Designing optimal investment trajectories for the energy transition of industrial clusters in the Netherlands

Master of Science in Complex Systems Engineering and Management

Stijn van Dullemen

Delft University of Technology

TU Delft

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Stijn van Dullemen
Student number: 5414903

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Graduation committee

Chairperson: Dr.ir. R.M. Stikkelman, Engineering Systems and Services
First Supervisor: Dr.ir. R.M. Stikkelman, Engineering Systems and Services
Second Supervisor: Dr. P.W.G. Bots, Technology, Policy and Management
External Supervisor: Ir. R. Slaghek, Sitech Services BV

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With this, I present you my master's thesis. With this, the last step will be concluded of my Master in Complex Systems Engineering and Management. It will also finalize my educational journey I have got to enjoy at the TU Delft. However, without the rightly deserved acknowledgements, I would not be where I am today. Therefore, I would like to express my gratitude to the following people:

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Executive Summary

Because of the climate crisis the world is facing, all sectors must move towards a more sustainable future. In the Netherlands, the industry sector emits large amounts of CO_2 because of the heavy reliance on fossil-fuels and large electricity demand. The Paris agreement and the Green Deal forces the industry sector to rapidly transition towards more sustainable practices, which can be achieved if the correct synergies are established. The multi-actor nature and the technical and operational dependencies that industrial clusters have, makes optimal decision-making extremely important in working towards that net zero future. Innovations that reduce the emissions are limited, but they exist and provide (intermediary) solutions to adhere with the imposed regulations. Furthermore, the industrial clusters are subject to numerous different factors that influences the behaviour of actors within the cluster. The issue faced is to understand how the transition of an industrial cluster is influenced by exogenous factors and how actors in such an integrated environment should invest, while keeping in mind that both the industrial clusters and the individual actors have to remain profitable and have differing investment behaviour.

Current studies fall short in identifying, analysing and understanding how multi-actors in an institutional environment relate to the technical options and the exogenous factors engaging with that system in an industrial setting. Identifying an optimal investment trajectory that such an industrial cluster should follow to adhere with the regulations whilst staying profitable with a multi-actor configuration requires different integrated methods and other tools. This thesis will address that problem through the following main research question:

What is the effect of multiple exogenous factors on the optimal investment trajectories of industrial clusters in the Netherlands with multiple investment options?

This question has been answered through exploratory research combined with a modelling approach. The first step in the exploratory research required attaining insights in what the current state of is multi-actor investments. This in combination with looking at how they are structured contractually has been the main foundation for the literature review. A case study analysis has been conducted of an industrial cluster located in Geleen, called Chemelot. This allowed for analysing decarbonizing investment options and looking at what exogenous factors influence the industrial cluster. The investment options attempt to move Chemelot away from fossil-fuels as energy source and move towards lower emitting sources such as electricity.

The information gathered served as an input to put together a methodology which captured the exogenous factors, interactions in the industrial cluster and the sustainable investment options in an optimization model. Using this, the optimization model was constructed using Linny-R, a Mixed Integer Linear Programming optimization software developed by Dr. P.W.G. Bots. The model produced quantifiable results as well as serve as a proof of concept for the methodology that is presented to incorporate exogenous factors and sustainable investment options in the energy transition. The model also gives insights in what effect the exogenous factors have on the investment behaviour of actors within industrial clusters by showing cash flows, both individually and collectively and through an investment curve for the cluster. The economic performance is considered to be the leading metric in this research. Finally, using the results, the implications of implementing exogenous factors and sustainable investment options in an optimization model are discussed.

The research outcomes show that CCS and electrification are favourable investments for Chemelot to remain profitable and cope with increasing prices of commodities and CO_2. The model results has provided insights in the effect that exogenous factors have on the energy transition of an industrial cluster. More specifically, it showed that a cap on CO_2 and increasing the price of CO_2 emitted really accelerates the rate at which actors make investments in sustainable options. Added to that, increasing the price of other commodities such as natural gas and naphtha also forces actors to move away from those commodities and look for alternatives that provide the same product or energy without having to compensate the CO_2 emissions related to them. Other factors such as limited infrastructure restrict industrial clusters in the amount of products they can produce and restrict them from innovating towards less emitting processes. Electrification of certain processes is possible, but increases the electricity demand with enormous amounts. With limited electricity infrastructure to provide those amounts, the innovation cannot be realized and therefore, halting the transition for an industrial cluster. The findings suggest that because of these exogenous factors, the actors will move towards electricity demanding innovations that do not make use of fossil-fuels and invest in CCS options. However, the methodology presented should be used as directing future research in looking at how industrial clusters should engage in the energy transition. The dependencies existing between actors in an industrial clusters and how different investments

may adjust these dependencies are identifiable using the methodology presented in this research.

Ending with a general conclusion, the investment behaviour of industrial cluster changes because of multiple exogenous factors that influence the system. The increase in commodity prices combined with CO_2 capping regulations cause actors to invest more quickly into sustainable investment options to adhere with the regulations, but it also causes them to compromise their production levels in some scenarios to remain profitable. Actors downstream are dependent on the investments made by actors upstream since they rely on the output of those upstream actors to develop the final products that they sale. This combination generates valuable insights from a systems perspective but also from a multi-actor perspective.

With the conclusion of this research, suggestions are made for future research. First, future research should be committed to optimizing the investment structure presented in this research as well as performing the research on a different industrial cluster to look determine whether some industrial clusters are more resilient than other industrial clusters. Furthermore, performing the research at a different industrial cluster can also give rise to the identification of different exogenous factors and determine the relative impact of the exogenous factors. Other future research could be committed to using more relevant input data, increasing the level of detail in the model and by including market demand developments to gain more insights in how they will influence the investment behaviour. Finally, extending the regulations implemented in this research to also include other emissions such as NOx will give rise to new investment trajectories, which in turn will support industrial clusters in their energy transition.

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1 Introduction

1.1 Importance of the industrial sector energy transition

Industrial processes consume over one third of the total energy worldwide and its associated emissions (Sharifzadeh et al., 2015). With the commitment to the Green Deal and Paris Agreement, road maps with key policies have been created for the EU and the Netherlands to start a revolutionary transition path to reduce the CO_2 emitted by 55% in 2030 and 95% in 2050 (Agreement, 2015; Siddi, 2020). It requires all industries to reduce their CO_2 emissions drastically in the coming decades such that the average global temperature increase can be maintained below 2 degrees. The industrial sector in the Netherlands was responsible for 18.9 MTon of CO_2 (CBS, 2020) in 2020, accounting for 11,5% of the total emissions of the Netherlands (CBS, 2021), but was also responsible for generating roughly 1.8% of the Dutch gross national product (Kwaak et al., 2021). Currently, the Netherlands rank third largest chemical industry in Europe (Topsectorchemie, 2020), and keeping this competitive position is important because of the revenue it generates (Vanthillo et al., 2018). The problem is that this industry is very energy intensive and extremely fossil-fuel reliant, making the energy transition a complex problem.

