constant
Steam Pipe CAPEX (€)	$12*10^6$	$6*10^6$	$12*10^6$	Constant

6.4.1 Linear time series

For the gas price, CO_2 emission price and the hydrogen price, multiple linear time series are generated using their reference values and sampling ranges for 2030. This generation process uses a generic equation to define the development of an uncertain factor (f) as a function of time (t) for every sampled value (s):

$$f(t)_s = \frac{s-c}{T} * t + c$$

For

$$\{s \mid B_L \leq s \leq B_U\}$$

Within this equation, the gradient of the linear function is given by subtracting the reference value (c) from the sampled value (s) and dividing it by the time horizon (T). The sampled value is taken from a set of values between the lower bound (B_L) and the upper bound (B_U). Figure 6.2 demonstrates how this generic equation works and what the resulting functions may look like.

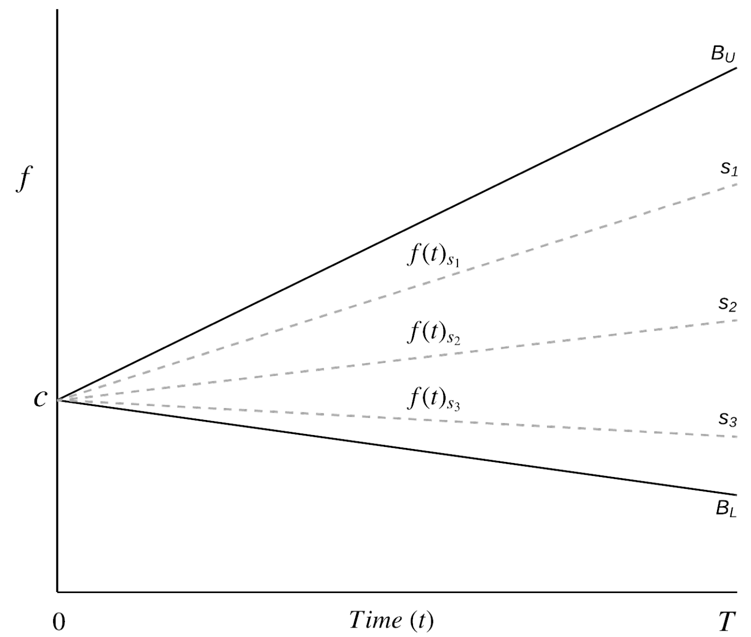


Figure 6.2: Technique for the generation of multiple linear time series

6.4.2 Scaling time series

For the uncertain factors involving the imbalance and day-ahead electricity markets, *scaling* time series are used. The generation of this data type requires two time series: a historical (empirical) time series as a reference scenario and a forecast (for 2030) time series created with the help of the scaling factor. Using linear functions between the data points of these two time series, multiple time series can be generated for each intermediate year. As an example, Figure A.2 illustrates how this method works for a three year forecast for the day-ahead electricity price.

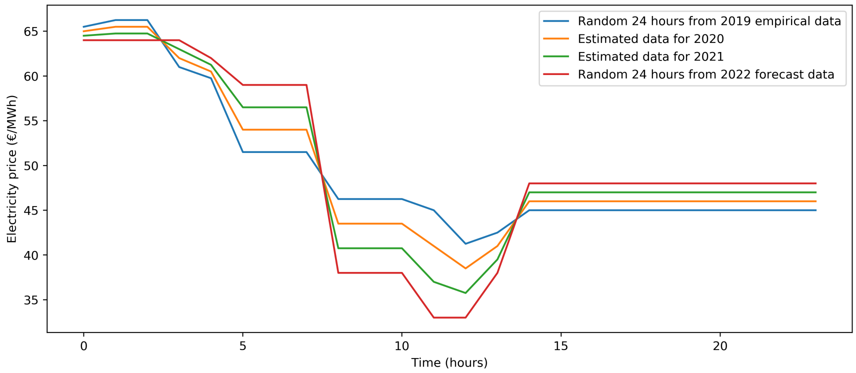


Figure 6.3: Illustration of the methodology for scaling time series

6.4.3 Cyclical time series

The price of 50% caustic soda (NaOH) has fluctuated heavily over the past few years. However, finding decent data on this topic is relatively hard. Stakeholder consultation resulted in the identification that the uncertainty is mainly located in the frequency of these fluctuations. Assuming there is some kind yearly cyclicality in the behaviour of the NaOH price, it is possible to capture its future development with a generic sine function:

$$y(t) = A * \sin(B * 2\pi * (t + C)) + D$$

This function has an amplitude (A), a cyclical frequency (B), time (t), horizontal shift (C) and vertical shift (D). Based on research, values were estimated for these variables (see Appendix A). As an example, Figure 6.4 illustrates how multiple time series can be generated for the NaOH price, by changing its cyclical frequency to a lower and upper bound.

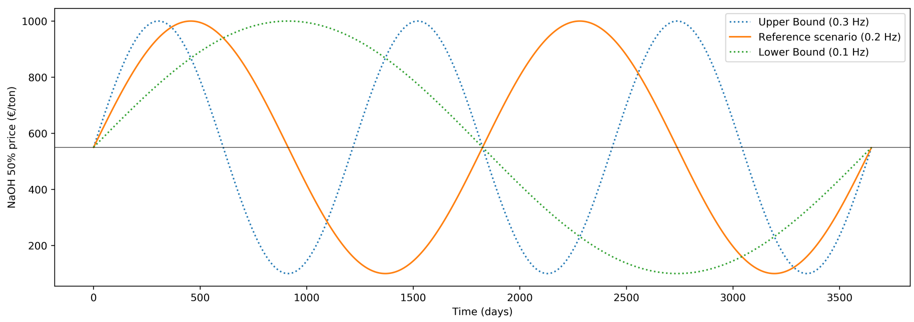


Figure 6.4: Illustration of technique for creating multiple cyclical time series

Chapter 7

Uncertainty analysis

In this chapter the uncertainty analysis is addressed. The first section explains the experimental design by discussing its most important components and by illustrating the design in a flow diagram. The subsequent sections discuss the results of different parts of the uncertainty analysis.

As a means of establishing a solid foundation in terms of consistent concept use, it is paramount to define some of the core concepts of this uncertainty analysis:

- Uncertain factors: factors that cannot be directly controlled by the stakeholders. These were identified in the previous chapter.
- Scenario: a set of values, one for each uncertain factor.
- Alternatives: options that the stakeholders can choose to implement (decision variables). In this case, these are the three Power-to-X options.
- Policy: a set of values, one for each alternative.
- Experiment: the required input for a model run, consisting of a certain scenario and policy combination.
- Outcome: an output variable of the model that has been identified as an performance indicator.

7.1 Experimental design

To create an effective experimental design, it is important to look back at the research questions that are expected to be answered by this uncertainty analysis:

3. *To what extent do the external uncertain factors affect the performance of the alternatives?*
4. *What strategies are optimal in terms of economic feasibility and decarbonization and what strategies are robust?*
5. *What are the key trade-offs among the strategies from individual and collective points of view?*

Before the experimental design can be put together, it is paramount to define its components. The following five subsections will discuss these components in detail. Afterwards, the different components are combined in a flow diagram that also explains the techniques used to answer each research question.

7.1.1 Uncertain factors

The uncertain factors with their reference values and sampling ranges were identified in the previous chapter and are now shown in Table 7.1. To enhance the readability of certain visualizations later on, each factor is given an abbreviation label. The set of uncertain factors entails a twelve-dimensional uncertainty space. To explore this space, Latin Hypercube Sampling (LHS) is used to make a twelve-dimensional sample of 100 alternative future states of the system.

Table 7.1: Sampling ranges of the uncertain factors

Uncertain factor	**Abbreviation**	**Reference Value**	**Lower Bound**	**Upper Bound**
Scaling factor day-ahead electricity price (-)	SF-DAE-P	0	0.7	1.3
Gas price in 2030 (€/Nm^3)	Gas-P-2030	0.28	0.16	0.32
CO_2 emission price in 2030 (€/ton)	CO2-P-2030	25	21	150
Hydrogen price in 2030 (€/Nm^3)	Hydro-P-2030	0.18	0.12	0.30
Cyclical frequency of NaOH 50% price (cycle/year)	CyFr-NaOH-P	0.2	0.1	0.3
Scaling factor up- and downward balancing electricity prices (-)	SF-(U/D)BE-P	0	0.7	1.3
Scaling factor electricity supply/demand on imbalance market (-)	SF-(S/D)IM	0	0.7	1.3
E-boiler CAPEX (€/MW)	Eb-CAPEX	$2*10^6$	$1.4*10^6$	$2*10^6$
E-boiler OPEX (€/MW/year)	Eb-OPEX	4000	2800	4000
Steam Pipe CAPEX (€)	SP-CAPEX	$12*10^6$	$6*10^6$	$12*10^6$

7.1.2 Alternatives and policies

The alternatives or decision variables are the three Power-to-X options as previously introduced. Table 7.2 shows that all of these variables are booleans, which in this case means that their value can be either 'implemented' or 'not implemented'.

Table 7.2: Alternatives

Alternative	**Variable type**	**Possible values**
E-boiler	Boolean	Implemented / Not implemented
Steam Pipe	Boolean	Implemented / Not implemented
Chlorine storage	Boolean	Implemented / Not implemented

Furthermore, policies are formed by different configurations of these alternatives. Table 7.3 shows how the full factorial set of these alternatives results in eight different policies:

Table 7.3: Policies

Policy	**E-boiler**	**Steam Pipe**	**Chlorine Storage**
None of the options	Not implemented	Not implemented	Not implemented
Only Steam Pipe	Not implemented	Implemented	Not implemented
Only E-boiler	Implemented	Not implemented	Not implemented
Only Chlorine storage	Not implemented	Not implemented	Implemented
Steam Pipe and E-boiler	Implemented	Implemented	Not implemented
Steam Pipe and Chlorine storage	Not implemented	Implemented	Implemented
E-boiler and Chlorine storage	Implemented	Not implemented	Implemented
All options	Implemented	Implemented	Implemented

7.1.3 Actor optimization perspectives

To answer the fifth research question regarding the individual and collective perspectives, four different versions of the original model are used. One version financially optimizes the production processes from a collective cluster perspective. Apart from the main stakeholders, this collective perspective includes other less-involved actors as well. Three other model versions optimize from the individual perspective of one the main stakeholders. Table 7.4 shows the different "optimization perspectives" and corresponding models used in this uncertainty analysis. Before moving on, it is paramount to discuss these optimization perspectives in more detail. When the objective function of the MILP problem is altered to minimize the costs of an individual actor or group of actors (see Section 4.3.3), it means that the remainder of the actors will do anything in their power (as far the boundaries of their products and processes allow it) to ensure the lowest possible production costs for the actors included in the optimization perspective. In other words, one could argue that the actors not included in the optimization perspective become "enslaved". This state of affairs might not be considered a valid representation of reality, because these actors are unlikely to behave this way. Nevertheless, since it is key to consider both the individual actor and cluster level during decision-making in this field (see Section 3.1.1), the optimization perspectives can potentially reveal interesting trade-offs that contribute towards a balanced decision-making process.

Table 7.4: Model versions

Optimization perspective	**Model file name**	**Financial optimization actor(s)**
Collective	botlek_model_collective.lnr	All the actors in the system
Air Liquide	botlek_model_airliquide.lnr	Air Liquide
Nouryon	botlek_model_nouryon.lnr	Nouryon
Huntsman	botlek_model_huntsman.lnr	Huntsman

7.1.4 Outcomes

Within the stakeholder analysis, three Key Performance Indicators (KPIs) were identified for the Power-to-X alternatives: economic feasibility, decarbonization and security of supply (see Section 5.5). In terms of model output, economic feasibility translates to the cash flow of the entire cluster as well as the clash of flows of individual actors. Decarbonization can be evaluated by looking at the total CO_2 emissions of the system. Regarding security of supply, this is not a realistic performance indicator to evaluate with a MILP problem. By default, the solver already satisfies the lower bounds (contractual obligations) of product delivery. Therefore, this KPI is excluded from the analysis. An overview of the included outcomes is displayed in Table 7.5.

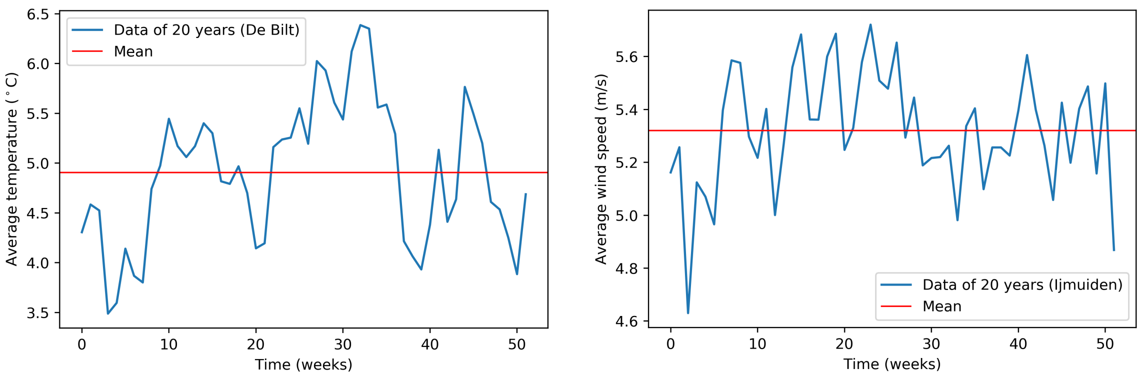
Table 7.5: Outcomes

Outcome	**Abbreviation**	**Corresponding KPI**	**Original output type**
Cash flow of the cluster (€)	CF Cluster	Economic feasibility	Time series
Cash flow of Air Liquide (€)	CF Air Liquide	Economic feasibility	Time series
Cash flow of Nouryon (€)	CF Nouryon	Economic feasibility	Time series
Cash flow of Huntsman (€)	CF Huntsman	Economic feasibility	Time series
CO_2 emissions (ton)	CO2 Emissions	Decarbonization	Time series

7.1.5 Model run-time

During the modelling of the future development of the uncertain factors, a time horizon of ten years was chosen for the uncertainty analysis (see Section 6.4). However, simple experiments with the model revealed that running these full ten years results in unmanageable long run times. Hence, a different creative approach was required. The implemented solution is to run one characteristic week for each of the ten years. This time period of one week is carefully chosen based on the cycle time of the different model variables. For the validity of this approach, it is paramount that the cycle time of these variables fits within the chosen period.

The characteristic week is identified based on variables that have a major influence on the seasonal fluctuations of the uncertain factors. Within this analysis, the uncertain factors surrounding the electricity market are the only factors whose future trajectory is based on empirical or forecast data that is characterized by this seasonality. In a country with moderate summer temperatures like the Netherlands, electricity demand generally peaks in the winter and shows a minimum in the summer. However, within a study performed by Hekkenberg et al. (2009), a trend was identified indicating that higher temperatures can nowadays lead to a higher electricity demand due to the increased use of cooling applications. Furthermore, due to the expected increase in off-shore wind energy, the wind speed becomes a increasingly relevant variable, because it influences the day-ahead electricity prices (Mulder & Scholtens, 2013). Hence, weekly averages of the temperature and wind speed of the past twenty years are used to identify the characteristic week (see Figure 7.1).



(a) Weekly average temperature

(b) Weekly average wind speed

Figure 7.1: Identification of the characteristic week (Data from KNMI)

The required data was retrieved from weather stations at different locations (KNMI, 2019). For the average temperature, a station located in the middle of the country was used (De Bilt). The wind speed data was retrieved from a weather station near the coast (Ijmuiden). When ranking the weeks in Figures 7.1a and 7.1a based on the absolute difference between their corresponding value and mean (red line), week nine is present in the top three of both the temperature and wind speed rankings. Therefore, this week is identified as characteristic for the average behaviour of the electricity market and will be used for further simulation.

While applying this approach to decrease the run-time, two problems surfaced. To begin with, the chosen period of one week is not enough to fully justify the uncertainty surrounding the cyclical frequency of the caustic soda price. This the only variable that is characterized by a cycle time that does not fit into one week. More specifically, its cycle time varies from three to ten years, based on the sampled value for its cyclical frequency. The implemented workaround for this problem is using the average caustic soda price of a certain year throughout its corresponding week. Furthermore, the initial the idea was to run ten weeks from different years consecutively in one model run. However, this resulted in unrealistic transitions from one week to another in terms of differences in prices and the supply/demand of products. Since the solver of the MILP problem has the ability to look into future, this may cause an actor to obtain unrealistic profits using storage opportunities. This problem is resolved by running the ten weeks separately in different models.

7.1.6 Linear solver

The MILP problems created by the models are solved using a block structure methodology (Martin, 1999). Each simulated week is divided into different blocks. Every block captures a number of time steps, given by the sum of the *period* and the *look-ahead*. In a system with storage, an appropriate value for the period is determined by looking at the cycle time of the storage system. The chlorine storage system at Nouryon entails a cycle time of 24 hours, based on certain safety restrictions. Since the time step corresponds to one quarter of an hour, this number is multiplied by four, resulting in a period of 96 time steps.

The look-ahead entails the number of time steps that the solver can look into the future. This is important for the efficient performance of the Demand Side Management (DSM) aspect of the chlorine storage alternative. However, larger values for the look-ahead can drastically increase the run-time of the model. Hence, multiple experiments were performed to see how different values for the look-ahead affect both storage behaviour and model run-time. To ensure that all other variables stay constant in these experiments, one specific combination of optimization model, policy and scenario is used. Figure 7.2 shows the results for one week (672 quarters).

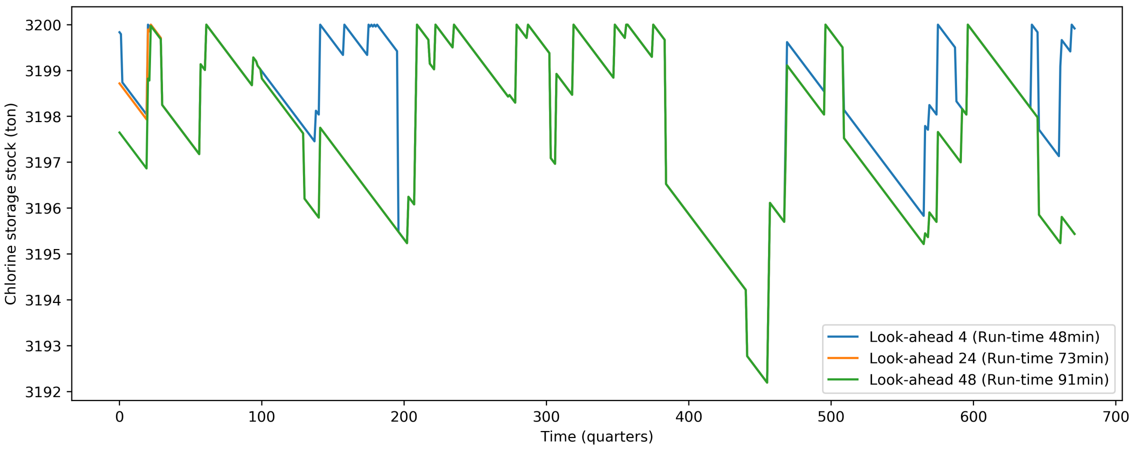


Figure 7.2: Chlorine storage stock for different values of the look-ahead

It is important to note that at the beginning of every week the initial value of the chlorine stock is equal to the maximum storage capacity. This decision was made to enhance the interpretability of the results, as experiments with various scenarios showed indistinguishable linear increases of the chlorine storage stock, due to its robust profitability and restricted amount of storage per time step. Starting each week with maximum storage allows for the identification of different storage behaviour. Figure 7.2 shows that look-aheads of 24 and 48 time steps achieve equal results in term of storage behaviour. Since a look-ahead of 48 time steps corresponds to a longer run time, this option can be excluded. To choose between the remaining values for the look-ahead, it is paramount to consider which corresponding storage behaviour is more valid. The look-ahead of 24 time steps is more profitable in terms of chlorine storage, since it is able to anticipate six hours of future market prices instead of one hour. Under the assumption that Nouryon would be able to make accurate forecasts for this relatively small time frame, it is considered the more valid option.