1.2 Industrial clusters

A way to enhance the sustainability of an industrial company is by combining multiple companies in an industrial cluster (IC) (Domenech et al., 2019). **Industrial clusters** can be defined as follows: "An **industrial cluster** is a cluster of a geographically proximate group acting as an integrated system that reduces waste generation and GHG emissions by closing the loop on manufacturing processes of all sorts through recycling of waste from different processes and industries and using it as feedstock for other processes" (Domenech et al., 2019; Foundation, 2013; Sun et al., 2017). Industrial clusters enhance sustainability within industries which are hard to decarbonize due to less pressure on the raw materials used and reduction in GHG emissions due to reusing waste (Domenech et al., 2019). Furthermore, industrial clusters allow for maintaining a competitive position by increasing revenue (Sun et al., 2017) due to the reduced waste and less pressure on raw materials (Domenech et al., 2019). A difference can be made between the implementation of industrial clusters in Europe and within the Netherlands. In Europe, the implementation of industrial clusters is happening at a disappointing rate (Domenech et al., 2019), whereas in the Netherlands, multiple industrial clusters already exist for a few decades. Through case studies, (Taddeo et al., 2012) has developed a list of the largest barriers for IC implementation in Europe, and state that it is mainly obstructed by financial obstacles, lack of on ground support and the regulatory and legislative barriers related to the country it is situated in (Zander et al., 2016). An industrial cluster can consist of many different processes and products, but is defined by having an integrated structure. For the sake of this research, the term industrial clusters will encompass the largest industrial clusters in the Netherlands, with a focus on the petrochemical aspects such as chemical production, chemical cracking and generation of required energy.

1.3 Industrial clusters in the Netherlands

In the Netherlands, six large clusters can be identified: Delfzijl, Emmen, Amsterdam, Rotterdam-Moerdijk, Zeeland and Chemelot, with Chemelot having the largest petrochemical production. Combined they have over 400 active companies within those clusters and around 46.000 employees (Topsectorchemie, 2018) (Chemische-industrie.nl, 2022). The chemical industry in the Netherlands is not only important for the jobs they create, but they also provide economic benefits because of the revenue they generate. The Dutch chemical industry is largely concentrated into those industrial clusters (Topsectorchemie, 2018). The majority of the Dutch chemical industry is situated in industrial clusters, putting them in advantage to other related countries because of the added benefits that industrial clustering bring (Domenech et al., 2019; Kwaak et al., 2021). The current fossil fuels used in the industrial clusters in the Netherlands serve two purposes, providing energy for the different processes in an industrial cluster and providing the feedstock for various processes. The clusters require naphtha, natural gas, biomass, and pyrolysis oil as feedstock. The different companies acting in an industrial cluster can belong to the same owner or multiple different owners. This is referred to as **single-actor industrial cluster** and a **multi-actor industrial cluster**. With the single-actor industrial cluster referring to a cluster largely owned by either a single or few actors, whereas, the multi-actor industrial cluster refers to industrial clusters existing of a large number of different companies owned by different owners.

1.4 Investment decisions in industrial clusters

Becoming more sustainable as an industrial cluster is complex, the clusters have to invest in new technologies that reduce emissions drastically. However, little literature is available on how industrial clusters should invest to adhere with the regulations of 2050. Literature such as Janipour et al. (2022) highlights that companies acting alone and have a short-term focus are 'traps' within industrial clusters that hinder reaching deep emission reductions, however, it does not show what the influence can be of coordinated investment operations. Other literature such as Wang et al. (2022) and Mazzoni et al. (2020) focus on a single aspect which may affect the emission levels. The investment decisions can be made on a collective level, a high systems level and taking into account all active companies in the cluster, but also on an individual level. The individual companies residing in an industrial cluster also need to reduce their individual emission levels (Cuppen et al., 2021). The difficulty resides in moving towards more sustainable processes whilst still being able to meet market demand. Furthermore, the investments need to be profitable over a very long amount of time. The multidisciplinary nature and individualistic investment behaviour of companies within the multi-actor industrial clusters are large factors influencing the investment trajectory that the industrial companies can take Janipour et al. (2022). Investment decisions are based on the functional, institutional, legal and economic relationship actors have who are interconnected. Changes made to the operation level of a certain actor may alter the overarching cluster, reducing the flexibility of the entire system (Cuppen et al., 2021). Because the single-actor industrial clusters can function largely as one entity, and therefore, perform actions with a higher systems level perspective, the focus of this thesis will be on multi-actor industrial clusters. More specifically, the focus will be mainly on multi-actor industrial clusters in the Netherlands with large petrochemical production sites.

1.5 Knowledge gap on investments for the transition in industrial clusters

The knowledge gaps identified firstly show that the current literature focuses on either single investments, or CO_2 reducing solutions that are already in place in the industrial clusters in the Netherlands. Secondly, different factors that influence the industrial clusters need to be identified and categorized to fully comprehend the effect they have. The goal of this thesis is to research how industrial clusters are influenced by different factors and how it influences the investment behaviour. To specify the knowledge gap a bit more, there is lack of knowledge on what influences the investment behaviour and how can the influences be identified and analyzed. Literature on increasing the sustainability of industrial clusters is limited in multiple ways. It suggests that companies within industrial clusters should integrate their inputs and outputs to increase sustainability (X. Chen et al., 2020), industrial clusters should focus on innovation (Wang et al., 2022) and that (local) governments should induce policies that limits the clusters to emit more than a certain amount of CO_2 (Mazzoni et al., 2020; Wang et al., 2022). Furthermore, more micro-level literature focuses on replacing single processes to increase sustainability, such as usage of carbon capture and storage to capture and use CO_2 for other companies in the industrial cluster (Bui et al., 2018), the use of excess H_2 for the production of methanol (CH_4O) following a gasification-method using biomass, or how using sequential combustion in a steam methane reforming hydrogen plant can reduce both costs and allow for decarbonized industrial clusters to generate H_2 and electricity downstream (Herraiz et al., 2020). However, literature lacks to provide knowledge and insights on two aspects for multi-actor industrial clusters in the Netherlands:

- The clusters already have a (relatively) high level of interdependency (VNCI, 2020), have innovation hubs to increase sustainability (Chemelot, 2021) and are already subject to CO_2 reducing policies, such as the Green Deal and the Paris Agreement (Agreement, 2015).
- The literature focuses on replacing a single process or implementing a single innovation to reduce CO_2 emissions (Bui et al., 2018) (Herraiz et al., 2020) and not on the possibility of adding multiple innovations, or focus on the investment behaviour of multiple actors if multiple innovations should be implemented across those actors.

The knowledge gap is now further specified by looking at other influences that determine the investment behaviour of industrial clusters.

1.5.1 Additional problems that hinder the investment behaviour

Multi-disciplinary nature

A large barrier for engaging in the energy transition of industrial clusters is the multidisciplinary nature of multi actor industrial clusters. Especially in examples of clusters where some companies have multiple international owners. They may be more hesitant to engage in the energy transition if it may risk the economic benefits (van Benthem, 2021; Gunantara, 2018). In addition, because of the distance between the owners and the physical location of the company, it may be harder to implement certain CO_2 reducing initiatives due to the owners not sensing the urgency to reduce the CO_2 or lack of loyalty to the country (Warnock, 2019). New investment options are carefully evaluated in industrial clusters due to the large costs and implementation time, and having to provide a profitable return. Actors within the cluster should be aware that their operation within the cluster may not always provide advantages. It could well be that in the cluster, a phenomenon called "co-opetition" arises, which is a situation where an actor may have a competitor that also complements the competitors economic position because of the integrated structure (Teychené et al., 2019). This also results in certain investments not being an option due to compromising that integrated structure. This micro-level consideration of companies within clusters versus the macro-level consideration of the IC itself and the social responsibility that the IC carries makes creating a single transition path for the industrial cluster that everyone benefits from difficult.

Alternative fuels and raw materials

Besides searching for alternative fuels and raw materials, certain processes also have to adapt to these new fuels and materials. The majority of the processes will still require high temperatures to function, but working towards 2050, they cannot be fueled using fossil-fuels. Industrial clusters currently use naphtha, natural gas, biomass and pyrolysis oil as feedstock to both generate the required energy for the processes and to use it as raw materials for producing products such as plastics (*Netbeheer2022ii*, n.d.). However, in the path towards 2050, the feedstock has to be changed to reduce the CO_2 emissions. Firstly with regard to the use of alternative fuel like combustion of biomass, the EU ETS does not penalize the CO_2 emitted through combustion of biomass as long as the companies using it can provide proof that the biomass being combusted adheres to the European sustainability criteria starting in 2023 (NEA, 2022). Meaning that biomass can still function as a feedstock towards reaching the CO_2 policy of 2050 and beyond. However, it is projected that the availability of biomass is not sufficient to supply the demands of the industrial clusters (Spijker et al., 2020). Therefore, other alternative fuels and raw materials have to be used as well. Furthermore, because of the interdependencies in industrial clusters, by-products and emissions of feedstock and raw materials are essential to keep the competitive position industrial clusters have with other European clusters. By deviating from the current feedstock and raw materials, companies downstream may suffer from lack of input due to new feedstock and raw materials not providing the necessary input. So, another big challenge is overcoming the lack of necessary input, or producing the input without emitting CO_2. High temperature processes fueled by fossil-fuels will have to look into the possibility of electrification. However, companies with high temperature processes that have high energy demands such as melting, furnacing, and drying are unsure in whether electrification may be an alternative for natural gas in the long term, or that combustion of natural gas or biomass are the only possible feedstocks to comply with the demanded process conditions (Chemelot, 2021). Due to the uncertainty of this issue, companies may also look into the possibility of H_2 usage for those processes besides electrification and whether it is technically feasible or affordable (Chemelot, 2021). H_2 is currently also a large feedstock for other industrial clusters in the Netherlands. The 2050 policy forces the clusters to make use of green hydrogen, which is hydrogen made using renewable electricity. This also comes with issues, such as the intermittency of solar and wind energy, losses due to transportation and lack of storage infrastructure (Slaghek, 2021).

Lack of infrastructure

Current infrastructures cannot handle these amounts (Wiggelinkhuizen et al., 2021) and thus, adjustments to the infrastructure are necessary to continue with producing the same amount of products without using CO_2 emitting fuels. An alternative could be using electricity, but it would require large amounts of electricity to reach these high temperatures. It is expected that the average electricity usage of the Netherlands will increase by 300% (*Netbeheer2022ii*, n.d.), and the industrial clusters demand increasing with even more. However, current infrastructures cannot handle these amounts (Wiggelinkhuizen et al., 2021) and thus, adjustments to the infrastructure are necessary to continue with producing the same amount of products without using CO_2 emitting fuels. Furthermore, the infrastructure within industrial clusters also needs to be adjusted to incorporate those large amounts of electricity (Chemelot, 2021). Another issue is that certain industrial clusters in the Netherlands are not situated near a port, thus acquiring offshore generated renewable electricity might be less efficient due to losses. The use of H_2 in those same clusters may also be less efficient due to the necessity of transportation from the H_2 ports to the clusters (Aakko-Saksa et al., 2018) (Jackson et al., 2019). Implementing technology such as local H_2 storage in the industrial clusters would require adjustments to the infrastructure inside and outside of the cluster to overcome the issue of transportation losses. The difficulty of the infrastructure issue is that it requires cooperation of the DSO's and TSO's together with industrial clusters to realize the electricity infrastructure (Chemelot, 2021), and cooperation between H_2 importing companies, industrial clusters and the government to realize the H_2 infrastructure (Tarkowski, 2019). Furthermore, companies within industrial clusters need to cooperate to realize the electricity and H_2 infrastructure locally whilst maintaining a competitive position with respect to other industrial clusters in Europe (Chemelot, 2021).

1.5.2 Factors influencing the energy transition of industrial clusters

The energy transition of industrial clusters in the Netherlands face the problems described above. Breaking down the different factors that influence the energy transition for industrial clusters in the Netherlands allow for better understanding. The factors that influence the industrial clusters can act from within the system boundaries, or outside of the system boundaries. These are referred to as *Internal factors* and *Exogenous factors*. Depending on the system boundaries of an industrial cluster, or the research approach that is taken, there might be some overlap between internal and exogenous factors. Misalignment of (commercial) interests, lack of social responsibility and duration of alignment of economic interests are usually considered as internal factors (Plyaskina et al., 2017). Whereas, factors happening outside of the system boundary and that are induced by external parties and occurrences such as gas prices, low efficiency of government policy encouragement and limited opportunities to attract investment resources are usually considered exogenous factors (Plyaskina et al., 2017). Categorizing the internal and exogenous factors will allow for a better overview of the characteristics of the factors such as rate of change and impact. Relevant literature uses different frameworks for assessing different rules or institutions within complex systems. Stepney (2010) uses the IAD framework by Polski & Ostrom (1999) to describe the interactions between participants under certain circumstances. Koppenjan & Groenewegen (2005) use the Williamson scheme by Williamson (1989) to describe the efficiency and effectiveness of different institutions on the regulation and coordination of the behaviour of actors in complex networks. Furthermore, Abba et al. (2022) uses a holistic risk management framework to consider the multi-dimensional perspective of risk, the interactions and interdependencies within said complex system, the dynamic nature of risk and a holistic approach to the priority risks. chapter 2.4 will elaborate on the framework that is chosen to categorize the factors. Internal factors can be influenced by an industrial cluster, or the companies situated in the industrial cluster. Exogenous factors influence the entire industrial cluster and they are not influenceable by the industrial cluster. The exogenous factors form the playing field and the rules to which the industrial clusters must adhere when becoming more sustainable. Therefore, this research will only consider the exogenous factors.