7.1.7 Flow diagram

To illustrate how all the previously discussed components come together and are used to answer the research questions, Figure 7.3 shows a flow diagram of the experimental design.

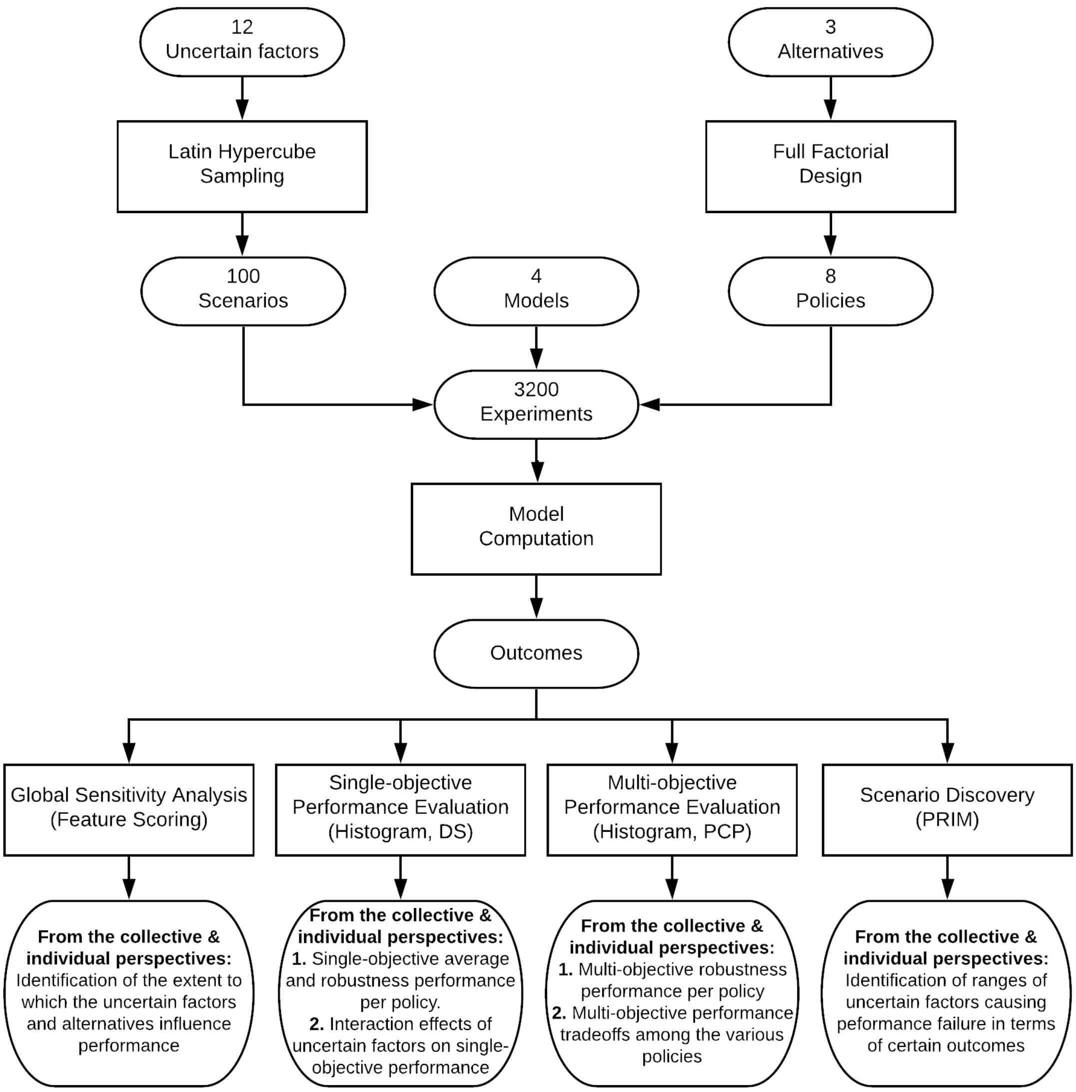


Figure 7.3: Flow diagram of the experimental design

The thousand scenarios, eight policies and four models together form a set of 3200 experiments. The outcomes of these experiments are analyzed using four different methods. Before discussing these methods, it is important to realize that each of the four models results in a different financial optimization perspective. It means that the results of every analysis method can be viewed from collective and individual actor perspectives. This extra dimension allows for a multi-perspective uncertainty analysis which can be used to answer the fifth research question.

Using Feature Scoring, a global sensitivity analysis is performed that identifies the relative effects of the uncertain factors and alternatives on the outcomes. This information provides an answer to the third research question. Feature Scoring is a family of techniques often used in machine learning to identify the most relevant features to include in a model. Its main advantage is that it imposes no specific constraints on the experimental design (Kwakkel, 2019). Based on any unsuspected or remarkable results of this sensitivity analysis, it is possible to perform model verification to reveal potential defects.

The single-objective performance of the policies is evaluated by visualizing both average performance and single-objective robustness from the different optimization perspectives in histograms. Based on the average performance, policies can be identified that are optimal in terms of decarbonization and economic feasibility, thereby answering the "optimal" part of the fourth research question. Furthermore, each policy is given a robustness score based on the numbers of scenarios in which it satisfies a certain *performance condition*. For example, using the condition "CO_2 emissions $< X$", one can evaluate the robustness of policies in terms of decarbonization. This information is part of the answer to the "robust" part of the fourth research question. In addition, Dimensional Stacking (DS) is used to visualize the interaction effects of the uncertain factors most influential in achieving a certain level of single-objective performance.

The multi-objective performance of the policies is evaluated by looking at multi-objective robustness. This different type of robustness is quantified and visualized using the same methodology as applied during single objective performance evaluation, only now the condition is based on more than one outcome. This analysis provides the other part of the answer to the "robust" part of the fourth research question. Following the steps of the Multi-Objective Robust Decision Making (MORDM) framework by Kasprzyk et al. (2013) (see Section 3.3.3), a Trade-off Analysis can be performed. In this case, Parallel Coordinate Plots (PCP) are used to illustrate the multi-objective performance trade-offs among the different policies. This is an answer to the third research question.

Lastly, "scenario discovery" is used to identify ranges of uncertain factors causing performance failure in terms of certain outcomes. This specific approach was introduced by (Bryant & Lempert, 2010) and can be used as address the challenges of characterizing and communicating deep uncertainty associated with simulation models (Dalal et al., 2013). More specifically, the Patient Rule Induction Method (PRIM) algorithm is used to identify one or various rectangular subspaces of the model input space within which the values of a single output variable are considerably different from its average values over the entire model input space (Kwakkel & Cunningham, 2016).

7.2 Global sensitivity analysis

The feature scoring technique used to perform the global sensitivity analysis is based on a statistical machine-learning approach called "extremely randomized trees" (Extra-Trees). It was introduced by Geurts et al. (2006) and uses decision trees to estimate regression coefficients. The global sensitivity analysis of the outcomes of the first set of experiments showed a number of unexpected results. Hence, model verification was performed and a number of problems were found (see Appendix B). Unfortunately, not every problem could be resolved in the available time frame. Nevertheless, one defect was resolved and all of the experiments were run again. Figure 7.4 shows the global sensitivity analysis performed using the outcomes of this experimental iteration.

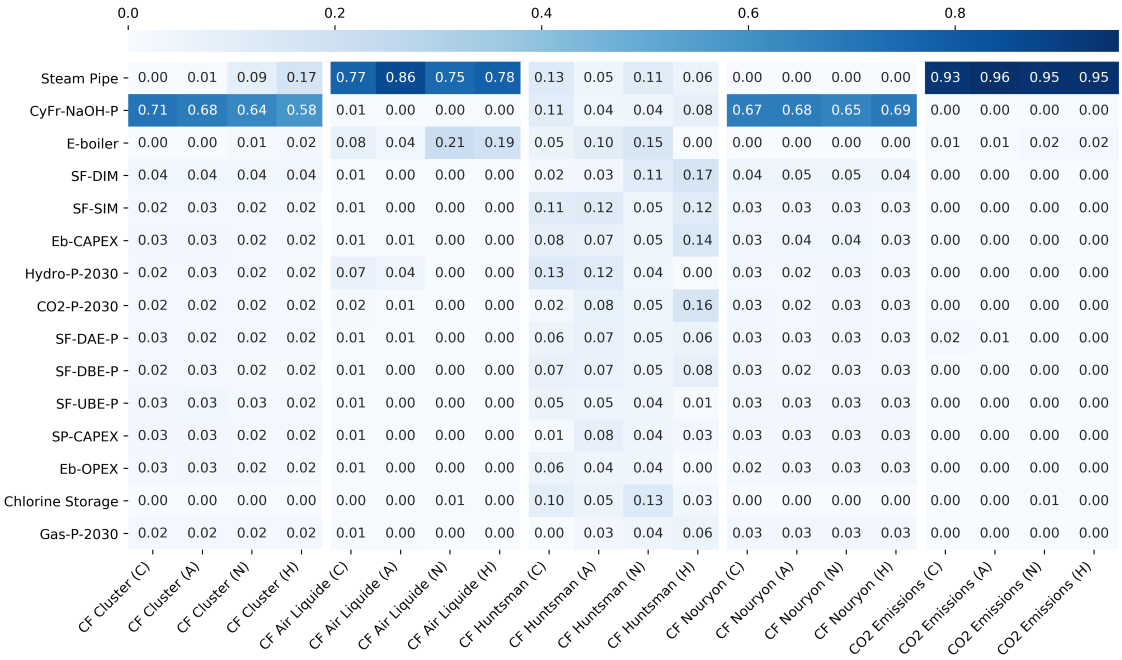


Figure 7.4: Feature scoring diagram

The vertical axis contains the uncertain factors and alternatives, ranked in descending order based on the sum of their estimated regression coefficients. The horizontal axis contains the outcomes grouped by optimization perspective. It is important to note that the estimated regression coefficients do not indicate the direction (increase or decrease) of an effect. They are merely indicators of the extent to which an uncertain factor or alternative influences a certain outcome.

By inspection of Figure 7.4, it is clear that some of the uncertain factors and alternatives still show behaviour which deviates from valid expectations. For example, all the uncertain factors have very little influence on any outcome compared to the influence of the cyclical frequency of the NaOH price on the cash flows of Nouryon and the entire cluster. Furthermore, the E-boiler seems to have a very low effect on the CO_2-emission outcome. In general, this means that there are still unexplained and unresolved problems within the model influencing the results. The extent to which this affects interpretation will be reflected on during the discussion in the next chapter.

7.3 Single-objective performance

In this section, the single-objective performance of the policies is evaluated based on average outcomes and robustness analysis. With respect to the uncertain factors, interaction effects on single-objective performance are identified using Dimensional Stacking (DS). First, economic feasibility is evaluated based on the cash flow of the entire cluster. Afterwards, the CO_2-emission outcome is used to look at decarbonization performance.

7.3.1 Economic feasibility

To identify policies that have good overall performance in terms of economic feasibility, the average value for the "Cash flow of the cluster" outcome is calculated per policy for the collective and individual optimization perspectives. Figure 7.5 shows the results of these calculations in a histogram.

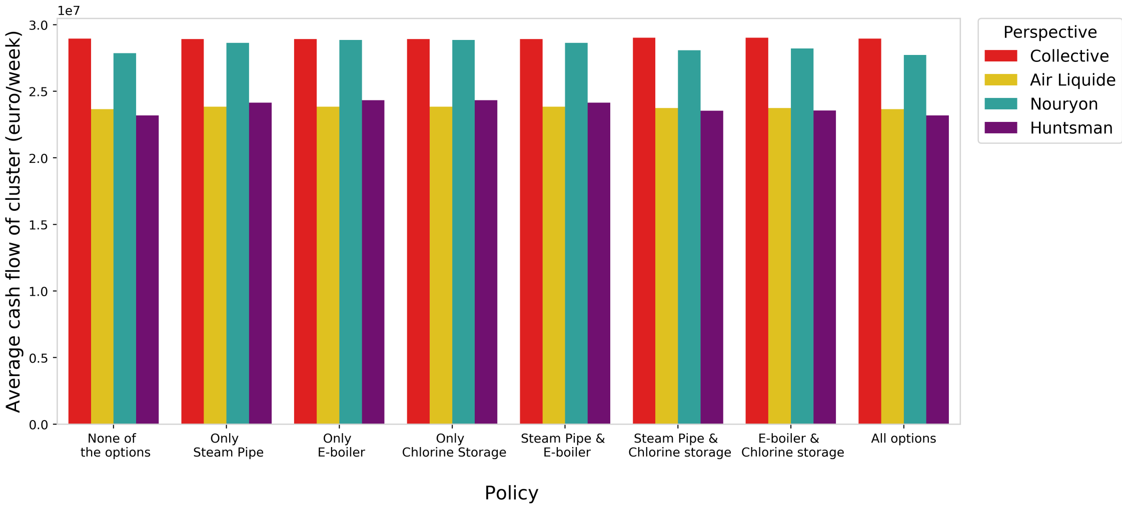


Figure 7.5: Histogram of average cluster cash flow per policy and perspective

The results in Figure 7.5 show that the differences between the average outcomes of the cluster cash flow are minimal across the set of policies. In terms of the differences among the four optimization perspectives, it is clear that average cash of the cluster is always higher when the model is financially optimized from the perspective of the Collective or Air Liquide. It is important to note that the exact numbers of the cash flow outcomes are not valid, because various kinds of costs were not included in the model. Hence, these numbers can only be used for comparison.

To further evaluate the economic performance of the policies, one can look at their robustness in respect to this performance indicator. In order to identify the economic robustness of the policies, the total set of experiments and outcomes is filtered based on the condition that the "Cash flow of the cluster" outcome is larger than its 80th percentile. This percentile is based on the entire set of outcomes and not per individual optimization perspective in order to discover the overall robustness per combination of policy and perspective. Next up, each of the eight policies is given an "Economic robustness score" per optimization perspective, based on the fraction of the total amount of scenarios in which it satisfies the performance condition. Figure 7.6 shows a histogram of the results.

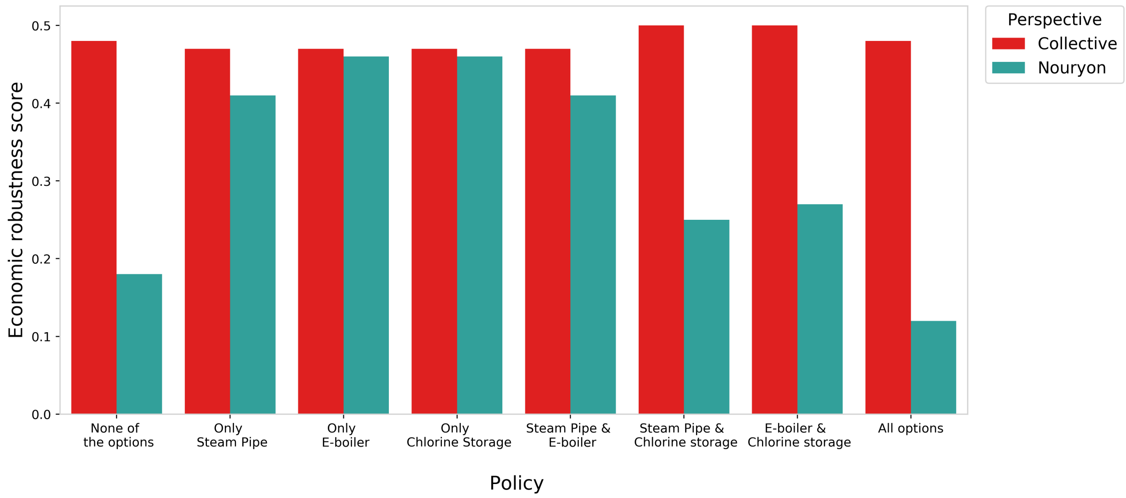
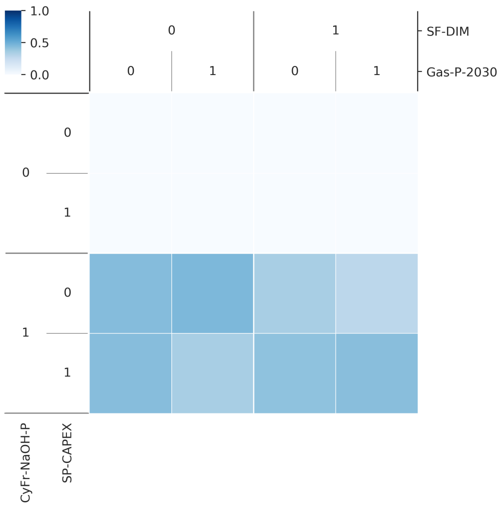


Figure 7.6: Histogram of economic robustness per policy and perspective

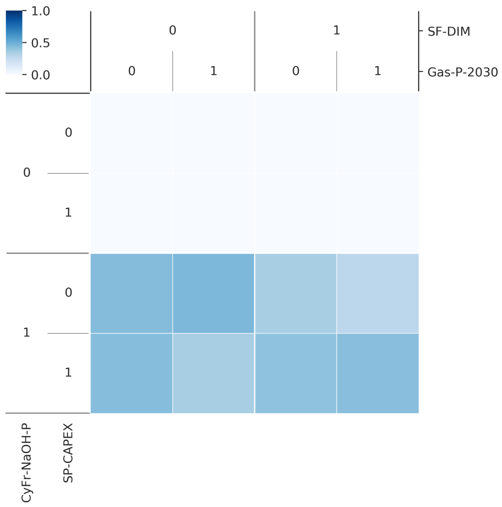
The results of the economic robustness analysis show that cluster cash flows above the 80th percentile are only realized from the Collective and Nouryon optimization perspectives. Overall, it can be observed that financially optimizing from the Collective perspective results in a higher level of economic robustness across the different policies compared to the Nouryon perspective. The economic robustness scores per policy from the Collective perspective are all around 0.5, meaning the policies achieve the desired robust performance in 50% of the evaluated scenarios.