1.5.3 Modelling the investment behaviour for the transition of industrial clusters

Currently, no literature takes into account the multi-disciplinary and interdependency nature of industrial clusters, and combines it with the exogenous and internal factors that influence the energy transition to develop optimal investment paths such that the goals of 2050 will be reached. Furthermore, literature on energy system modelling falls short in grasping the relation between the technical level and the institutional multi-actor structure of an industrial cluster (Fleiter et al., 2018). These models highlight either the policy details or the technological innovations. The high technological detailed models fail to consider the policy instruments in place, whereas the focusing on the policy instruments, do not optimize the technological performance (Fleiter et al., 2018). The conventional energy system modelling approaches lack the ability to integrate the technological with the policy, resulting in lack of identifying future uncertainties arising from the interactions between the technological and, in this research, the multi-actor nature of industrial clusters (Melese et al., 2015). The industrial clusters require to develop an investment trajectory, showing their planned investment options over a set time span. The main goal of the investments for the individual level should be to generate positive cash flow, and on the cluster level to reduce CO_2 without negatively impacting other companies. Several studies have focused on applying optimization models on industrial clusters to develop investment paths, but they focused on risk-sharing (Jamal & Montemanni, 2018) or cross-plant precaution investments (Reniers et al., 2012) and not on the energy transition and its related investments.

By using relevant literature, the knowledge gap has been specified. The knowledge gap is that the macro-level literature provides outdated solutions and the micro-level literature focuses on single innovations, whereas a macro-level perspective is required with multiple innovations to be able to transform the entire system towards the requirements of 2050. This gap shows that no clear investment trajectories currently exist for industrial clusters trying to become CO_2 neutral in 2050 and that the effects that different exogenous factors have on the system have not been identified and analyzed. Resulting in industrial clusters not knowing how they should invest in new sustainable technologies under different circumstances and scenarios. Furthermore, the energy system models used in relevant literature fails to capture both the technological and policy elements of the industrial clusters. These knowledge gaps are summarized and addressed in chapter 1.10 as the main research question and sub-questions for this research.

1.6 Scope

This research aims to demonstrate the influences of multiple exogenous factors on the optimal investment trajectories for industrial clusters in the Netherlands with multiple investment options. The scope of this research includes the petrochemical departments of multi-disciplinary industrial clusters in the Netherlands and it extends towards the exogenous factors that influence them. However, it must be noted that the system cannot influence the exogenous factors. The exogenous factors are dependent on decisions made by actors outside of the scope such as local governments, regional governments, the EU and volatile market influences such as the price of commodities. To achieve this, a modeling approach will be formulated that can engage with this problem and future similar problems. Furthermore, a case study will be performed on an industrial cluster in the Netherlands to test the modeling approach in a real life situation, and to get a closer look at the dynamics and exogenous factors. This will then be used to determine the influence that certain exogenous factors have on the system and in turn on the investment trajectories for the industrial clusters, under different future scenarios.

1.7 Research questions

Provided below are the research questions regarding the influences of multiple exogenous factors on the optimal investment trajectories for industrial clusters in the Netherlands with multiple investment options.

1.7.1 Main research question

How to determine the effect of multiple exogenous factors on the optimal investment trajectories for industrial clusters in the Netherlands with multiple investment options?

1.7.2 Sub-questions

The main research question is broken down into the following sub questions:

Sub-question 1: What can be learned from the current state of multi-actor investments trajectories?

Sub-question 2: Which exogenous factors influence industrial clusters?

Sub-question 3: How can investment option representations be integrated in an optimization model?

Sub-question 4: How can the effects of different investment strategies be examined in a structured way?

Sub-question 5: How can the proposed modeling methodology be tested in a structured manner?

Sub-question 6: What form of validation can be performed to determine the effectiveness of the investment model?

Sub-question 7: What is the effect of exogenous factors on the investment behaviour for the transition of industrial clusters towards a CO_2 neutral future in 2050?

The first and second sub questions are part of the exploratory phase of this research. The identification of the current state of multi-actor investment trajectories requires knowledge on the state-of-the-art of investment trajectories in different sectors, the effect of exogenous factors and the different investment options available. By performing a desk research, textual sources can be used as input for the literature review. A literature review can be limited because of its sole reliance on published literature, and the quality of those papers (Snyder, 2019). It is also possible to miss studies containing the insights required for the research, therefore, a case study analysis will be performed to overcome this limitation (Snyder, 2019). Case studies are a valid exploratory method and allow for the observation of patterns in real life situations and including them to the analysis of theoretical findings derived from previously published literature (Yin, 2012). This will provide an answer to

SQ1 and SQ2. The exploratory phase will also serve as a basis for answering SQ5 later on.

To achieve the goal of this research, the output of the literature review will be used to develop a simplified model of the interactions between different actors on an industrial clusters. By using the answered sub questions as a guide to develop the constraints related to the investment behaviour and the effect of the exogenous factors on the actors. For the model, a time span of 30 years will be taken, starting at 2020 and ending in 2050. This time span provides the necessary data and because the 2030 regulations are getting closer, requiring an increase in RD activity, performing pilots and deciding on final investments to reduce the emissions of the cluster without affecting the overall structure. The model to be used will be based on Mixed Integer Linear Programming (MILP), which has proven itself to be suitable for similar cluster optimization studies (Assis et al., 2021; Zatti et al., 2019). The model is able to capture a representative of the real dynamics in a cluster, whilst having some degree of simplification applied. This is the sole limitation of this model, and it should not be used as a predictive model for future investment behaviours, but as a proof of concept of the of the exogenous factors on the investment behaviour for industrial clusters. The model to be used should also allow for comparing a situation where the actors have full knowledge of future prices versus having no knowledge of future prices. This comparison can give interesting insights on the optimal investment trajectory versus the investment trajectory that will happen most likely. The model will be developed in Linny-R, a software tool designed to incorporate industrial processes whilst relying on a MILP solver. Linny-R is able to produce systems as clusters of processes, allowing it to modelling processes within firms within companies. It also allows for the visualization of the impact that certain interventions or investments may have on the performance of the cluster, financially and technically. The model allows for the optimization of cash flow for individual companies as well as for the entire cluster, making it suitable for incorporating the exogenous factors on the investment behaviours. The implementation of different exogenous factors has never been applied in Linny-R, adding much to the research on multiple investment trajectory options and will provide an innovative design. By comparing the investment trajectories, with knowledge of future prices and without knowledge, the effect of different exogenous factors on investment behaviour under different scenarios can be analysed, answering SQ3 and SQ4 and forming the basis for SQ7. The investment decisions can be quantified by looking at the cluster's performance in terms of CO_2 and by looking at the cash flow on a cluster level and individual level. This will provide a solid basis to answer the main research question.

For the case study, an industrial cluster in the Netherlands will be selected as the cluster to study, providing relevant insights in the current state of multi-actor investments as well as the influences of exogenous factors and how they look at the regulations of 2030 and 2050. The industrial cluster that is chosen will be based on different factors such as location, infrastructure, is the cluster highly integrated and other relevant factors. Furthermore, the industrial cluster should be advanced in terms of being an integrated multi-actor cluster, this makes the observations to be made relevant to this study. For the simplification of the case study, only the petrochemical parts of industrial clusters will be considered, due to having the largest share in the emissions, the given time constraint and the complexity of entire clusters. For the case study, grey literature and available reports combined with expert interviews will be served as input data and to define the boundaries of the system in which will be acted. The case study will allow for answering SQ5 and the combined insights with the modelling chapter will be used for answering SQ7. With the combined output of the literature review and the performed case study, the validation of the model can be performed, answering SQ6. With the answers to all sub-questions together, the main research question can be answered.

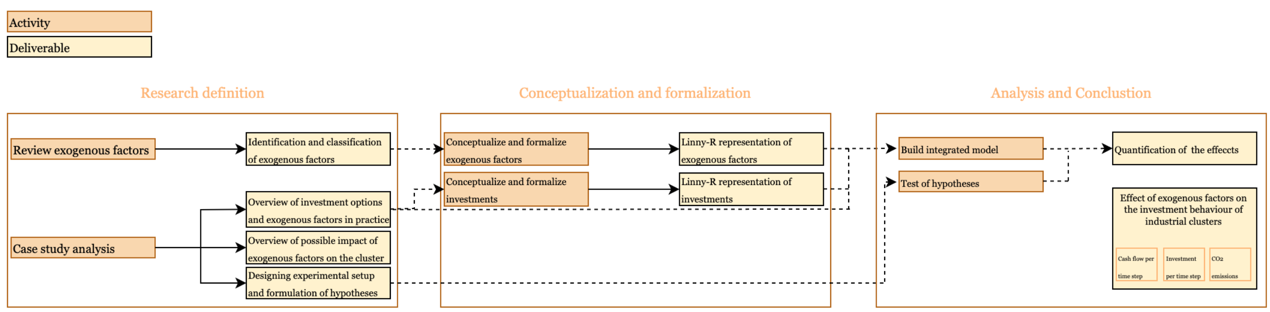

Figure 1: Research flow diagram

1.8 Thesis structure

Having provided the problem at stake, the research will continue with the following structure: In chapter 2, a literature review is provided on the current state of investments and what can be learned from them, on renewable energy alternatives for industrial clusters and the exogenous factors of importance within industrial clusters to consider. In chapter 3, the methodology is identified through conceptualizing and combining all the information that has been acquired so far. This methodology allows to incorporate exogenous factors and investment options in an optimization model. chapter 4 will focus on the influence that exogenous factors have in practice by looking at an industrial cluster, as well as identifying sustainable investment options for that industrial cluster. chapter 5 provides an example of applying the methodology presented in this research by developing a model based on the selected industrial cluster. This model is used as a testing tool to determine the effects that exogenous factors have on the investment behaviour. The results derived from this model are presented in chapter 6, where the limitations of the study are also discussed. Finally, chapter 7 will provide a conclusion and recommendations for further research.

2 Literature review

In chapter 2, a literature review is provided on the current state of investments, how they are preformed and what can be learned from them. Furthermore, existing literature on factors influencing industrial clusters to consider is reviewed. The following sub-questions are answered in this section:

- What can be learned from the current state of multi-actor investment trajectories?
- Which exogenous factors influence industrial clusters?

Answering these sub-questions will provide the insights on multi-actor investments, cluster dynamics and exogenous factors. These insights combined will provide the basis for the theoretical basis to answer the remaining sub-questions.

2.1 Reviewing literature for multi-actor investments and exogenous factors

Collaboration opportunities and other interesting dynamics are present in industrial clusters. To understand the dynamics, potential opportunities and other influences, multiple theories have been critically read. Scientific literature has been reviewed, by making use of databases such as Google Scholar, Scopus and Science Direct. Besides that, (backward) snowballing has been used to identify other literature regarding topics such as game theory within industrial clusters. The papers were selected and then scanned on whether the paper would provide theoretical relevance regarding multi-actor investments and exogenous factors within industrial clusters. The papers selected were used to identify the coordination issue: how should industrial clusters react to exogenous factors when engaging in the energy transition. After looking more into the coordination issue, the IAD framework was followed to identify exogenous factors and determine the effects. From the exogenous factors, the simple contracting scheme by Williamson (1989) was used to categorize the factors and create the focus of the research. Provided below is the structure followed for the literature review.