Apart from the policies, it also is important to analyze how the uncertain factors influence the economic feasibility performance. A potentially interesting method for the visualization of these effects is called Dimensional Stacking (DS). In terms of computation, this method performs feature scoring using random forests (see Section 7.2), selects a number of high scoring factors based on the specified number of levels and creates a pivot table for visualization (Kwakkel, 2019). Within this table, one can observe how various uncertain factors interact while achieving a certain level of an outcome of interest. Figure 7.7 shows these tables per optimization perspective for the same condition as used for the robustness analysis. Within each table, the vertical and horizontal together contain four of the most influential factors for the outcome of interest. Furthermore, the numbers zero and one indicate low and high values respectively for these factors.

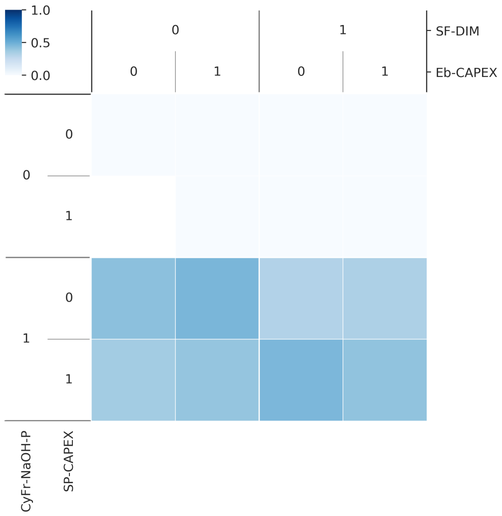
The pivot tables in Figure 7.7 show that for every optimization perspective, a high cyclical frequency of the NaOH price has a significant effect on realizing “Cash flow of the cluster” outcomes larger than its 80th percentile. This in line with the results of the global sensitivity analysis. Furthermore, while the cyclical frequency is high, the other uncertain factors identified as most influential seem to have little effect. Nonetheless, the CAPEX of the Steam Pipe and the scaling factor of the electricity demand on the imbalance market have been identified for all four of the optimization perspectives. The fourth influential uncertain factor varies across the perspectives. For the Collective and Nouryon it is the gas price in 2030, while for Nouryon and Huntsman the CAPEX of the E-boiler is more important in realizing a relatively high economic feasibility for the entire cluster.



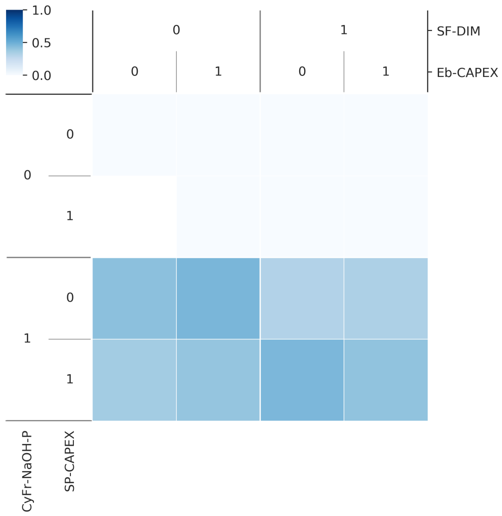
(a) Collective



(b) Air Liquide



(c) Nouryon



(d) Huntsman

Figure 7.7: Dimensional stacking economic feasibility per optimization perspective

7.3.2 Decarbonization

The same approach is applied to the decarbonization objective. First, the average value for the "CO_2 emission" outcome is calculated per policy for the collective and individual optimization perspectives. Figure 7.8 shows the results.

In contrast to the average economic performance, Figure 7.8 shows that there are differences among policies and between perspectives in terms of average CO_2 emissions. More specifically, optimizing from either the Nouryon or Huntsman perspective, results in significantly lower CO_2 emissions for every policy. Furthermore, it can be observed that the alternatives are only effective in terms in CO_2 reduction when they are implemented together. Remember that the numbers in Figure 7.8 can only be used for comparison purposes, since various kinds of CO_2 emission sources were not accounted for in the model.

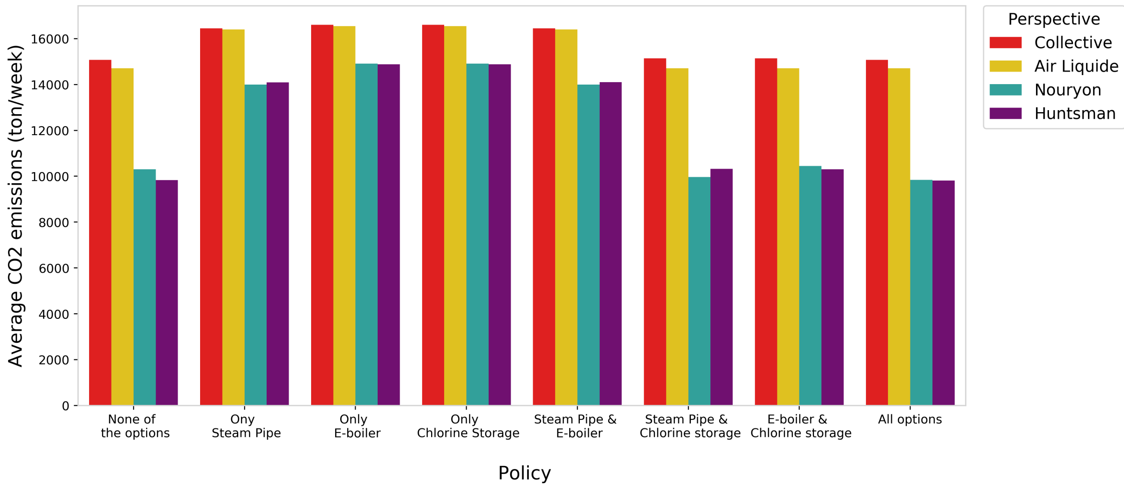


Figure 7.8: Histogram of average CO_2 emissions per policy and perspective

The robustness in terms of decarbonization performance is evaluated by filtering the total set of experiments and corresponding outcomes based on the condition that the "CO_2 emissions" outcome is lower than its 20th percentile. Afterwards, each of the eight policies is given a "Decarbonization robustness score" per optimization perspective, based on the fraction of the total amount scenarios in which it satisfies the performance condition. Figure 7.9 shows a histogram of the results.

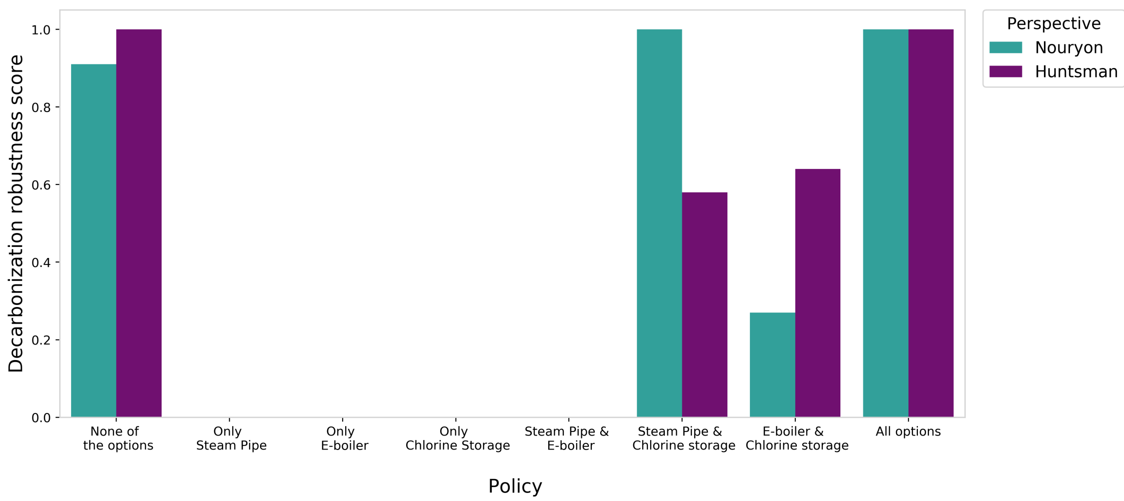
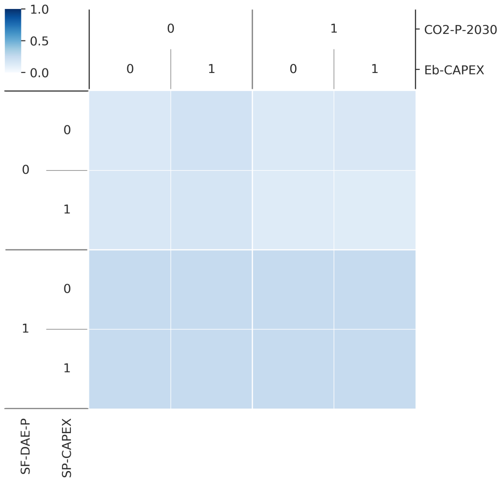


Figure 7.9: Histogram of decarbonization robustness per policy and perspective

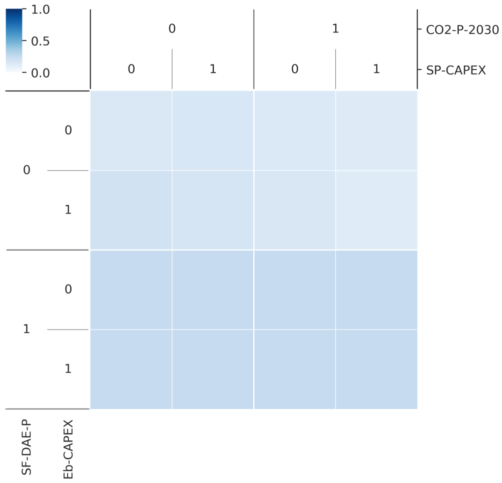
The results of this analysis show that relatively low CO_2 emissions are only achieved when the model is optimized from the financial perspective of either Nouryon or Huntsman. Furthermore, it is obvious that some policies do not have the ability to realize these outcomes. In contrast, the policies that do possess this ability have very high or maximum robustness scores. A maximum decarbonization robustness score (1.0) for a specific policy means that it honors the specified condition of relatively low CO_2 emissions in all of of the scenarios included in the experimental setup. In other words, when optimizing from either Nouryon's or Huntsman's perspective, implementing none of the options or implementing all options is an extremely robust choice in terms of decarbonization.

Similar to the evaluation of the economic feasibility performance, it also is important to analyze how the uncertain factors influence decarbonization. Using Dimensional Stacking, the interaction effects among the most influential factors are visualized per optimization perspective in Figure 7.10 using the same condition as applied during the robustness analysis.

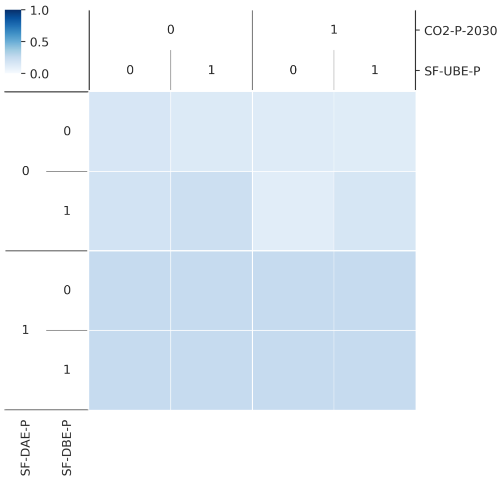
The results show that all the interaction effects of the identified factors are close to equal in terms of their effect on realizing low CO_2 emission outcomes. This is true for every optimization perspective. Nevertheless, it seems like a high scaling factor for the day-ahead electricity price has the largest influence. This factor is also identified in every optimization perspective. This is also true for the CO_2 emission allowances price in 2030 and the CAPEX of the Steam Pipe.



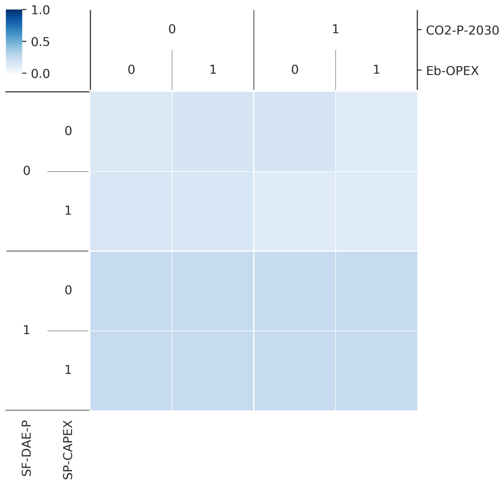
(a) Collective



(b) Air Liquide



(c) Nouryon



(d) Huntsman

Figure 7.10: Dimensional stacking for decarbonization per optimization perspective

7.4 Multi-objective performance

In this section, the performance of the policies is evaluated based on multi-objective conditions. In this case, the goal is to find policies that are robust in terms of both economic feasibility and decarbonization. Hence, the multi-objective conditions use outcomes related to both KPIs. First, a multi-objective robustness analysis is performed and visualized in a histogram. Afterwards, Parallel Coordinate Plots (PCPs) are used to illustrate the multi-objective performance trade-offs amongst the different policies and optimization perspectives.

7.4.1 Overall robustness analysis

To identify policies that are robust in terms of both economic feasibility and decarbonization, the total set of experiments and corresponding outcomes is filtered based on the following two-fold performance condition: the "Cash flow of the cluster" outcome is larger than its 70th percentile and the "CO_2 emissions" outcome is smaller than its 30th percentile. Afterwards, each of the eight policies is given a "Multi-objective robustness score" per optimization perspective, based on the fraction of the total amount scenarios in which its outcomes satisfy the performance condition. The results of this analysis are visualized in Figure 7.11.

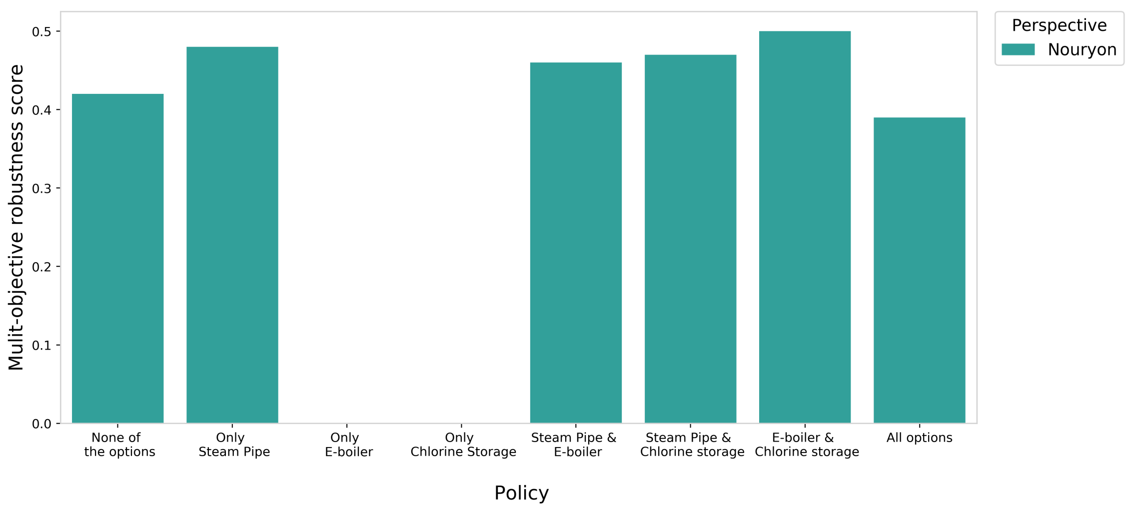
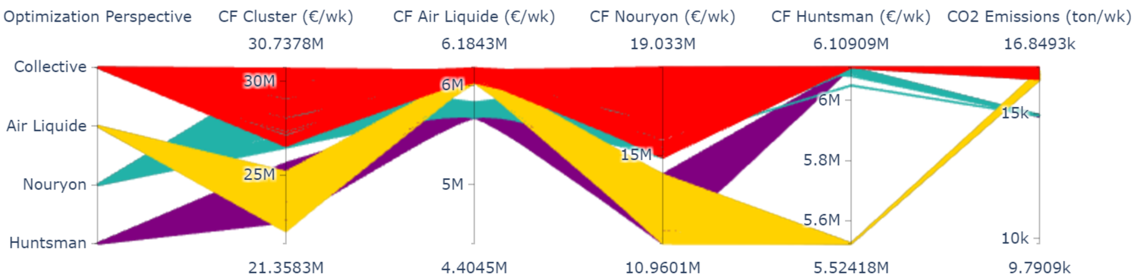


Figure 7.11: Histogram of multi-objective robustness per policy and perspective

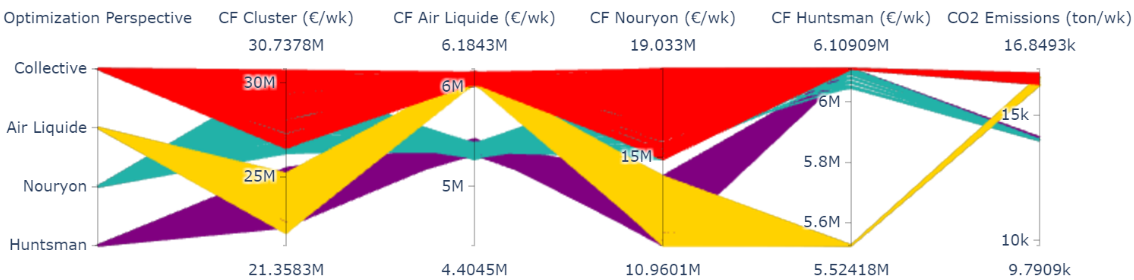
The histogram shows that only when the model is financially optimized from Nouryon's perspective, outcomes are retrieved of relatively high cluster cash flows and low CO_2 emissions. This observation is in line with the average outcome histograms in Sections 7.3.1 and 7.3.2. Furthermore, the policies that only implement the E-boiler or Chlorine storage have a robustness scores of zero for all perspectives. This means that these two policies will not result in the desired outcomes from any of the optimization perspectives. In contrast to the high decarbonization robustness scores for some of the policies (see Section 7.3.2), this multi-objective condition results in robustness scores around 0.45. This number entails that in roughly 45% of the tested scenarios, the remaining six policies honored the specified condition of a relatively high cluster cash flow and low CO_2 emissions.