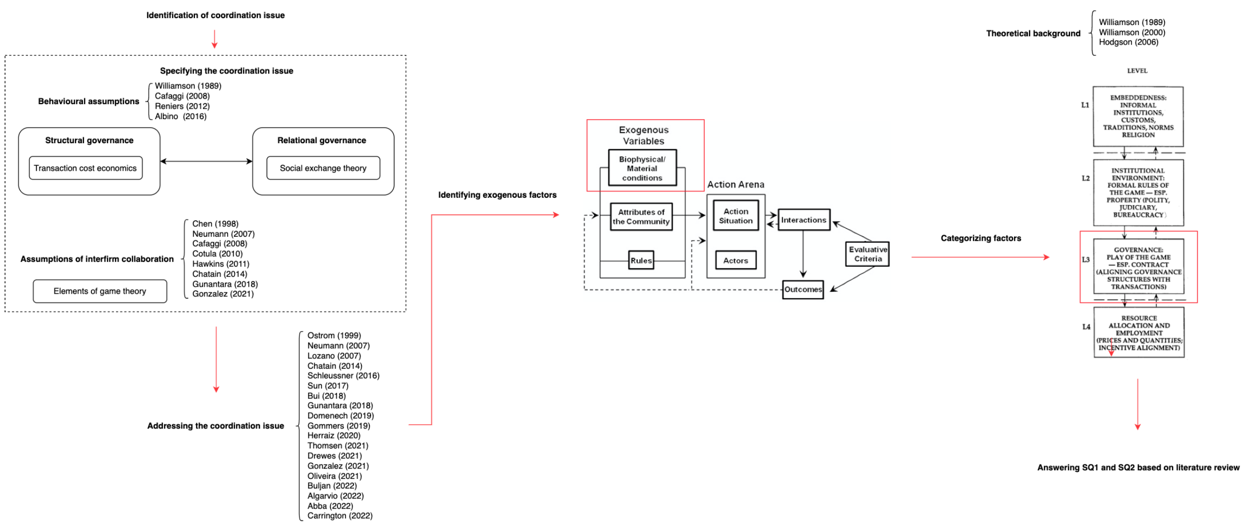

Figure 2: Literature review structure

2.2 Current state of multi-actor investments and structures

The idea of a multidisciplinary investment is not new, numerous investments as such have been performed in the past and currently some are being decided upon right now. Because the world is moving towards a sustainable future, large investments need to be performed to accomplish this. Looking at previous multi-actor sustainable investments can provide insights in the investment behaviour, investment structure, macro-level approach and insights in the factors taken into consideration. Following is a summation of multidisciplinary projects which are analysed on what they do, from where do they originate, how does their management structured (do they have an overarching organization, or different structure such a bilateral structure.) and what does their investment structure look like?

Energy Island

Denmark has set out to develop an artificial island 80 kilometers of the coast of Jutland, Denmark called VindØ. This island is set to be finished by 2031 and it is designed to connect 3 GW of offshore wind in the beginning, and eventually connect 10 GW of offshore wind (Thomsen, 2021). This will then be transported to the mainland in the form of electricity using High Voltage Direct Current Transmission (HVDC Transmission) or in the form of H_2. With this island, the aim is to provide 10 million European households with their power consumption (Buljan, 2022). It is a collaboration between the Danish government, EnergiNet and Andel. Furthermore, the investors consist of PensionDenmark and PFA, with the financing package being evaluated by Nykredit. Copenhagen Infrastructure Partners, a global fund manager mainly focused on investing in renewable energy and offshore wind, will act as the project developer on behalf on the investors (Drewes, 2021).

Figure 3: Energy Island VindØ

Hydrogen network in North Sea Port

The North sea port, combined with GasUnie (NL) and Fluxys (BE) have collaborated on the development of a hydrogen netwerk in the port. Both companies are in collaboration with individual companies such that they can be coupled to the network. Furthermore, the two large networks will be coupled in the North sea port on the border of the Netherlands and Belgium. This will be one of the first border crossing hydrogen networks with open access in Europe. The current demand and supply of the North sea port is around 580.000 ton H_2. GasUnie and Fluxys are the investors of this project, where GasUnie is owned by the Dutch state and Fluxys is a private company backed by various stakeholders.

Hydrogen pipe between Pernis and Maasvlakte

The port of Rotterdam, combined with Gasunie have started with investing in developing hydrogen transportation pipes which will be situated between Pernis and the Maasvlakte, having a length of 32 km. The plan is to connect this pipeline to the national hydrogen network to be developed as mentioned above, and once operational, individual companies can make use of this hydrogen pipeline between Pernis and the Maasvlakte. The investment structure is to be decided on later this year, however, the port of Rotterdam generally does not invest in infrastructures, they mostly rent out their ground, so it is expected that the largest investment comes from Gasunie.

Green ammonia import terminal Maasvlakte
As mentioned earlier, green ammonia will be required as a carrier for green hydrogen, since the demand will be higher than the H_2 production in the Netherlands will be. Gasunie, HES International and Vopak are currently developing an import terminal for green ammonia, called ACE Terminal. The investment structure is to be decided on later this year, however, it will most likely be based on customer contracts, it will be in possession of the required permits and a procedure focussing on the sustainability and environment will be held. The infrastructure will be independent and open access, and neither of the developing companies will be owner of the green ammonia. The supply, storage and transit will be performed by interested parties who are currently in a tendering process. These companies are mostly international.

Hydrogen value chain Northern-Netherlands with HyNL
In the Northern-Netherlands, ENGIE has joined forces with OCI and EEW to develop a hydrogen based value chain. ENGIE will build an electrolyzer to produce the green hydrogen. EEW will develop an installation to capture CO_2 and integrate it with the existing waste-to-energy installation already owned by EEW. OCI will invest in a production facility for e-methanol by using the green hydrogen provided by ENGIE and the biogenic CO_2 from EEW. In this value chain, ENGIE will be the producer of the green hydrogen and OCI will be the customer. EEW plays a vital role by providing the biogenic CO_2 captured from the combustion of biomass.

2.3 Behavioural dynamics within industrial clusters

What can be see from the multi-actor investment examples, is that large projects involving infrastructure such as the development of a hydrogen network is largely financed by a state-owned company, in the Netherlands an example is Gasunie who will be the owner of the hydrogen infrastructure in the Netherlands. Whereas, 'smaller' investments in for example an electrolyzer are done individually, but do need to be connected with other companies to create a value chain. What can be seen from the examples is that because of the multi-actor dependencies, combined with the technical and institutional limitations in place, reaching CO_2 neutrality is quite the objective. It requires a collaboration between all active companies in the clusters. The problem is that all the actors within the companies have different goals, subject to their own constraints and therefore, it might even be possible that some conflicts arise (Lozano, 2007). Furthermore, every company will react differently to exogenous factors, fluctuations in the markets and changes in regulations, making the investment behaviour a company has because of the action of another company very uncertain (Melese et al., 2017).