7.4.2 Performance trade-offs

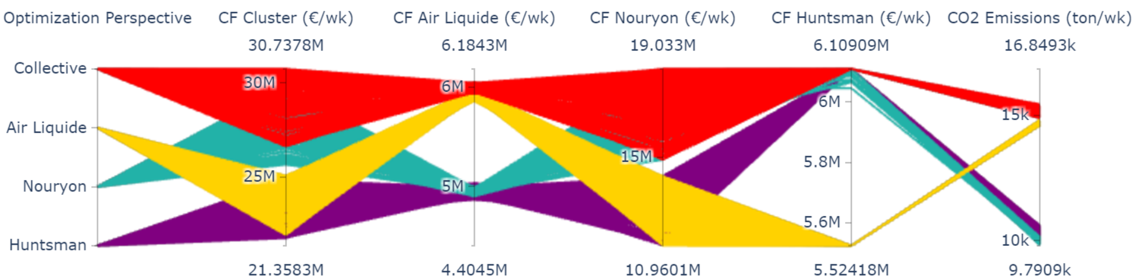
So far, two out of five outcomes have been analyzed: "CO_2 emissions" and "Cash flow of the cluster". However, it is paramount to also analyze how the individual cash flows of the main stakeholders change over the different policy and perspective combinations. As a means of visualizing all of these important trade-offs, Parallel Coordinate Plots (PCPs) were constructed (see Figure 7.12). In terms of average outcomes, the histograms in Sections 7.3.1 and 7.3.2 showed relatively small differences among policies and much larger differences across optimization perspectives. Therefore, the PCPs are designed to focus on illustrating trade-offs among the latter category. This decision results in eight plots, one for each policy. Each outcome is given its own axis with a unique scale that remains constant over the different plots to allow for a fair comparison. The outcomes of a specific experiment are plotted as a single line connecting all the axes. Each optimization perspective is given a different color. Instead of using a legend, an additional axes is created at the left-hand side to demonstrate which perspective belongs to which color. It is paramount to note that the exact values on the axes are not meant to be interpreted in isolation, because they are not valid representations of the real-world system. Rather, the idea is to perform an overall comparison of the trade-offs and differences among the optimization perspectives and across the various policies.



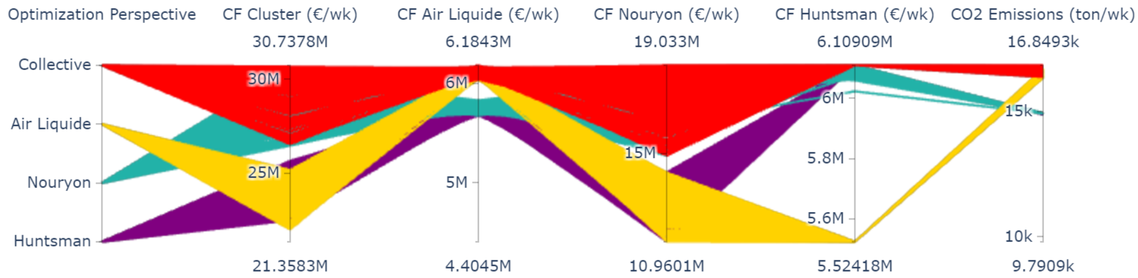
(a) None of the options



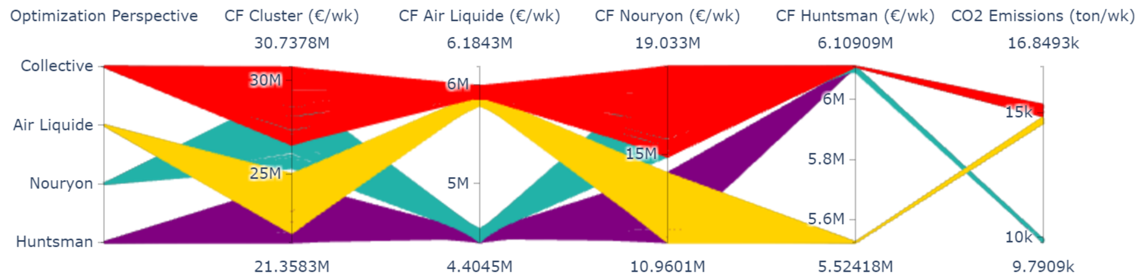
(b) Only E-boiler



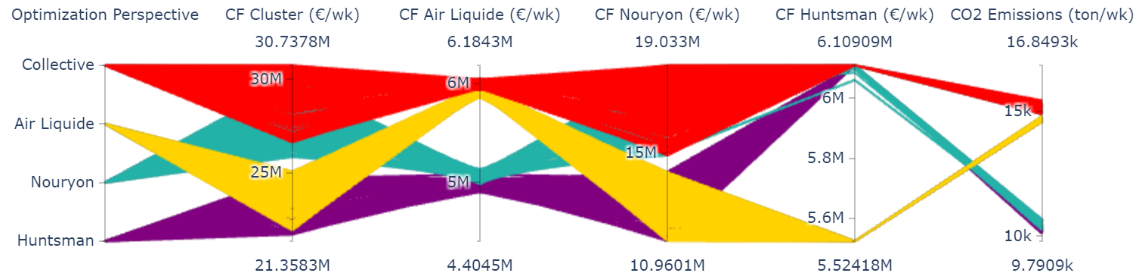
(c) Only Steam Pipe



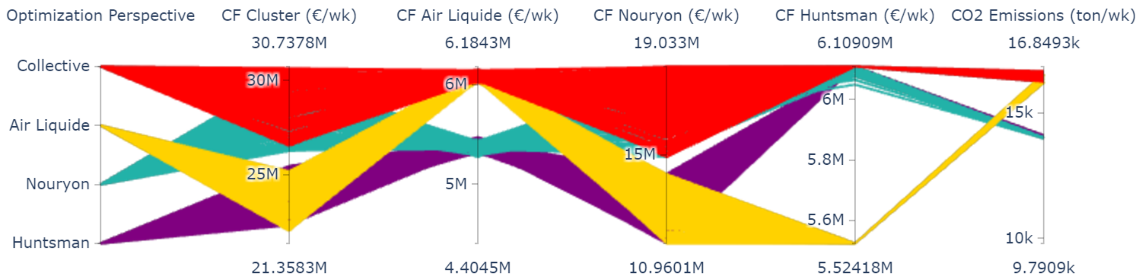
(d) Only Chlorine storage



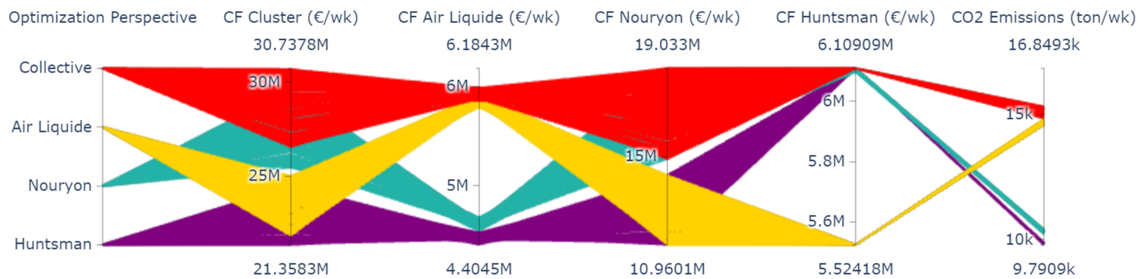
(e) Steam Pipe and E-boiler



(f) Steam Pipe and Chlorine storage



(g) E-boiler and Chlorine storage



(h) All options

Figure 7.12: Parallel coordinate plots per policy

The PCPs in Figure 7.12 show that when the model is optimized from the collective perspective, all cash flows are relatively high, but it also results in a relatively large amount of CO_2 emissions. Optimizing from the perspective of Nouryon or Huntsman generally results in a relatively low cash flow for Air Liquide, while realizing low CO_2 emissions. Optimizing from Air Liquide's perspective results in relatively low cash flows for the other stakeholders and a large amount of CO_2 emissions, but means a high cash flow for the company itself.

In terms of the trade-offs among the policies, it is clear that each policy realizes roughly equal cash flows for Nouryon and Huntsman. However, there are differences across the policies in terms of Air Liquide's cash flow when the model is optimized from either Nouryon's and Huntsman's perspective. More specifically, when either the Steam Pipe and the E-boiler or all the options are implemented, the cash flow of Air Liquide is relatively low, thereby decreasing the total cash flow of the cluster. Furthermore, there are significant trade-offs in terms of CO_2 emissions. The E-boiler and the Chlorine Storage alternatives seem to have no effect on this outcome in any of the policy configurations. However, whenever the Steam-Pipe option is implemented, the CO_2 emissions are relatively low, especially when the model is optimized from Nouryon's or Huntsman's perspective.

7.4.3 Robustness trade-offs

What is robust for one actor, may be not robust for the others. Hence, it is important to look at robustness trade-offs. Until now, the percentiles used for the robust performance condition were based on the total set of experiment outcomes. However, it might also be interesting to estimate unique percentiles per actor optimization perspective. This is done by dividing the total set of experiments into four subsets, based on the model used for computation (see Section 7.1.3). Then, within each actor optimization subset the percentiles are estimated and applied to calculate the robustness scores per policy. This new approach allows to see the policy robustness scores per actor optimization perspective in a different light, since the unique percentiles ensure that the outcome differences across the optimization perspectives are normalized. Using the same condition as in Section 7.4.1, Figure 7.13 shows the results of this analysis in a parallel coordinate plot. The axes represent the robustness scores per actor perspective and the lines represent the policies.

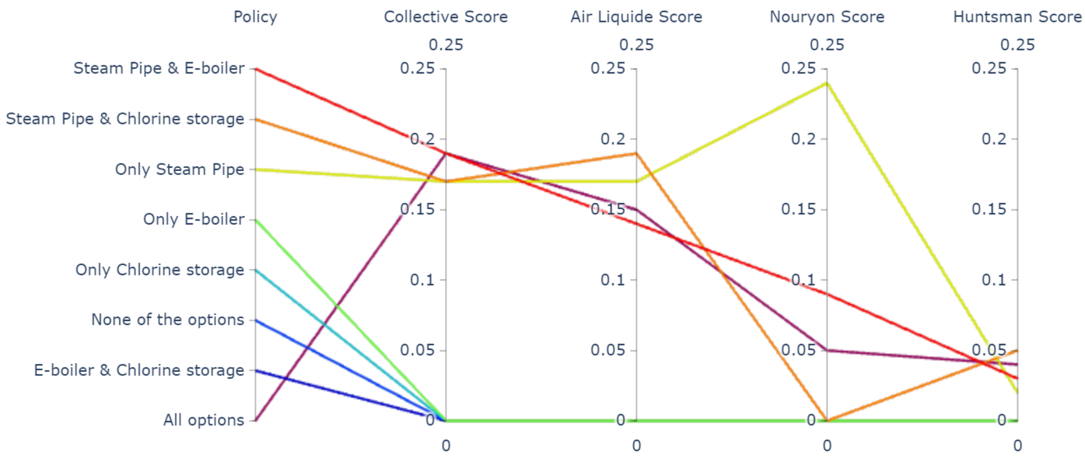


Figure 7.13: Robustness trade-offs between the actor perspectives for each policy

The results in Figure 7.13 show an entirely different picture compared to the histogram in Figure 7.11. It is clear that when the policy robustness scores are estimated based on unique percentiles per actor optimization perspective, the policies are not merely robust from Nouryon's perspective. More specifically, the perspectives of the Cluster and Air Liquide show relatively high robustness scores for some of the policies. Furthermore, four policies are not considered robust in any of the actor perspectives: only implementing the e-boiler or the chlorine storage, the combination of the two alternatives and implementing none of the options. In contrast, implementing only the Steam Pipe alternative scores a high overall robustness, because it performs well from Nouryon's perspective.

7.5 Scenario discovery

The results of the global sensitivity analysis (see Section 7.2) have shown that the cyclical frequency of the NaOH price is dominantly influencing the cash flows of both Nouryon and the entire cluster. Due to the identified problems within in the model and the implemented workaround to deal with the fact that the cyclical frequency of the caustic soda price does not fit into the characteristic week used to decrease the model run-time (see Section 7.1.5), it is unclear whether this behaviour is valid. Nevertheless, it can be interesting to analyze what values for this uncertain factor result in performance failure. For this type of analysis "scenario discovery" can be a useful tool. Scenario discovery was introduced by (Bryant & Lempert, 2010) and can be used to address the challenges of characterizing and communicating deep uncertainty associated with simulation models (Dalal et al., 2013).

The main algorithm that is used for scenario discovery nowadays is the Patient Rule Induction Method (PRIM) (Friedman & Fisher, 1999). It can be used to find combinations of values for input variables that result in similar characteristic values for the outcome variables. More specifically, this method identifies one or various rectangular subspaces of the model input space within which the values of a single output variable are considerably different from its average values over the entire model input space (Kwakkel & Cunningham, 2016). These subspaces of the total model input space are often referred to as "boxes". To further illustrate how PRIM works, Figure 7.14 shows its process broken down into three steps.

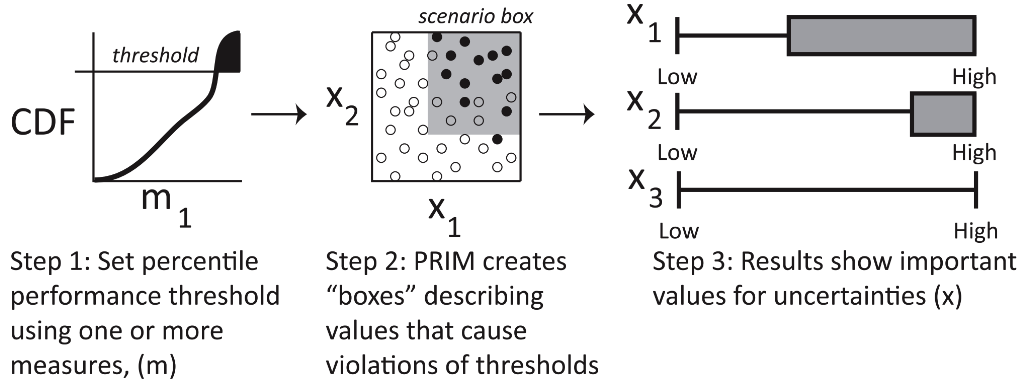


Figure 7.14: Three main steps of scenario discovery using the Patient Rule Induction Method (PRIM). Copied from "Many objective robust decision making for complex environmental systems undergoing change", by Kasprzyk et al., 2012, p.59.

In the first step of the PRIM process, it is paramount to define a certain performance threshold for one or more of the outcome variables. In this case, the goal is to identify ranges for the cyclical frequency of sdsdfsdf the NaOH price that result in performance failure in terms of Nouryon's and the entire cluster's cash flow. Since it is potentially interesting to analyze these outcomes independently, this results in two distinct thresholds that are analyzed separately by the PRIM algorithm. Incorporating the different optimization perspectives, this number is multiplied by four, resulting in eight runs. By default, in the next step the algorithm searches for boxes that violate the thresholds. Hence, the thresholds for both outcomes are defined at the 80th percentile of the total set of cash flow values.

In the second step, PRIM uses a non-greedy or patient, and hill climbing optimization procedure to identify the boxes. By keeping track of the route followed by this optimization procedure, the so-called "peeling trajectory", manual observations can reveal how the *number of uncertain factors* that define the box varies as a function of *density* and *coverage* (Kwakkel & Cunningham, 2016). The number of uncertain factors that make up the box is often used as a measure for interpretability. Furthermore, density is the fraction of cases within the box that is of interest, while coverage is the fraction of all the cases that are of interest that fall within the box (Kwakkel & Jaxa-Rozen, 2016). This allows the decision maker to carefully choose a certain box based on the trade-offs among these variables. Figure 7.15 shows an example of a graph that conveniently visualizes these trade-offs. Density and coverage are on the vertical and horizontal axes respectively, while the color bar on the left-hand side of the graph visualizes the number of uncertain factors. Each data point in the graph corresponds to one of the identified boxes.

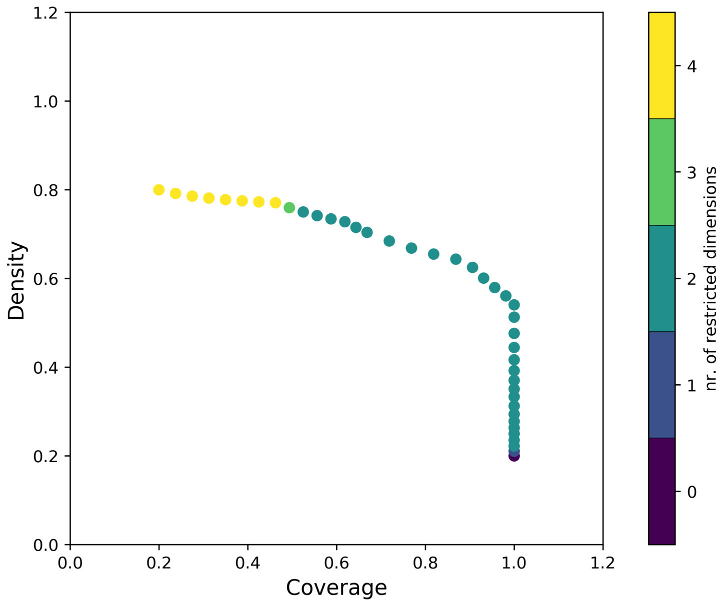
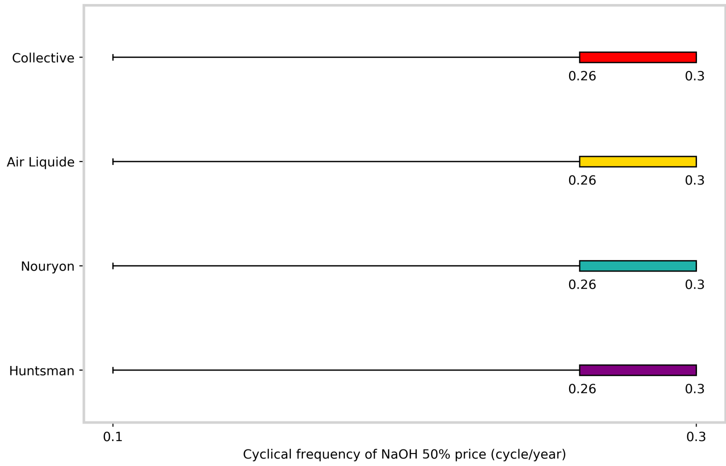
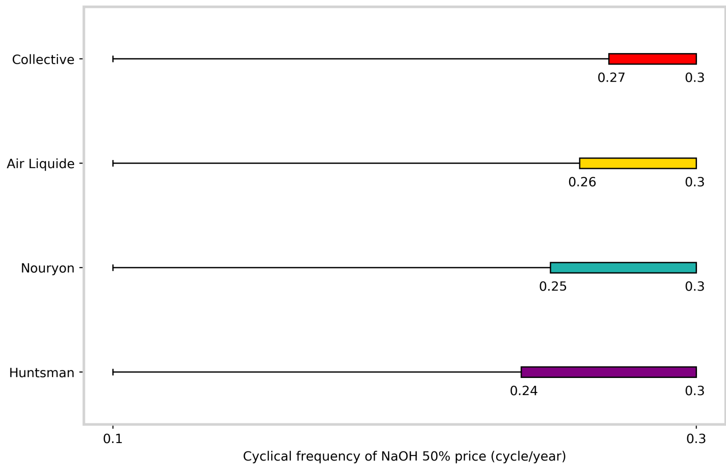


Figure 7.15: Boxes trade-off plot from PRIM algorithm of the EMA Workbench

The strategy used to decide on the boxes for each of the eight PRIM runs is based on two rules. To begin with, the number of uncertain factors (dimensions) of the box is not considered important, since this analysis focuses merely on the cyclical frequency of the NaOH price. This factor is always in the box, as the results of the global sensitivity analysis have shown that it is very dominant in its influence on the outcomes of interest. Furthermore, a high density (precision) value is preferable, but the coverage variable is not allowed to decrease below a threshold of 0.7. Using the PRIM algorithm in combination with these rules, ranges of the cyclical frequency of the NaOH price have been identified that are responsible for the performance failure of both Nouryon's cash flow (see Figure 7.16a) and that of the entire cluster (see Figure 7.16b). In these figures, the ends of the horizontal axes indicate the lower and upper bound of the sampling bandwidth of the uncertain factor. The vertical axes display the four optimization perspectives. The colored boxes indicate the ranges of the uncertain factor responsible for performance failure.



(a) Ranges responsible for the performance failure of Nouryon's cash flow



(b) Ranges responsible for the performance failure of the cluster's cash flow

Figure 7.16: Results from the PRIM analysis

Considering the results of both cash flow outcomes, it is obvious that in this model it is a relative high cyclical frequency (0.24 - 0.30) of the caustic price that causes performance failure. In terms of the cluster's cash flow, it is clear that this range changes slightly across the optimization perspectives. More specifically, when the model is optimized from the cluster's perspective, this range is significantly smaller compared to the perspective of Huntsman. Regarding Nouryon's cash flow, the results show that the range of the cyclical frequency does not change over the optimization perspectives.

Chapter 8

Discussion

This chapter elaborates on the meaning of the results obtained in the previous chapters. To begin with, the implications of this research for analyzing uncertainty in industrial electrification systems are addressed. Afterwards, implications are provided for combining Exploratory Modelling and Analysis (EMA) with Mixed Integer Linear Programming (MILP) models. Finally, the limitations of this research are discussed based on the different steps taken.

8.1 Implications for analyzing uncertainty in industrial electrification systems

Based on the results of this research, it is safe to argue that exploring the effect of uncertainty on industrial systems undergoing electrification is a feasible goal. More specifically, using EMA to achieve this goal has been a successful endeavor. However, it is important to realize that the results remain very dependent on the scope, the assembly of simplifying modelling assumptions and the constraints of the experimental design. In other words, attempts to translate the results of a case-study into a bigger picture must be performed with great caution.

Apart from using EMA, various other steps have been taken during this research. Now it is paramount to reflect on their contribution to the uncertainty analysis process, as a means of composing an effective plan of action. To begin with, the development of the theoretical framework was key in understanding the specifications of the Power-to-X alternatives, the cluster characteristics of the system and the various dimensions of uncertainty. It allowed for a well-founded academic approach to analyzing uncertainty in industrial electrification systems. Furthermore, the stakeholder analysis helped to understand the interests and interconnected responsibilities among the actors within the industrial cluster. These interests are a great source of information for the identification of the Key Performance Indicators (KPIs) for the uncertainty analysis. In addition, knowing the actor network is a must to understand on the implications of the results. Therefore, it is advisable to include some form of actor analysis for this type of research.

The uncertain factors were mainly identified based on a literature review. In addition, the model was observed for any uncertain assumptions that might greatly influence the results. This combination of methods was successful in identifying a comprehensive set of uncertain factors. Nonetheless, it has to be noted that a different choice of identification methods might have led to a different set of factors. Hence, it is recommended to carefully approach this process and to attentively consider the specific scope of the contemplated analysis. During the determination of this scope, extra attention must be payed to the level of detail at which the model is a representative version of reality (Fraiture, 2020). A highly detailed analysis results in specific insights into the effect of the uncertain factors, but requires a model that is able to translate detailed conclusions to the real-world. In contrast, analyses that try to capture the bigger picture allow for a model that is representative on a higher level. Overall, this remains a complicated topic and decisions in this area should be communicated clearly by the analysts.

Considering the uncertainty analysis, it is interesting to reflect on the extent to which the methods chosen for the analysis of the experimental results provided a sufficient amount of insight. In general, the decision to look at optimization perspectives of different (groups of) actors resulted in some interesting trade-off visualizations. This is very convenient for electrification systems where stakeholders form an industrial cluster, because in these situations it is key to consider both the individual actor and cluster level during decision-making (see Section 3.1.1). However, it remains very important to explicitly discuss the implications of these optimization perspectives, as they can potentially influence model dynamics. The implications of using different optimization perspectives in MILP models are explained in the next section. Furthermore, the global sensitivity analysis provided results based on regression coefficients indicating the amount of influence that factors have on performance relative to each other. Apart from answering one of the main research questions, this information proved to be valuable, as it allowed for the identification of certain modelling defects which could either be resolved or their implications thoroughly explained. The single- and multi-objective robustness scores per policy visualized in histograms were efficient in conveying trade-offs among policies and optimization perspectives, but provided no insight into the underlying dynamics of these results. Hence, it is recommended to dive into the latter topic first, to avoid unnecessary misunderstandings and faulty interpretations. Finally, the scenario discovery performed using PRIM provided insight into ranges of uncertain factors responsible for performance failure. In this research, it was only used to a limited extent, while it has great potential. Future research could focus further utilization of this method for analyzing uncertainty in industrial systems undergoing electrification.

8.2 Implications for combining EMA and MILP

Over the last decade, MILP has often been used to model systems characterized by uncertainty (Cristóbal et al., 2013; Moreno et al., 2015; Pazouki et al., 2014). These studies have in common that uncertainty is often approached in a stochastic manner. Using EMA (Kwakkel & Pruyt, 2013) to deal with uncertainty in MILP models seems to be a novel approach (Fraiture, 2020). Hence, it is paramount to discuss the implications for this approach based on the results and experience obtained in this research.

8.2.1 The connection

Before deriving these implications, it is important to understand how EMA and MILP have been combined in this study. Through the means of a “connector” script written in Python, the MILP model developed in “Linny-R” (Bots, 2020) is able to interact with the “EMA Workbench” module (Kwakkel, 2019). Within this module, policies and sampling ranges for the uncertain factors are defined. During each experiment, the Workbench samples through the uncertainty space and sends a collection of sampled values to the connector. The connector consists of two components: a generic part and a system-specific part. The generic part enables exchange of information and executes the model runs. The system-specific part is optional and has the ability to transform the sampled values into usable input data for the model. For example, when the E-boiler alternative is sampled “False”, the system-specific part of the connector transforms this binary information into a multi-factor input that ensures that the upper bounds of the processes within the E-boiler are set to zero, meaning it cannot be used during that run.

8.2.2 Benefits and limitations

Now it is key to consider the benefits and limitations of combining EMA and MILP models. To begin with, the stochastic approaches used in the aforementioned studies often require perfect knowledge about the probability distribution functions (PDFs) of the uncertain factors, which can be very difficult to obtain in practice (Zare et al., 2018). Within the EMA implementation used in this research, a so called “open exploration” is performed that evaluates the full distribution of each uncertain factor across the domain of all other parameters. In contrast to stochastic methods, this type of analysis requires only limited information in the form of sampling bandwidths. In addition, it entails a broader measurement of a system’s sensitivity to uncertainty (Jaxa-Rozen & Kwakkel, 2018). A downside to this approach is that it often requires a large amount of model runs. According to both Puigjaner et al. (2002) and the experience obtained in this research, the main limitation of using MILP to model process industry systems is the large computational effort required to solve problems of practical size. Depending on the computational recourses available, the combination of this MILP limitation and the large amount of runs required by the EMA approach might result in problems where the total run-time exceeds the amount of time available.

Apart from parallel computing, there are a number of ways to mitigate these excess run-time problems. One can change the properties of the linear solver (see Section 7.1.6) by applying a block structure methodology (Martin, 1999). However, this has to be done carefully, as it can drastically influence the dynamics and outcomes of the model based on the cycle times of the different variables. Furthermore, creative approaches can be developed for the efficient handling of the chosen time horizon. For example, in this research the decision was made to run one characteristic week for each year within the time horizon. A downside to this approach was that it required an extension of the system-specific part of the “connector”, thereby increasing its complexity and making it harder to trace back potential defects. In addition, due to the ability of the solver to see into the future, it was necessary to run each week in a separate model, thereby increasing the required memory when running in parallel. Another option might be to move away from EMA and consider a less computationally demanding approach. Research performed by Zare et al. (2018) proposes a novel Distributionally Robust Chance Constrained (DRCC) model to account for the uncertain factors in their MILP model. Apart from a low computational demand, this approach offers multiple interesting advantages: it requires limited information about the uncertain variables (rather than perfect knowledge of their PDFs), it immunizes the solution against all realizations of the distributions of the uncertain factors defined within a moment-based ambiguity set and it enables the decision maker to effectively control the degree of conservatism of the solution.

Another potential benefit is that MILP allows for easy implementation of different optimization perspectives. More specifically, the objective function of the MILP problem can be altered to contain only variables of one specific actor or group of actors. Combined with EMA, it is relatively simple to perform an uncertainty analysis from these different perspectives. This is a great opportunity in systems such as an industrial cluster, where it is key to consider both the individual actor and cluster levels during decision-making (see Section 3.1.1). It is important to note, however, that when a MILP problem is solved from the perspective of a certain actor, it means that the remainder of the actors will do anything in their power (as far the boundaries of their products and processes allow it) to ensure the highest possible outcome for that actor. In other words, one could argue that the actors not included in the optimization perspective become “enslaved”. This state of affairs might not be considered a valid representation of reality, because individual actors in a competitive environment are unlikely to behave this way. Nevertheless, the optimization perspectives can potentially reveal interesting trade-offs among actors that contribute towards a balanced decision-making process.

An important limitation of combining EMA and MILP models that surfaced during this research, is that the linear solver has to satisfy the boundaries of processes and products during its optimization process. These boundaries can entail specific capacity of machinery, contractual obligations, market supply/demand, etc. In mathematical optimization, these boundaries are called “constraints” and the set of all possible solutions that satisfy the problem’s constraints is called the “feasible region” (Beavis & Dobbs, 1990) (see Section 3.2). When this multidimensional space is relatively small in size, the effect of the uncertain factors on the constrained decision variables can only be measured to a limited extent. One can question whether these measurements are a valid representation of reality, as actors are likely to undertake some kind of (unmodelled) action if their current constraints result in undesired outcomes. Furthermore, a process planning study by Liu & Sahinidis (1995) indicated that as long as adjustments in production levels, purchases and sales are allowed, uncertainty in prices and demands does not seem to have any major impact on the quality of the solution of the MILP model. In other words, the feasible region allows the model solver to find an optimal solution that tends to minimize the effect of these uncertain factors. In such a case, one can question whether its justified to conclude that the impact of uncertainty is low, as the real-world system at hand might be unlikely to optimize itself in this way, especially in a multi-actor environment with multiple conflicting interests. Therefore, further research should focus on exploring whether the optimization characteristics of MILP described above allow for a valid uncertainty analysis in these type of environments.

A last point of interest entails the linear characteristic of MILP models and how it might influence the results of the uncertainty analysis performed using the EMA approach. In recent research, Fraiture (2020) uses the exact same combination and argues that the implementation and representation of the uncertain factors remains very much dependent on the model specification. In this case, the modelling approach assumes linearity and therefore requires simplification of non-linear transition dynamics. In a manufacturing environment, this process can lead to unsatisfactory or unfeasible solutions (Puigjaner et al., 2002). Nevertheless, these simplifying linear assumptions have the ability to decrease the required computational effort compared to non-linear models. Hence, during future research it might be interesting to compare the results of EMA applied to different models of the same system with both linear- and non-linear specifications to estimate trade-offs amongst computational effort and the validity of the results.

8.2.3 Conclusion

In conclusion, when the goal is to perform a broad uncertainty analysis that allows for easy implementation of actor optimization perspectives while requiring only limited information about the uncertain factors in the form of sampling bandwidths, combining EMA and MILP might be a good idea. However, there are some points of attention. Depending on the type of environment, a large computational effort may be required to solve MILP problems of practical size. Hence it is recommended to use this combination for systems that allow for a model which is relatively small in size or to have access to an extensive amount of computational resources. Furthermore, it is important to pay attention to the feasible region defined by the constraints of the MILP problem. If this multidimensional space is relatively small in size, the effect of the uncertain factors on constrained decision variables can only be measured to a limited extent. Moreover, in a multi-actor environment with multiple conflicting interests, it is key to observe the optimization process that takes place within the model and to question whether its dynamics allow for a valid uncertainty analysis. A last general piece of advise is to evaluate the extent to which the linear characteristics of the MILP model are able to validly represent the uncertainty of the real-world system.

8.3 Limitations of this research

Although the results of this research provide valuable insights, the different steps that have been taken are subject to limitations. To be able to draw reasonable conclusions, this section provides a reflection on those limitations. First, the limitations of the methodology are considered. Afterwards, the choices made during the stakeholder analysis are observed for any weaknesses. Then, the constraints of the identification of the uncertain factors are addressed. Finally, the limitations of the uncertainty analysis are explored.

8.3.1 Limitations related to the methodology

Regarding the limitations of the methodology, three main topics are paramount to consider: the case-study, the model and the method used for the uncertainty analysis (EMA). Case studies are a widely recognized method for data collection in many different disciplines. However, it is also an approach that remains very controversial. The most important limitation of using a case study for this specific research is that it provides a weak basis for scientific generalization, because it uses a small number of subjects (Yin, 1984). In the proposed case study, more than one subject is used, because the model concerns three different companies in the Port of Rotterdam.

Nevertheless, it is just one case and other cases in the world might entail completely different values and dynamics. Therefore, it is paramount to think about the extent to which the results allow for generalization. In terms of the implications of the effect of uncertainty on industrial electrification performance, the results of this research allow for a limited amount of generalization, as the analyzed system represents only a small part of the bigger picture. Nevertheless, considering the implications for combing EMA and MILP models, the results can be generalized to a larger extent, because these derivations are less dependent on the specific case.

The model itself is subject to a large number of limitations. However, this is considered an inherent property of models in general. As Box (1979) put it: “all models are wrong, but some are useful”. Hence, it is important to discuss the limitations that are a direct threat to its usefulness. In this case, the intended purpose of the model is to help describe the effect of various uncertain factors on the system which it tries to represent. Following this line of reasoning, three main limitations are worthwhile to discuss. To begin with, during this research a problem was discovered within the model that remains unsolved (see Appendix B.2). The current hypothesis is that this defect causes a significant amount of invalid behaviour. Hence, the results of the uncertainty analysis were only interpretable to a very limited extent and it was not possible to make any case-specific conclusions or recommendations. Furthermore, a more generic limitation was already addressed in the previous section and entails that the simplifying assumption of linearity might lead to unsatisfactory or unfeasible solutions (Puigjaner et al., 2002). The extent to which this limitation has influenced the validity of the uncertainty analysis is yet unclear and might be an interesting topic for further research. Finally, by default the actors in the model pay so called “cost prices” for the products produced by other actors within the cluster. In other words, the model does not account for any profit or loss margins. Consequently, if a product becomes more expensive to produce due to increased prices for its materials, the guaranteed sales price increases with an equivalent amount. This means that product prices have no effect on the cash flow of the actors. Moreover, it entails that actors have no incentive to lower their production costs, which results in an unrealistic financial optimization process. The software that defines the MILP problem (Linny-R) does contain an option to include profit margins for certain products, by setting a specific price on them that has the ability to change according to a specified equation. For example, this option could be utilized to ensure that a certain product is always sold at price that is 10% higher than its cost price, thereby increasing the cash flow of the actor that sells the product. However, this option was not implemented during this research, because there was no data on specific profit margins beforehand and the various actors were deemed unlikely to provide this information.

Using EMA does not result in many limitations since its “open exploration” implementation imposes very few constraints on the uncertainty analysis. This is due to the fact that it evaluates the full distribution of each uncertain factor across the domain of all other parameters. Nevertheless, something that can arguably be considered either an advantage or limitation to EMA, is that it provides “foresight” and not “forecasting”. There is an important difference between these two concepts. Forecasting attempts to predict the future as accurately as possible, whereas foresight places several realizable or desirable futures side by side (Mietzner & Reger, 2005). On the one hand, this introduces limitations in the sense that the results can never be used as if they provide certain knowledge about the future. On the other hand, it incentivizes the development of robust solutions that perform well over a wide range of scenarios.

8.3.2 Limitations related to the stakeholder analysis

Considering the stakeholder analysis, its scope is potentially its main weakness. This scope is crucial, as the results of the stakeholder analysis are used to identify the Key Performance Indicators (KPIs) of the Power-to-X alternatives. In addition, it is used to understand the interconnectedness among the actors and their entwined responsibilities. Decisions were made to include a limited number of actors, based on the four categories of uncertainty in electrified industrial systems as defined by Thijsen (2018): policy, market, technology and process. To begin with, one can question whether this list of categories is comprehensive enough to be used for an actor identification process. If not, then this might have resulted in the fact that some actors were overlooked. Furthermore, due to the complexity of the market category and the impossible task to include all its actors, a generic "markets" actors was included. Obviously, it is impossible for this generic actor to represent the variety of interests of responsibilities of all the actors within this category. Consequently, the actor network diagram developed to reveal the important relationships between the actors might have been too simplistic, resulting in an incomplete understanding of the total set of responsibilities. Yet another limitation might be that not all the actors present in the model were included. Some of these actors were considered too small in scale or too insignificant in terms of power to incorporate them into the analysis. Overall, it is clear that a different scope for the stakeholder analysis might have resulted in different KPIs and a different understanding of the actor network.

8.3.3 Limitations related to the identification of the uncertain factors

The identification of the uncertain factors is also subject to a number of limitations. To begin with, the industrial cluster and energy systems in general are always evolving. Consequently, the uncertain factors identified in this research may no longer be applicable after a certain period of time, thereby limiting the future usability of the results. Hence, it is recommended to not unquestioningly copy any conclusions, but rather to put them into a current perspective for a critical review.