2.3.1 Game theory within industrial clusters

Making decisions aimed at increasing the sustainability in the chemical industry is complicated because the main objective is to achieve economic benefit. However, actions taken in this matter also have an influence on the social and environmental sectors. Decision-making processes have increasingly included the green chemical industry, attempting to consider the environmental impact and social aspects of their decisions, but still a difficult trade-off exists (Gonzalez-Ramirez & Rodriguez-Gonzalez, 2021). Three dimensions can be identified in the search for sustainable development decision making: Environmental, Social and Economic, where the objectives of each dimension differ from each other (Gonzalez-Ramirez & Rodriguez-Gonzalez, 2021). The difference in objectives from each dimension makes it a complex sustainable decision-making problem. The game-theory of trade-offs for single-actor industrial clusters is relatively easy, because of full cooperation between the different processes within the cluster. Adhering with the 2050 regulations is a very complex puzzle, but trade-offs between companies within the cluster are of a minimum. For multi-actor industrial clusters, the game-theory of trade-offs become increasingly more complex. There is no single solution, but rather a set of points on the boundary of the feasible region, the Pareto Optimal (W. Chen et al., 1998). The difficulty lies in that entities in the industrial clusters are not willing to give up part of their economic benefits to support a global benefit (Gunantara, 2018). Game theory allows for the assessing of situations involving multiple decision-makers where the objectives of each are partially or completely opposite from the others (Von Neumann & Morgenstern, 2007), thus also in the case of the energy transition of the industrial clusters in the Netherlands. Because of the situation in industrial clusters involves multiple decision-makers with opposite targets, either partially or totally, non-cooperative game theory becomes a suitable tool to approach this type of problem (Mazo et al., 2020). A non-cooperative game is a game which focuses on moves players should rationally make (Chatain, 2014). Sustainable decision-making problems can be treated as such non-cooperative games (Gonzalez-Ramirez & Rodriguez-Gonzalez, 2021). The companies within industrial clusters mainly behave on a what other companies do and adapt their behaviour to those actions (acting on micro-level and consider micro-level trade-offs with a focus on economic benefits), whereas, the industrial cluster mainly behaves on what the government does and what the large suppliers of feed stock does (acting on macro-level and considering macro-level trade-offs with a focus on CO_2 levels). Reaching the CO_2 regulations of 2050, requires a switch of going from a non-cooperative game towards a cooperative game, but a misalignment incentive problem must be prevented in which certain actors enjoy a large positive payoff and others suffer a negative payoff (Albino et al., 2016). So, using negotiations and agreements in the form of contracts, which pushes the actors to behave in a desirable way for all actors, industrial clusters should be able to achieve a Pareto-optimal outcome. From this, we can look at the different types of contracts that exist in industrial clusters in terms of legal forms (Cafaggi, 2008)

The game theory gives insights in how actors within industrial clusters behave. Because the focus of this research it is assumed that the actors within an industrial clusters act according to a cooperative game, where the cluster positive payoff combined with no negative individual payoff is the goal.

2.4 Potential renewable energy alternatives for industrial clusters

The feedstock currently used in industrial clusters are naphtha, natural gas, biomass and pyrolysis oil. These materials are used both for the generation of energy, as well as used as raw materials for producing products such as plastics (*Netbeheer2022ii*, n.d.). The industrial clusters in the Netherlands are fully adjusted to the current mix of feedstock such that the by-products arising from the production processes and the energy generation can be used down-stream as input for other processes (Foundation, 2013). These kind of value-chains are very important to industrial clusters since they already reduce the amount of emissions and create economic benefits due to less materials having to be purchased (Domenech et al., 2019; Sun et al., 2017). However, with the current operations and the feedstock that it uses, the targets of 2030 and 2050 will not be reached. Therefore, alternatives to the current mix of fossil-fuel feedstock need to be implemented to work towards the decarbonization, however, this is not easily performed. The change of feedstock mix can cause problems downstream due to waste products not being available anymore, causing problems for the actor needing those waste products, and may result in short-term solutions having to be implemented such as importing said product to adhere with the bilateral/multi-actor contract those actors might have. It may also be a problem because the facilities have not been developed yet to implement the new feedstock (Bui et al., 2018; Herraiz et al., 2020). The relevant renewable energy alternative and its investments for industrial clusters in the Netherlands are provided below:

- **Green hydrogen** is defined as producing H_2 using an electrolyzer with renewable electricity and is especially useful in processes in the industrial clusters that are hard to electrify due to its required energy or temperature (A. M. Oliveira et al., 2021). The biggest advantage of green H_2 is that it can be produced on site, allowing for the possibility to remove H_2 imports from the cluster site. Utilizing green H_2 in an industrial cluster requires an investment to be made in an electrolyzer if not present, and requires a H_2 network infrastructure, with the size depending on the number of actors to be reached (A. M. Oliveira et al., 2021).

- **Green ammonia** has proven to be an efficient carrier for H_2 and allows for safe transportation in large volumes. Offshore H_2 generation is increasing rapidly, but the distance the H_2 has to travel also increases. Transporting the (green) H_2 over a large distance causes large amounts of energy to be lost, up to 40% (Jackson et al., 2019), therefore, an efficient carrier is needed to reduce this energy loss. Ammonia has a history of large-scale cost optimised industrial production and its used globally as a refrigerant, chemical raw material and as a fertiliser, meaning that in times of overproduction, it can also be used in other sectors. Furthermore, the transportation of liquid ammonia is currently already being performed with good economics (Jackson et al., 2019), making green ammonia technically and economically viable as a carrier for green H_2. Green H_2 reacts with N_2 to form the green ammonia, and after storage, the green ammonia is converted back to green H_2.

- **Renewable naphtha** is a natural byproduct that comes from processing renewable feedstock into diesel. Renewable naphtha can also be decomposed using heat and separated to create propylene and ethylene, used for making plastics (Grubb, 2022). It has seen an increase in demand over the last few years because of its reduced GHG footprint compared to petroleum feeds, depending on the feedstock (Laird, 2022). Renewable naphtha is especially interesting for the industrial clusters because it can be used as feed for steam crackers in the plastic production, the paraffinic molecules and the little to no oxygen or contaminants make it especially attractive. It can also be used in integrated hydrogen units that convert renewable feed sources to H_2 with low GHG emissions. Furthermore, it is also suitable to use as a gasoline blending component, increasing the renewable percentage of said gasoline (Grubb, 2022). The renewable naphtha can replace the naphtha without any complications. The global market for renewable naphtha reached $422 million world wide in 2021 and is set to surpass $1 billion in 2030 (FMI, 2021).

- **Biomass** is a renewable energy source of fixed carbon, an essential component in numerous consumer goods and fuels. The main biomass sources are wood, agricultural and forestry residues and annual crops. Other sources are the biodegradable components of municipal solid waste and industrial and commercial wastes can also be considered significant bio-energy resources, however, they require heavy processing before it can be converted (Bridgwater, 2006). In industrial clusters it can be used as a source for heat, but can also be used for other processes such as methanol production (Holmgren et al., 2014). Biomass does need to be transported by road transport, railways or waterways, the transportation relies on established infrastructures and currently, fossil-fuels are used to transport the biomass, emitting CO_2 (Sun et al., 2017). Biomass will reach a carbon neutral status if the transportation involved also reaches carbon neutrality. However, studies have projected that the future demand of biomass may not be supplied, causing a mismatch between the supply and demand of biomass (Spijker et al., 2020).
- **Renewable electricity** is one of the biggest requirements for the energy transition of industrial clusters in the Netherlands. The demand for electricity is expected to increase with at least 1% per year per IC, which can be even more depending on other investments such as an electrolyzer or the electrification of other processes (*Netbeheer2022ii*, n.d.). The problems faced by the industrial clusters is the lack of infrastructure able to handle the demand capacity (Chemelot, 2021) and the current energy losses in transporting offshore renewable electricity to onshore (Gil et al., 2015). However, the utilization of renewable electricity is a large requirement for industrial clusters to reach the CO_2 emission reductions of 2030 and 2050.
- **Pyrolysis oil** or also knows as bio-crude or bio-oil is a renewable alternative to petroleum and is created by heating biomass in the absence of air to a temperature of 450-550 degrees Celsius, with subsequent cooling (Q. Zhang et al., 2007). Pyrolysis oil has experienced a large increase of interest from large energy organizations all over the globe for their characteristics as fuels used in gas turbines, engines and combustors as well as being used as a resource in various chemical industries (Q. Zhang et al., 2007). Under certain conditions, products can be formed from this with a mixture of aromatics and olefins with very similar properties to the products of hydro-cracking naphtha in current conventional olefin processes (Sharifzadeh et al., 2015). The use of pyrolysis oil can easily be integrated in the current petrochemical network without large retrofitting costs (Sharifzadeh et al., 2015). Furthermore, H_2 can be produced by taking pyrolysis oil and using it as feedstock for the steam reforming process, allowing for excess pyrolysis oil to be effectively used in such cases.