Furthermore, the identified set of uncertain factors is undoubtedly incomplete in the sense that it does not represent the full scope of uncertain factors influencing the performance of industrial electrification systems. However, this was not the intention of this research, as the goal was to include "external" uncertain factors manifested outside of the cluster that have a significant influence on the performance of the Power-to-X alternatives. Nevertheless, within this specific scope, it is not unthinkable that some factors have been overlooked during the various steps of the identification process. More specifically, the uncertain factors were identified based on a literature review, stakeholder interviews and uncertain modelling assumptions. The literature review is very limited in its use of sources, as it is purely based on the content taxonomy of uncertainty in electrified industrial systems by Thijsen (2018). However, this specific study relates perfectly to this research and the content taxonomy itself is based on various academical sources. The stakeholder interviews are limited to the extent that not every actor in the cluster has been interviewed. Especially the missing interview of Air Liquide, being one of the main stakeholders, might have resulted in the risk that a certain factor has not been identified. Nonetheless, this risk was minimized by closely observing the responsibilities of this actor in both the network diagram (see Section 5.1) and within the model itself. Considering the factors that were identified based on uncertain modelling assumptions that significantly influenced the results, it is certainly possible that some of these factors were overlooked. This process was done by hand, by experimenting with different configurations of factors and processes surrounding the Power-to-X alternatives. In future research, it might be interesting to explore the possibility of performing a very broad sensitivity analysis for this purpose, where next to simple parameters entire model structures are changed.

8.3.4 Limitations related to the uncertainty analysis

Finally, it is important to address the limitations of the uncertainty analysis. This has everything to do with the constraints on the experimental design and how they might have influenced the results. To begin with, the applied sample size of 100 alternative future states of the system generated using Latin Hypercube Sampling (LHS) would ideally have been much larger. This would have resulted in an overall higher precision of the results. However, this was impossible due to the large amount of computational effort required by the model and the limited amount of computational resources. For the purpose of parallelization, a computer with a processor of 56 cores was used to run the total set of experiments. This still resulted in a total run-time of five entire days.

Furthermore, the applied method to decrease the run-time per experiment might have influenced the results of the uncertainty analysis. This method consisted of running one characteristic week for each year of the ten years within the time horizon. This time period was not enough to fully justify the uncertainty surrounding the cyclical frequency of the caustic soda price, as it varies from three to ten years. The implemented workaround for this problem was using the average caustic soda price of a certain year throughout its corresponding week. Nonetheless, its estimated regression coefficient during the global sensitivity analysis was relatively high (see Section 7.2). Hence, in further research it is recommended to include the amplitude of the NaOH price sine function as well, in order to decompose the origins of its influence more specifically. In addition, although the characteristic week was carefully chosen based on the weekly average temperatures and wind speeds of the past twenty years (see Section 7.1.5), it might still not be completely representative for the outcomes of each future year run by the model. This method could be improved by accounting for climate development, thereby allowing the characteristic week to change over time. For example, in simulation year one the characteristic week might be week number five, while in simulation year ten it is week number seven.

As discussed in the previous section, the properties of the linear solver must be carefully chosen based on the cycle times of the variables within the system of analysis. Based on this recommendation, values were chosen for both the “period” and the "look-ahead" of the solver. The value for the period (24 hours) was determined by the cycle time of the chlorine storage system and was therefore considered quite plausible. The value for the look-ahead (6 hours) was determined based on a trade-off analysis between its effect on the validity of the storage behaviour and the run-time of the model. The former variable remains a controversial topic of discussion, since it is hard to determine what kind of storage behaviour is valid. In the future, it would be wise to closely study the storage system at hand and to consult stakeholders about the time frame they use for forecasting.

Last, but definitely not least, it is paramount to address the limitations of the methods used to analyse the results of the experiments. First of all, the chosen set of methods covers a broad, but nevertheless limited area of all the potential different types of analyses that could have been applied in this case. If different methods were chosen, the results might have pointed roughly in the same direction, but the interpretation of the details might have been very different. Furthermore, the specific choice of parameter values *within* every applied method also limits the outcomes. For example, during the evaluation of the multi-objective robustness scores per policy, different objectives might have resulted in different scores. Hence, it might be worthwhile to apply other methods to the same set of results to reveal potential divergent patterns of interpretation.

Chapter 9

Conclusion

This final chapter summarizes the results obtained in the previous chapters and draws conclusions. First, answers are provided to each of the research questions presented in the introductory chapter. Afterwards, an overall conclusion is formulated. Finally, recommendations are presented for future research.

9.1 Answers to the research questions

Based on the knowledge gap identified in the first chapter, this research attempts to answer the following main research question:

"How does external uncertainty influence the performance of (combinations of) Power-to-X alternatives that increase the decarbonization of the steam supply and the flexibility of an integrated chemical cluster in the Port of Rotterdam?"

To answer this main research question, the following subsections provide answers to the sub questions in which the main research question was disaggregated.

9.1.1 What are the interests and responsibilities of the interconnected stakeholders?

During a study of the actor characteristics in the stakeholder analysis (see Table 5.1), three common interests were identified among the stakeholders: economic feasibility, decarbonization and security of supply. In terms of Key Performance Indicators (KPIs) for the Power-to-X alternatives, economic feasibility translated to the cash flow of the entire cluster as well as the clash of flow of individual actors. Decarbonization was evaluated by looking at the total CO_2 emissions of the system. Regarding security of supply, this was not a realistic performance indicator to evaluate with a MILP problem. By default, the mathematical solver already satisfies the constraints (contractual obligations) of product delivery (see Section 4.3.3). Therefore, this KPI was excluded from further analysis.

In terms of responsibilities, a network diagram was designed (see Figure 5.1). This diagram contained a number of interesting observations. First of all, it showed that the members of the chemical cluster heavily depend on each other and on trade with the markets. Furthermore, it is clear that the Steam Pipe option introduces a new actor into the arena, namely waste-processing company AVR. Another key observation from the network diagram is that the Steam Pipe alternative further increases the interconnectedness of the chemical cluster. This might not be favored by all actors, because it decreases the level of independence. On the other hand, it creates new sustainable possibilities.

9.1.2 What are the external uncertain factors in this case?

During the identification of the uncertain factors in Chapter 6, various factors were identified based on a literature review and by observation of the uncertain assumptions of the case-study model (see Table 6.6). The results entailed twelve uncertain factors originating from various backgrounds with medium or higher estimated uncertainty. To model the future development of these factors within the chosen time horizon, reference values and sampling ranges were identified (see Appendix A). To be able to translate these values into multiple plausible futures, various mathematical techniques were designed (see Section 6.4).

9.1.3 To what extent do these factors affect the performance of the alternatives?

To answer this question, a global sensitivity analysis was performed. During this analysis, the outcomes of the first set of experiments showed unexpected behaviour (see Figure B.1). Hence, model verification was performed where a number of problems were found of which some were resolved (see Appendix B.2). Unfortunately, the solution implemented to solve one of the identified problems did not result in more valid behaviour. Most importantly, the E-boiler still seems to have a very low effect on the CO_2-emission outcome. The current hypothesis is that this invalid behaviour is caused by another issue within the model that not could be resolved in the available time-frame (see Appendix B.3). In fact, it is not unlikely that this issue is responsible for the overall disturbance of the dynamics within the model. This means that the results of the global sensitivity analysis and the other methods used during the uncertainty analysis can only be interpreted to a limited extent. Consequently, with respect to the following two research questions, it will not be possible to make any case-specific conclusions or recommendations.

9.1.4 What strategies are optimal in terms of economic feasibility and decarbonization and what strategies are robust?

For the identification of policies that perform well in terms of economic feasibility, the total set of experimental results was used to calculate the average cash flow of the entire cluster per policy for the collective and individual optimization perspectives (see Figure 7.5). The results show that the differences between the average cluster cash flows are minimal across the set of policies. In terms of the differences among the four actor optimization perspectives, it is clear that the average cash flow of the cluster is always higher when the model is financially optimized from the perspective of the entire cluster or Air Liquide.

The same approach was applied to the decarbonization objective. More specifically, the average CO_2 emissions of the cluster were calculated per policy for the collective and individual optimization perspectives (see Figure 7.8). In contrast to the average economic performance, these results show significant differences among policies and between perspectives. Optimizing from either Nouryon's or Huntsman's perspective, results in significantly lower CO_2 emissions for every policy. Furthermore, it is observed that the alternatives are only effective in terms in CO_2 reduction when they are implemented in conjunction.

To identify policies that are robust in terms of both economic feasibility and decarbonization performance, the total set of experiments and corresponding outcomes was filtered using a performance condition based on percentiles. Afterwards, each of the eight policies was given a “robustness score” per optimization perspective, based on the fraction of the total number of scenarios in which its corresponding outcomes satisfied the performance condition (see Figure 7.11). The results show that only when the model is financially optimized from Nouryon’s perspective, outcomes are retrieved of both high cluster cash flows and low CO_2 emissions. From this perspective, implementing only the e-boiler or the chlorine storage alternative results in a robustness score of zero, meaning that in 0% of the tested scenarios the performance condition was satisfied. The other six policies have roughly similar robustness scores of around 45%.

9.1.5 What are the key trade-offs among the strategies from individual and collective points of view?

As a means of visualizing the performance trade-offs among the policies from individual and collective points of view, parallel coordinate plots were constructed (see Figure 7.12). These showed significant trade-offs between the optimization perspectives. When the model is optimized from the collective perspective, the cash flows of all actors are relatively high, but it also results in a relatively large amount of CO_2 emissions. Optimizing from the perspective of Nouryon or Huntsman generally results in a relatively low cash flow for Air Liquide and low CO_2 emissions. Air Liquide’s perspective results in relatively low cash flows for the other stakeholders and a large amount of CO_2 emissions, but means a high cash flow for the company itself. In terms of the performance trade-offs among the policies, it is clear that each policy realizes roughly equal cash flows for Nouryon and Huntsman. However, there are differences across the policies in terms of Air Liquide’s cash flow when the model is optimized from either Nouryon’s and Huntsman’s perspective. More specifically, when the steam pipe and the e-boiler or all the options are implemented, the cash flow of Air Liquide is relatively low, thereby decreasing the total cash flow of the cluster. Furthermore, there are significant trade-offs in terms of CO_2 emissions. The e-boiler and the chlorine storage alternatives seem to have no effect on this outcome in any of the policy configurations. However, whenever the steam pipe option is implemented, the CO_2 emissions are relatively low, especially when the model is optimized from Nouryon’s or Huntsman’s perspective.

Apart from these performance trade-offs, a different analysis was conducted to look at robustness trade-offs. After all, what may be robust for one actor, may not be robust for the other. For this robustness analysis, a slightly different approach was used, which ensured that the outcome differences across the actor optimization perspectives were being normalized. This new approach resulted in some interesting robustness trade-offs (see Figure 7.13). Overall, implementing only the steam pipe is a relatively robust solution for all the actors, especially for Nouryon. The steam pipe is also quite robust for Air Liquide and the chemical cluster as a whole when it is implemented in conjunction with either the e-boiler or the chlorine storage alternatives. However, these are less robust solution for Nouryon and Huntsman. Implementing all the options achieves more or less the same results. The remaining four policies scored robustness scores of zero for each actor optimization perspective.

9.1.6 What are the practical implications of this research for combining EMA and MILP models?

During the discussion in the previous chapter, various implications of this research for combining EMA and MILP models were addressed in detail (see Section 8.2). This resulted in different benefits, limitations and other points of interest. Using these concepts, a conclusion was formulated that indicates the circumstances under which this combination is convenient to apply. In summary, when the goal is to perform a broad uncertainty analysis that allows for easy implementation of actor optimization perspectives while requiring only limited information about the uncertain factors in the form of sampling bandwidths, combining EMA and MILP might be a good idea. However, there are some points of attention. Depending on the type of environment, a large computational effort may be required to solve MILP problems of practical size. Hence it is recommended to use this combination for systems that allow for a model which is relatively small in size or to have access to an extensive amount of computational resources. Furthermore, it is important to pay attention to the feasible region defined by the constraints of the MILP problem. If this multidimensional space is relatively small in size, the effect of the uncertain factors on constrained decision variables can only be measured to a limited extent. Moreover, in a multi-actor environment with multiple conflicting interests, it is key to observe the optimization process that takes place within the model and to question whether its dynamics allow for a valid uncertainty analysis. A last general piece of advise is to evaluate the extent to which the linear characteristics of the MILP model are able to validly represent the uncertainty of the real-world system.

9.2 Overall conclusion

In this research, a MILP model and EMA have been combined to analyze the effect of uncertain factors on the performance of electrification alternatives for an industrial cluster. This approach has resulted in a large amount of interesting results and insights. Hence, it is safe to argue that exploring the effect of uncertainty on industrial systems undergoing electrification is a feasible goal. Moreover, using both EMA and MILP can be a powerful combination to achieve this goal. The ultimate aim of this research was to create insights that would increase the efficiency of decision-making processes and the robustness of businesses cases, thereby contributing to an acceleration of the energy transition. At this point, the results of this research are less relevant for the specific industrial cluster in the Port of Rotterdam, because the model contains a number of unsolved problems. In addition, various potential limitations have been identified with respect to the research approach. Nevertheless, it is clear that this type of research deserves an increased amount of attention, as it possesses the ability to achieve the objectives described above, thereby contributing to the full adoption of the potential of electrification.

9.3 Recommendations for future research

This section presents various suggestions for future research based on the topics identified during the discussion of the implications and limitations of this research in the previous chapter.

To begin with, it would be worthwhile to resolve the remaining problems within the MILP model of the chemical cluster. This would allow for a more precise and valid uncertainty analysis. Based on the results of this analysis, it might be possible to make case-specific recommendations that can contribute to an acceleration of the implementation of electrification alternatives within the Port of Rotterdam.

Furthermore, a general limitation of MILP is that its simplifying assumption of linearity might lead to unsatisfactory or unfeasible solutions, especially in a manufacturing environment (Puigjaner et al., 2002). The extent to which this limitation influences an uncertainty analysis is yet unclear. Hence, future research could focus on exploring this effect by comparing the results of uncertainty analyses performed with different models of the same system with both linear- and non-linear specifications. Moreover, since the linearity assumption has the ability to decrease the required computational effort compared to non-linear models, it would be interesting to visualize trade-offs among computational effort and the validity of the results.

A different limitation of MILP models that surfaced during this research and which is confirmed by a process planning study by Liu & Sahinidis (1995), is that uncertainty in prices and demands does not seem to have any major impact on the solution of the MILP model. More specifically, the feasible region defined by the constraints of the MILP problem allows the solver to find an optimal solution that tends to minimize the effect of these uncertain factors. In such a case, one can question whether its justified to conclude that the impact of uncertainty is low, as the real-world system at hand is unlikely to optimize itself in this way, especially in a multi-actor environment with multiple conflicting interests. Therefore, further research can focus on exploring whether the optimization characteristics of MILP allow for a valid uncertainty analysis in these type of environments.

Considering the identification of the uncertain factors, the decision was made to also include uncertain modelling assumptions that might significantly influence the results of the uncertainty analysis. The process of finding these assumptions was performed by hand, by experimenting with different configurations of factors and processes surrounding the Power-to-X alternatives. Due to the manual characteristic of this process, it is not unlikely that some important uncertain assumptions were overlooked or the extent of their influence misjudged. In future research, it might be interesting to explore the possibility of performing a very broad sensitivity analysis for this purpose, where apart from simple parameters, entire model structures are changed over a wide set of experiments. This would contribute to a more comprehensive identification process of the uncertain factors.

When using MILP models that contain a Demand Side Management (DSM) system which uses storage opportunities, it is crucial to determine an appropriate value for the "look-ahead" property of the solver. This value entails the number of time steps which the solver can see into the future. In other words, it is the time-frame in which the solver has perfect information regarding the uncertain factors and other variables that change over time. In this research, the value for the look-ahead was determined based on a relatively simple trade-off analysis between its effect on the validity of the storage behaviour and the run-time of the model. However, the former variable remains a controversial topic of discussion, since it is hard to determine what kind of storage behaviour is valid. Since the value for the look-ahead has the ability to exert a huge amount of influence, it might be wise to study this topic in more detail and to include stakeholders in this process to access information about forecasting time-frames.

The caustic soda price is a very uncertain factor and therefore relevant to include in any uncertainty analysis of systems where it is influential. However, its future development is hard to model, as it is characterized by potentially large fluctuations over changing periods of time. In this research, the applied approach was to model the its potential future trajectories by using a generic sine function, where the cyclical frequency was identified as the uncertain factor. However, the applied method to decrease the run-time per experiment might have influenced the results of this approach. This method consisted of running one characteristic week for each year of the ten years within the time horizon. This period of one week was not enough to fully justify the uncertainty surrounding the cyclical frequency of the caustic soda price, as it sampling ranges varied from three to ten years. The implemented workaround for this problem was using the average caustic soda price of a certain year determined by the sine function throughout its corresponding week. Consequently, the specific effect of the cyclical frequency was only partly measured. In addition, the high regression coefficient estimated during the global sensitivity analysis indicated that the chosen amplitude for the generic sine function might have been very influential. Hence, for future research that applies the same approach in respect to modelling the future development of the caustic soda price, it recommended to include both the cyclical frequency and the amplitude of the sine function in order to decompose the origins of its influence more specifically.

A last suggestion for future research revolves around the utilization of the Patient Rule Induction Method (PRIM) for the performance of scenario discovery in industrial systems undergoing electrification. In this research, it was only used to a limited extent, while it has great potential. This potential originates from the fact that PRIM has the ability to identify ranges of uncertain factors or other variables most responsible for the performance failure of certain alternatives. Further research could focus on the increased utilization of this method to estimate and visualize the specific circumstances in which alternatives perform well.

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Appendix A

Identification of sampling ranges

Within this appendix, the reference values and sampling ranges of the uncertain factors are identified based on literature and market reviews. In addition, it explains various methodologies for using these variables to explore multiple futures.

A.1 Day-ahead electricity price

For the day-ahead electricity price, two data-sets are available which can be used to model its different plausible futures. Figure A.1 combines the empirical data from 2019 with the forecast data for 2030.

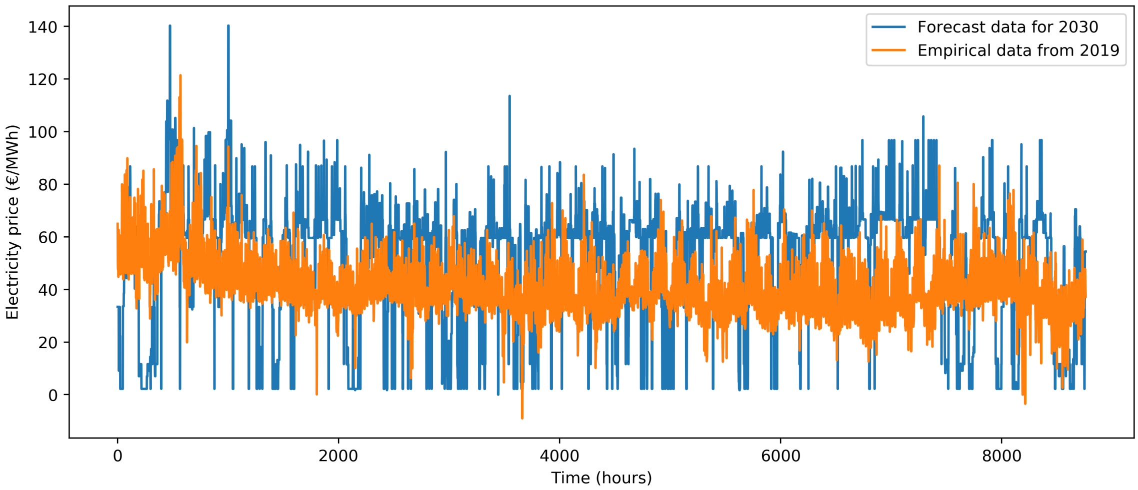

Figure A.1: Empirical data from 2019 and forecast data for 2030 of hourly day-ahead electricity prices. Data provided by PBL (2019) and Entsoe (2019) respectively.

The prices differences between these time series are mainly caused by the expected increase in offshore wind power. Due to the inherent variability of the wind, this form of energy generation is characterized by huge fluctuations in usable power. Through changes in the merit order, this fluctuating power source results in the fact that electricity becomes cheap whenever its supply is abundant and relatively expensive when it is scarce.

The targets for offshore wind power show that towards 2030 various wind parks are planned to be built and put into operation (Ministry of EACP, 2018). With every new wind park, the total amount of offshore wind power (GW) increases by a certain amount. The planning for the future shows that this increase is close to linear for the period between 2020 and 2030. Hence, under the assumption of this linearity, intermediate time series can be generated for the years between the empirical observation and the forecast, by using linear functions between the time related data points of these data sets. As an example, Figure A.2 illustrates how this method would work for a three year forecast for the day-ahead electricity price.

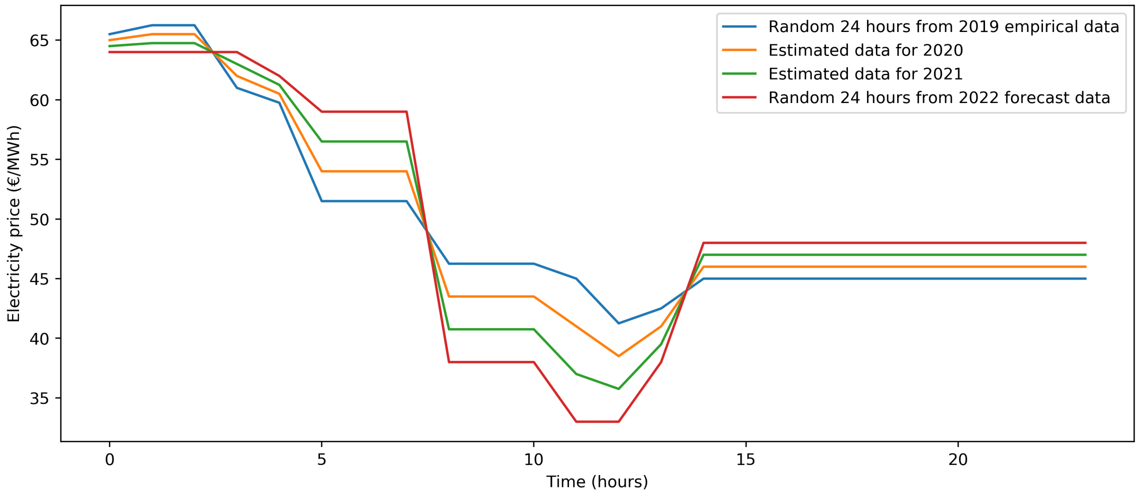

Figure A.2: Illustration of method for the estimation of hourly day-ahead electricity prices in years between empirical and forecast data.

In this case, the uncertainty is located in the accuracy of the forecast for the hourly day-ahead electricity prices of 2030. Hence, to create a sampling bandwidth for exploration of multiple plausible futures, every data point in this forecast time series is multiplied by a certain factor. The lower bound of this factor is 0.7 (-30%) and the upper bound is 1.3 (+30%).

A.2 Gas price

The reference value of the wholesale gas price is based on the preliminary gas price of the fourth quarter of 2019, which is 0.28 €/m^3 (CBS, 2020). The sampling ranges for 2030 are identified based on a forecast graph by PBL (2019) in Figure A.3. The lower bound is 0.16 €/m^3 and the upper bound is 0.32 €/m^3.

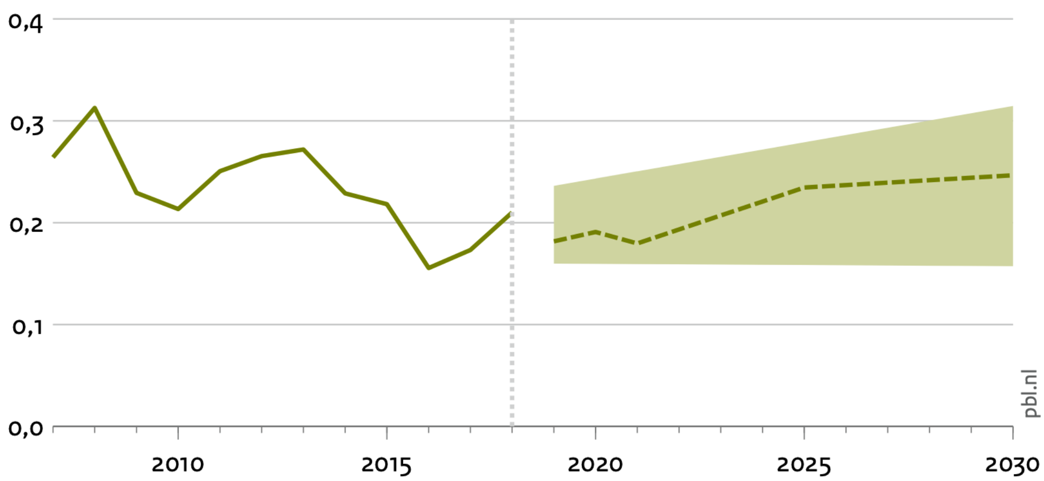

Figure A.3: Forecast of the wholesale gas price (€/m^3). Copied from "Climate and Energy Exploration", by PBL, 2019, p.35.

To be able to explore multiple plausible futures for the gas price within this sampling bandwidth, various linear time series are generated by using a generic equation to define the development of an uncertain factor (f) as a function of time (t) for every sampled value (s):

$$f(t)_s = \frac{s-c}{T} * t + c$$

For

$$\{s \mid B_L \leq s \leq B_U\}$$

Within this equation, the gradient of the linear function is given by subtracting the reference value (c) from the sampled value (s) and dividing it by the time horizon (T). The sampled value is taken from a set of values between the lower bound (B_L) and the upper bound (B_U). Figure A.4 demonstrates how this generic equation works and what the resulting functions may look like.

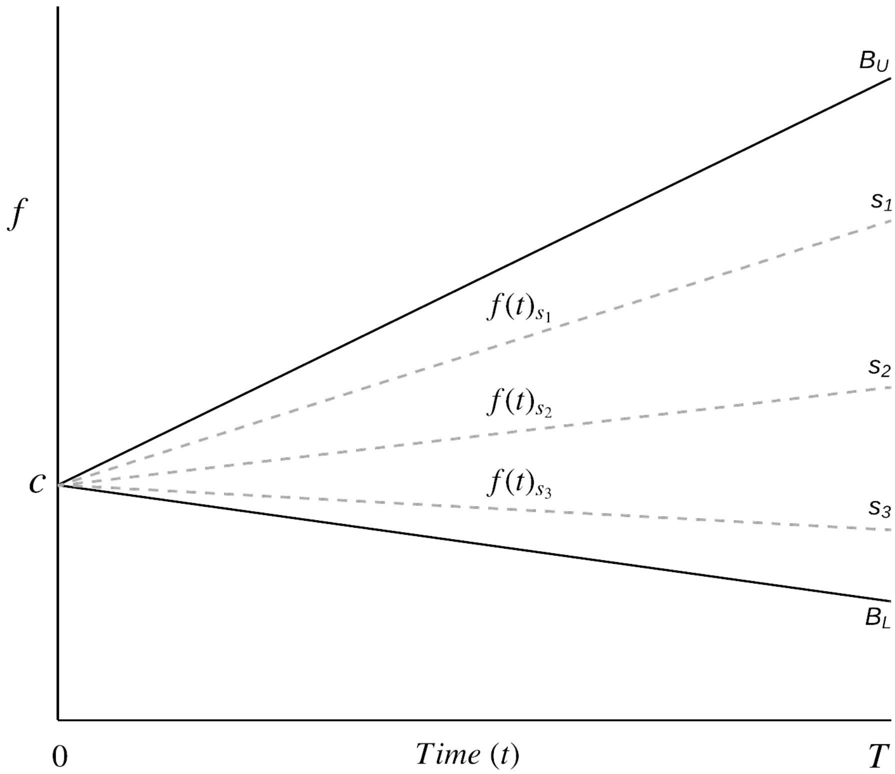

Figure A.4: Methodology for generating multiple linear time series

A.3 CO2 emission price

The reference CO_2 emission price is based on a market value in February 2020, which is 25 €/ton (Markets Insider, 2020). Figure A.3 shows a forecast graph by PBL (2019). The upper bound of this forecast is no longer accurate, as the recent national climate agreement announces a tax that could potentially cause the CO_2 price to rise to 150 €/ton (Ministry of EACP, 2019). Following this line of reasoning, the lower bound is set at 21 € /ton and the upper bound at 150 € /ton. Multiple futures for the CO_2 emission price are generated by using the same linear methodology as applied to the gas price in Figure A.4.

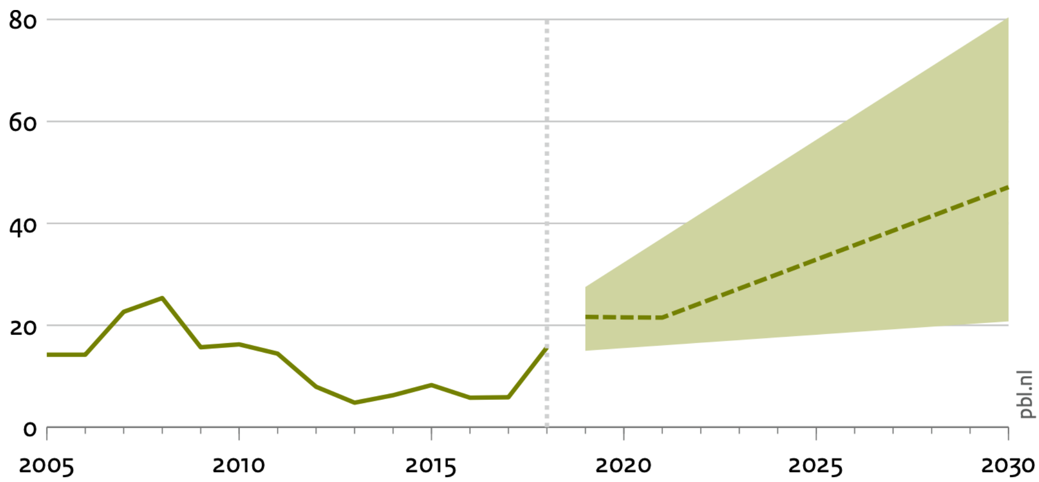

Figure A.5: Forecast of CO_2 emission allowance price. Copied from "Climate and Energy Exploration", by PBL, 2019, p.38.

A.4 Hydrogen price

To generate plausible numbers for the reference value and the bounds of the hydrogen price in 2030, only production from natural gas is considered, as hydrogen from electrolysis is expected to make its big entry after that period (Hydrogen Council, 2020).

Consultants from RoyalHaskoningDHV provided a simple excel sheet to calculate this hydrogen price. The calculation is based on the CO_2 emission price, the gas price and the CAPEX and OPEX of the Steam Methane Reforming (SMR) production process with Carbon Capture and Storage (CCS).

Stakeholders were consulted to make accurate estimations of the CAPEX and OPEX. For the calculation of the hydrogen prices, the previously identified reference values and bounds of the CO_2 emission price and gas price are used. This resulted in a reference value of 2.00 € /kg, a lower bound of 1.34 € /kg and an upper bound of 3.30 € /kg. Since 1 kg of hydrogen corresponds to a volume 11.13 Nm^3, the reference value can be expressed as 0.18 € /Nm^3, the lower bound as 0.12 € /Nm^3 and the upper bound as 0.30 € /Nm^3. Multiple futures for the hydrogen price are generated by applying the linear methodology from Figure A.4.

A.5 NaOH price

According to a presentation by industry group Ercros (2019), the price of caustic soda (NaOH) has fluctuated heavily over time. It is recognized to be very volatile, as it has been going up and down for years. As an example, Figure A.6 shows the historical prices of NaOH 50% between the period of 2013 and 2018.

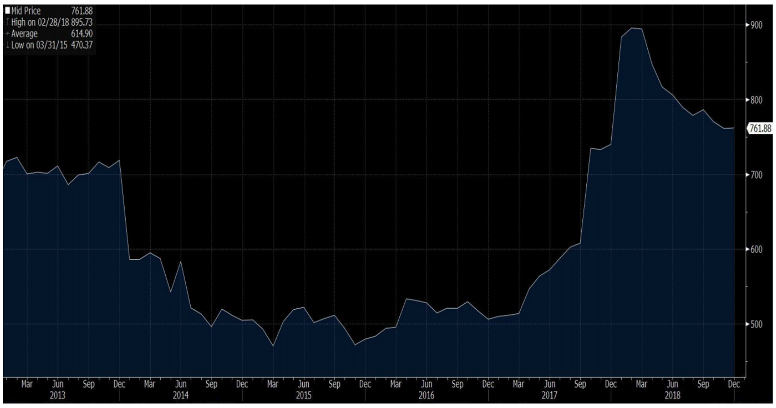

Figure A.6: Historical prices of 50% NaOH. Reprinted from "Outlook caustic soda and chlorine derivatives", by Ercros, 2019, p.20.

Assuming there is some kind yearly cyclicality in the behaviour of the NaOH price, it is possible to capture its future development with a generic sine function:

$$y(t) = A * \sin(B * 2\pi * (t + C)) + D$$

This function has an amplitude (A), a cyclical frequency (B), time (t), horizontal shift (C) and vertical shift (D). Stakeholder consultation resulted in the identification that NaOH prices fluctuate roughly between 100 €/ton and 1000 €/ton. Assuming a mean based on these numbers, the vertical shift of the sine function can be estimated at 550 €/ton and the amplitude at 450 €/ton. In this case, the uncertainty is mainly located in value for the cyclical frequency. Hence, a reference scenario is identified based on the graph in Figure A.6, which shows a cyclical frequency of one over five years (0.2 Hz). The NaOH price is likely to change daily, so this frequency is divided by the amount of days in a year. Since the reference 50% NaOH price is close to 550 €/ton, the horizontal shift is estimated to be zero (Kemcore, 2020). The analysis above results in the following sine function:

$$\text{NaOH 50\% price}(t) = 450 * \sin(\frac{0.2}{365} * 2\pi * t) + 550$$

Figure A.7 shows how multiple futures can be generated by using a lower bound of 0.1 Hz and an upper bound 0.3 Hz

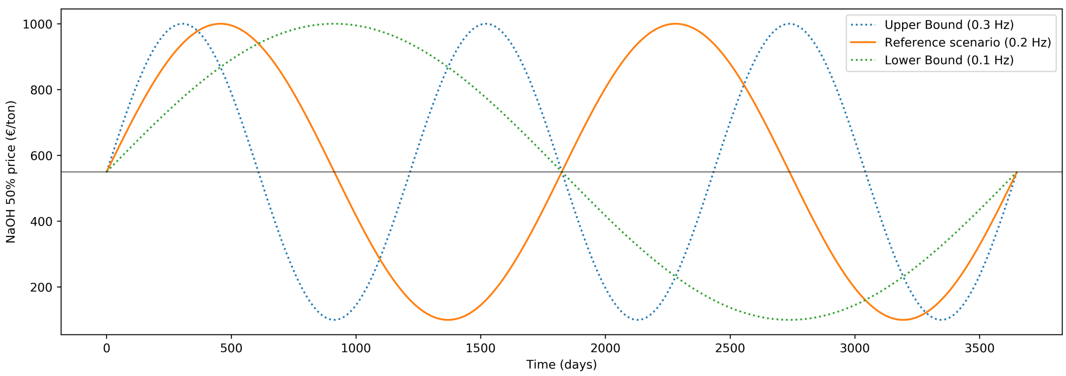

Figure A.7: Time series forecast of 10 years for the price of 50% NaOH.

A.6 Balancing electricity prices

Since the up- and downward balancing electricity price fluctuate heavily every fifteen minutes, a different approach is appropriate. As a reference scenario, the database prices of 2019 from TenneT (2019) are used. As an example, Figure A.8 shows the reference scenario for the downward balancing price.

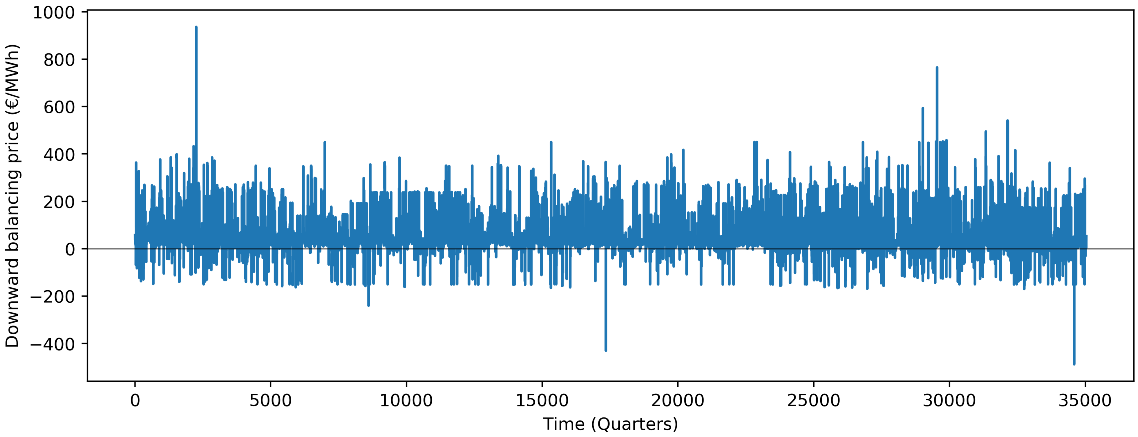

Figure A.8: Downward balancing electricity price per quarter of an hour in 2019. Data provided by TenneT (2019).

Figure A.9 shows the average downward balancing price per quarter of an hour per day to illustrate how forecasts for 2030 are generated by multiplying the time series by a scaling factor. This scaling factor has a lower bound of 0.7 (-30%) and an upper bound of 1.3 (+30%). It is important to note that this less dense average data is purely used for illustration purposes and will not be used in the uncertainty analysis. Instead, for the both the up- and downward balancing prices, the entire time series from 2019 is used to account for the peaks and negative prices. The time series for the intermediate years are estimated using the same approach as applied to the day-ahead electricity price.

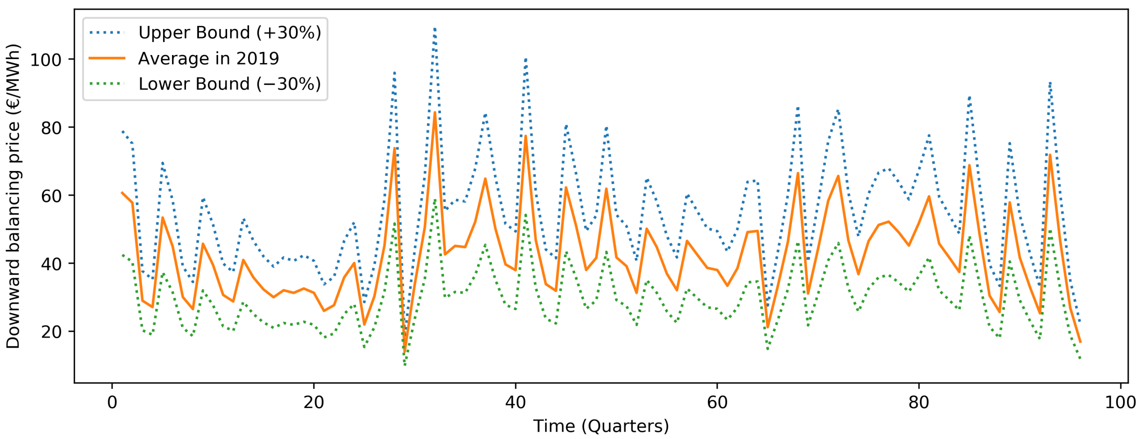

Figure A.9: Average downward balancing electricity price per quarter of an hour per day in 2019. Data provided by TenneT (2019).

A.7 Electricity on the imbalance market

The electricity supply and demand on the imbalance market also fluctuate significantly every fifteen minutes. Hence, the same approach is applied. Likewise, the database values of 2019 from TenneT (2019) are used to define the reference scenario. Figure A.10 shows this scenario, where positive and negative values represent the demand and supply respectively.

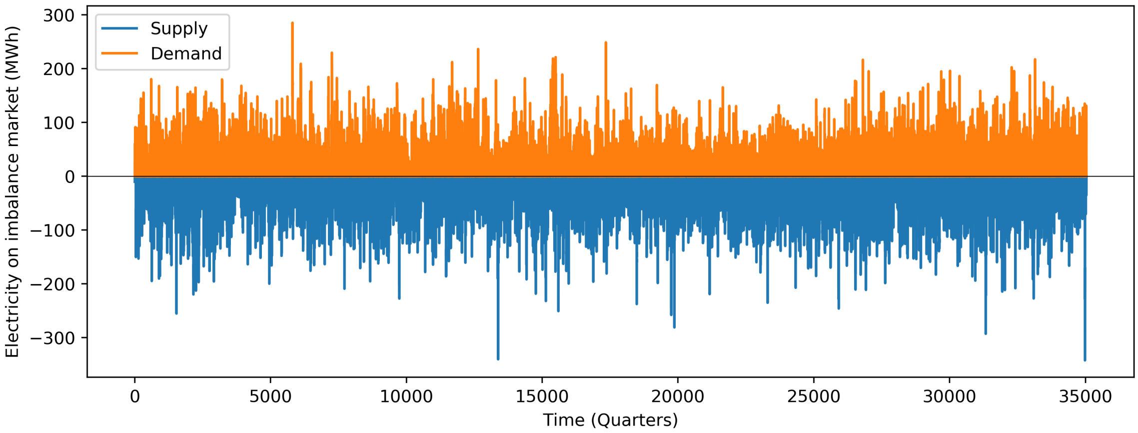

Figure A.10: Electricity supply and demand on the imbalance market per quarter of an hour in 2019. Data provided by TenneT (2019).

Figure A.11 shows the average demand per quarter of an hour per day to illustrate how forecasts for 2030 are generated by multiplying the time series by a scaling factor. This scaling factor has a lower bound of 0.7 (-30%) and an upper bound of 1.3 (+30%). Again, this less dense average data is purely used for illustration purposes and will not be used in the uncertainty analysis. Instead, for both the supply and demand on the imbalance market, the entire time series from 2019 is used to account for the many peaks. The time series for the intermediate years are estimated using the same approach as applied to the day-ahead electricity price.

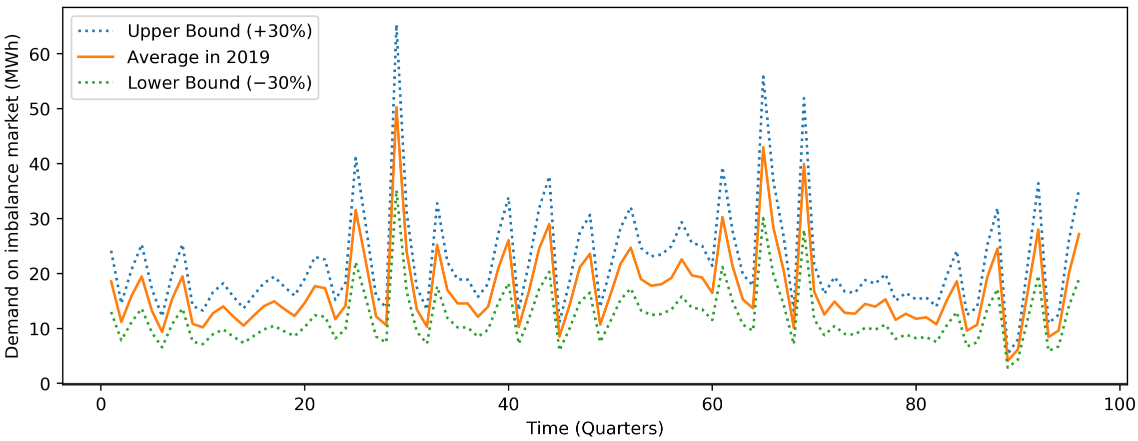

Figure A.11: Average electricity supply on the imbalance market per quarter of an hour per day in 2019. Data provided by TenneT (2019).

A.8 CAPEX and OPEX of the E-boiler

For the reference values of both the CAPEX and OPEX of the E-boiler at Air Liquide the default values in the model are used. This means that the reference value of the CAPEX is estimated at $2*10^6$ €/MW and the OPEX at 4000 €/MWh/Year. Since these values can only decrease through potential subsidy or technological innovation, the lower and upper bound of these factors are generated by multiplying the reference values by 0.7 (-30%) and 1 (-0%) respectively. For the CAPEX of the E-boiler this results in a lower bound of $1.4*10^6$ €/MW and an upper bound of $2*10^6$ €/MW. For the OPEX of the E-boiler this results in a lower bound of 2800 €/MW/Year and an upper bound of 4000 €/MWh/Year.

A.9 CAPEX of the Steam Pipe

The CAPEX of the Steam Pipe was not implemented in the original model. Hence, to estimate its reference value, the first step is to determine the potential length of the pipe infrastructure. Figures A.12 and A.13 show that the Steam Pipe consists of two parts. The first parts connects the existing steam pipe from AVR to the site where both Air Liquide and Huntsman are located. The second part connects the first part to Nouryon, which is located elsewhere in the Botlek area.

Figure A.12: Length estimation of the first part of the Steam Pipe, connecting Air Liquide and Huntsman (Google Maps).

Figure A.13: Length estimation of the second part of the Steam Pipe, connecting Nouryon (Google Maps).

The total length of the Steam Pipe infrastructure can be calculated by taking the sum of the length of both parts, which equals to 1.30 + 2.70 = 4.00 km. To find the reference value for the CAPEX of the Steam Pipe, this length is multiplied by a price factor of 3000 €/m, resulting in a reference value of $12*10^6$ €. Since this value can only decrease through a potential subsidy, the lower and upper bound are generated by multiplying it by 0.5 (-50%) and 1 (-0%) respectively. This results in a lower bound of $6*10^6$ € and an upper bound of $12*10^6$ €.

Appendix B

Model verification

This appendix contains model verification performed based on the unexpected results of a global sensitivity analysis of the first experimental results. In the first section, the results of this sensitivity analysis are shown in a feature scoring diagram. Within the second section, underlying model dynamics are explored to reveal potential defects. The third section discusses the results of a second global sensitivity analysis using an improved connector script.

B.1 Global sensitivity analysis

The feature scoring technique used to perform the global sensitivity analysis is based on a statistical machine-learning approach called “extremely randomized trees” (Extra-Trees). It was introduced by Geurts et al. (2006) and uses decision trees to estimate regression coefficients. Figure B.1 shows the results based on the outcomes of the first set of experiments.

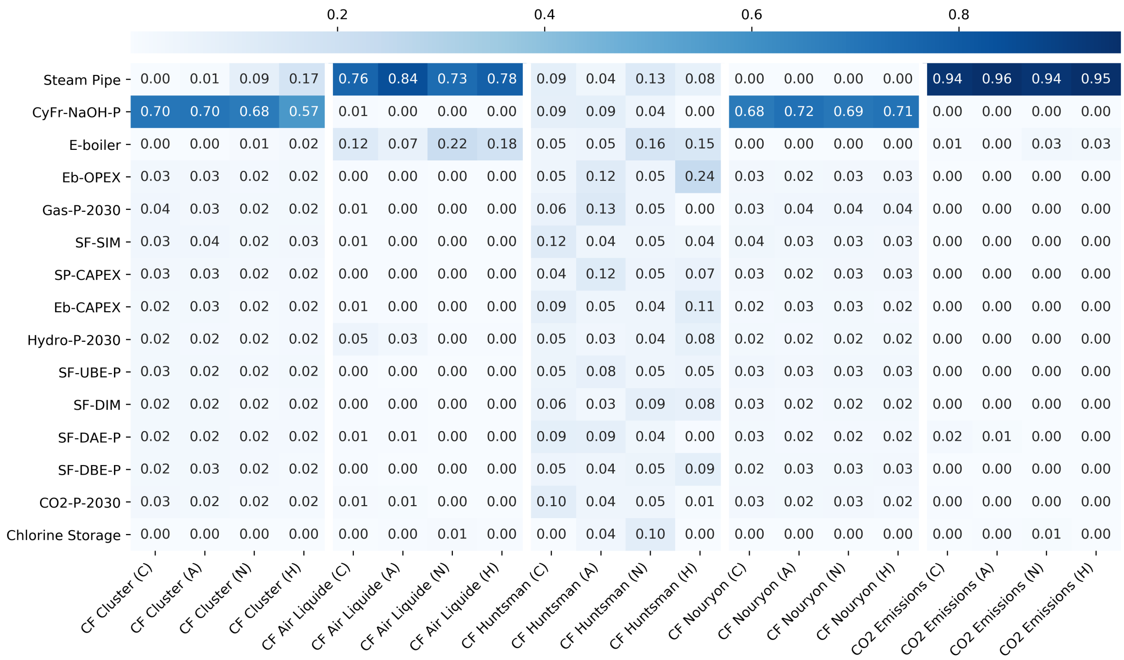

Figure B.1: Feature scoring diagram of first set of experiments

The vertical axis contains the uncertain factors and alternatives, ranked in descending order based on the sum of their estimated regression coefficients. The horizontal axis contains the outcomes grouped by optimization perspective. It is important to note that the estimated regression coefficients do not indicate the direction (increase or decrease) of an effect. They are merely indicators of the extent to which an uncertain factor or alternative influences a certain outcome.

By inspection of Figure B.1, it is clear that some of the uncertain factors and alternatives show unexpected and divergent behaviour. For example, all the uncertain factors have very little influence on any outcome compared to the influence of the cyclical frequency of the NaOH price on the cash flows of Nouryon and the entire cluster. Furthermore, the E-boiler seems to have a very low effect on the CO_2-emission outcome. Hence, the next subsection will explore the underlying dynamics of these remarkable results to find out whether a certain kind of behaviour is valid or whether it is caused by model imperfections.

B.2 Exploring the underlying dynamics of unexpected results

There are four main cases of results in Figure B.1 that require an explanation. To begin with, it is remarkable that the E-boiler has such a low effect on the CO_2-emissions. By closely observing a number of custom experiments with the model and by talking to its original developers, it was obvious that a mistake was made regarding the implementation of the E-boiler. More specifically, when the E-boiler was implemented during an experiment, the so called "cogens", which are machines that use gas to generate electricity and useful heat at the same time (co-generation), were not put out of operation. Consequently, they would still be used to generate these products, as their corresponding production costs are often lower than that of the E-boiler. The solution was an adjustment of the python script connecting the EMA Workbench and the model, which forces the model to put the cogens out of operation whenever the E-boiler is implemented during an experiment.

Furthermore, the Steam Pipe alternative scores very high in terms of its effect on the CO_2-emission outcome. When this behaviour was checked during simple model experiments, it was discovered that the implementation of this "green steam" alternative actually *increased* the amount of CO_2-emissions, instead of decreasing it. After a thorough search through the model, there were indications of where the origin of this problem might be located. However, the specific dynamics underlying the problematic behaviour found at this location were not well understood by the developers. Within the time frame available to this research, this problem could not be resolved at this point. Hence, potential future research that uses this model should initially focus on finding a solution to this problem.

Another remarkable result is the relatively large amount of influence exerted by the cyclical frequency of the NaOH price. Model inspection resulted in the conclusion that it was unlikely to be caused by an error within the causal relationships of the model. As discussed earlier, the cycle time (three to ten years) of this uncertain factor does not fit into the characteristic week used for each simulation year. However, a workaround was implemented for this problem by using the average caustic soda price of a certain year throughout its corresponding week. Following this line of reasoning, the behaviour of this factor might be explained by the large amplitude of the sine function used to model its future development. However, these choices were made based on information provided by stakeholders. Therefore, it is concluded that the influence of the cyclical frequency of the NaOH price is valid according to the extent in which the model is a representative version of the real-world system.

The relatively low effect of the gas price and CO_2-emission price on both the amount of CO_2-emissions and the cash flow of Air Liquide is also worthwhile to look into. The first category of behaviour can be explained by the relatively small decision space available to the actors due to their contractual obligations. For example, Air Liquide can only ramp down its production process to a certain extent, because of the bilateral agreements with both Huntsman and other market actors. Hence, the effect of such product prices on the amount of CO_2-emission is limited. Furthermore, the low influence of the gas price and CO_2-emission price on the cash flow of Air Liquide is related to the fact that the model does not account for any profit or loss margins. By default, the actors in the model pay so called "cost prices" for the products produced by other actors within the cluster. Consequently, if a product becomes more expensive to produce due to higher prices for its materials, the guaranteed sales price increases with an equivalent amount. This means that product prices have no effect on the cash flow of the actors. The software that defines the MILP problem (Linny-R) does contain an option to account for profit or loss margins. However, this option was not implemented at this point, because the actors were deemed unlikely to provide this kind of information.

B.3 Iteration using improved connector

After the implementation of the solution regarding the identified E-boiler problem, all experiments were run again using the improved connector script. Figure B.2 shows the results of the feature scoring analysis using the new results.

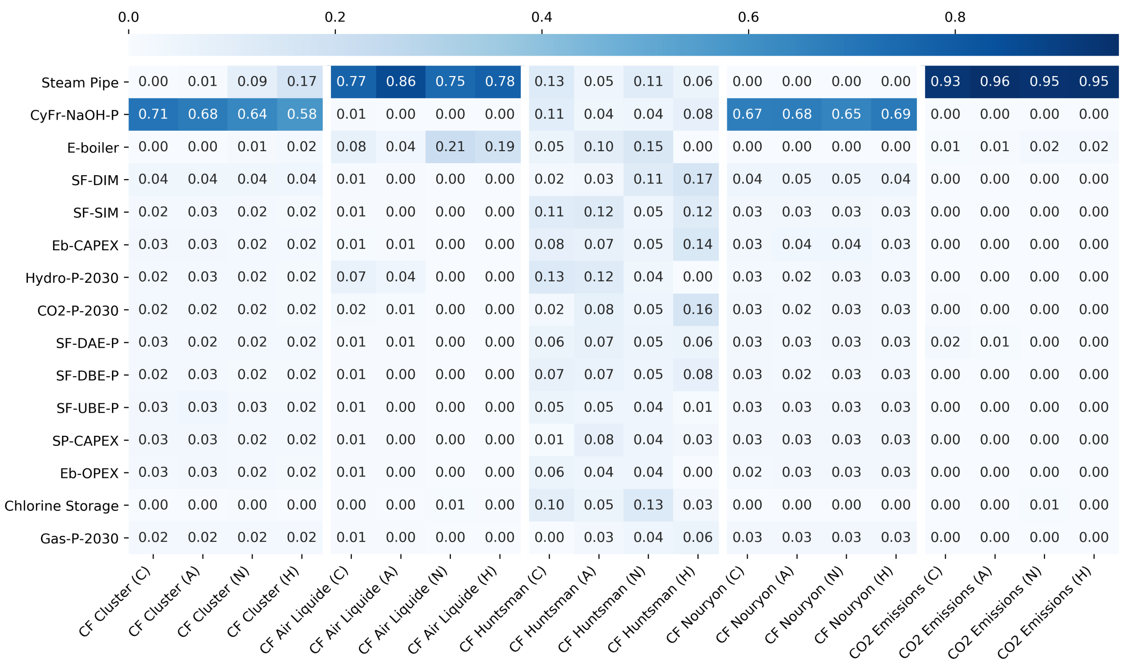

Figure B.2: Feature scoring diagram of second set of experiments

At first sight, the results in Figure B.2 look quite similar compared the previously presented feature scoring diagram. However, when one pays attention to the ranking of the uncertain factors and alternatives, it is obvious that a lot has changed. Most importantly, with the implemented solution, one would expect a significant increase in the effect of the E-boiler on the CO_2-emission outcome. However, in contrast, the results show only a slight increase of this effect from the perspective of Air Liquide and a decrease from the perspectives of Nouryon and Huntsman. Hence, the conclusion is that the potentially valid dynamics within the model are distorted by something else. The current hypothesis is that this is caused by the problematic behaviour found at the location where the Steam Pipe issue originates. Nonetheless, this remains a topic for future research.

Now it is clear that the model contains unsolved defects which invalidly influence the results, it is paramount to consider what this means for the remainder of the uncertainty analysis. In general, it means that the results of every method (including the feature scoring) can only be interpreted to a very limited extent. More specifically, it will not be possible to make any case-specific conclusions or recommendations. This translates to the fact that some of the research questions cannot be answered completely.

Appendix C

Code

The code used throughout this research is made available in a GitHub repository on the following web page:

`https://github.com/robroos/master_thesis_code`

This repository contains the following Python scripts:

- The "connector" script that allows for the exchange of information between the EMA Workbench and the Linny-R model (linnyr_connector.py).
- The open exploration script using the EMA Workbench (open_exploration.py).
- The Jupiter Notebook of the analysis of the results (analysis_of_results.ipynb).

Feel free to contact me on the e-mail address below if you have any questions:

`rob__roos@hotmail.com`