This shows that there are multiple different renewable energy alternatives to decarbonize industrial clusters. However, not every energy alternative is applicable to every industrial cluster, and the renewable energy alternatives are also subject to other barriers such as how much of the product is available and what would the industrial clusters require. From the alternatives given above, the following selection of the renewable energy alternatives to consider has been made based on their availability and ease of implementation in industrial clusters. They will be used for the rest of this research from this moment on:

- Green hydrogen
- Green ammonia
- Renewable electricity
- Renewable naphtha

2.5 Factors influencing industrial clusters

The industrial clusters in the Netherlands are subject to various factors influencing the energy transition possibilities and their investment behaviour. Using relevant literature as well as using information gathered from conducting expert interviews, a list has been created with relevant factors for this research. Furthermore, the factors will be further categorized using the simple contracting scheme by Williamson (1989) to differentiate between internal factors and exogenous factors. Where internal factors can be influenced by the system, and exogenous factors cannot be influenced by the system. As mentioned before, only exogenous factors will be considered since they influence the behaviour of actors in industrial clusters. From the list of factors, a selection of the most important exogenous factors will be made that will be considered for the model.

2.5.1 Identifying factors influencing industrial clusters

Emission reduction policies

As highlighted earlier, several emission reduction policies are already set in place. The main goal of these policies are to prevent the global average temperature to reach 2 degrees Celsius and aim to even limit this to 1.5 degrees Celsius (Schleussner et al., 2016). This is to prevent dangerous anthropogenic interference with the current climate system. Crop yield projections are becoming more uncertain due to uncertainty in the climate projections as well as the influence it has on the crops (Schleussner et al., 2016). This can in turn be of negative impact downstream for example on the availability of biomass (Schleussner et al., 2016). On a more national level, the Netherlands has set out goals to reduce CO_2 even further, going beyond the Paris Agreement. The Netherlands aims to reduce its CO_2 emissions by 49% compared to 1990 by 2030, and a 95% reduction by 2050 compared to 1990. Furthermore, the Netherlands has a climate plan that changes every 10 years and is revised and adjusted every 5 years. This climate plan covers a range of topics with a general guide to which the government wishes to reach their set out goals. It includes the economic consequences, the support base it requires, the cooperation and direction and the new tasks that the government will have to perform (Gommers et al., 2019).

Gas and oil prices

As can be seen by the war currently going on between Russia and Ukraine, the war has induced an enormous increase in the price for both gas and oil due to the supply from Russia being cut off (Żuk & Żuk, 2022). The consequences for the industrial clusters is that their variable costs have increased tremendously. Because of this increase in costs, renewable solutions may be put on hold due to lack of funds or because of angst for potential energy security compromises (Żuk & Żuk, 2022). However, the largest players of the fossil fuel industry have set out to open 195 new gigantic oil and gas projects, of which 60% has already started pumping. This can reduce the price of oil and gas on the short-term, but does have catastrophic consequences for the environment (Carrington & Taylor, 2022). The lower price may help to overcome the energy security angst and enabling the energy transition to continue, but the industrial clusters do need to balance the amount of fossil fuels they use with their CO_2 emissions such that they adhere with the regulations.

Misalignment of interests

What the Dutch government wants, and what the individual actors situated in an industrial cluster wants are quite often two completely different goals. This misalignment can cause initiatives induced from the government on industrial clusters that do not result in a profitable scenario, or that fines are incurred if they do not adhere to new regulations (Lorenzen, 2001). These regulations may be unattainable for certain companies situated in industrial clusters. The effect that misalignment of interests from outside the system on industrial clusters can have, may result in scenarios that actually hamper the energy transition.

Subsidies and funding

Subsidies can be seen as an enabler for industrial clusters to engage or speed up the energy transition. The subsidy is an investment made by the government allowing for companies within industrial clusters to reduce their CO_2 emissions (Rijksoverheid, 2022). Numerous subsidies currently exist allowing companies to deviate from their current operations to implement operations that provide the same output with a reduction in GHGs. The current subsidies such as the SDE++ allow for industrial clusters to acquire funds for different phases of becoming more sustainable. Other subsidies include subsidies for performing fundamental research into new techniques, subsidies for researching and developing, subsidies for demonstrations or subsidies for up-scaling and market introduction (Rijksoverheid, 2022). This enables companies within industrial clusters to become more sustainable as it makes sustainable investments profitable.

Renewable energy alternatives availability

As mentioned previously, the renewable energies provide a positive outlook for the future of energy, however, it also has limitations. Currently, the biomass demand cannot be met (Spijker et al., 2020), the total demand H_2 demand in the world is too much to be produced as green H_2, requiring fossil fuels to be used to generate the H_2 (Zhiznin et al., 2020), offshore electricity currently experiences large losses when transporting the electricity from offshore to onshore (Kucuksari et al., 2019), and certain technologies such as efficiently producing pyrolysis oil with the right properties are still in early stages of development (Sharifzadeh et al., 2015). Large investments in the renewable energies are required to overcome these obstacles. Luckily, these investments are happening, but require time to be fully operational. Because the CO_2 emissions are heavily dependent on the feedstock and fuels, the industrial clusters energy transition is heavily influenced by these developments. The industrial clusters have no direct influence on the development of the technologies of these renewable energy alternatives and its availability, therefore, it is considered as an exogenous factor.

Scale and speed of change
The demand for (half)products coming from the petrochemical industry has been growing for the past decades. This growth is projected to keep on rising in the future (Alshammari et al., 2016). This growth is dynamic however, and large imbalances due to external factors such as Covid-19 or the war in Ukraine can arise. Because the growth in demand is dynamic, it is hard for actors within industrial clusters to estimate the exact growth and its fluctuations. Expanding too quickly when there is no demand might compromise an actor, whereas expanding too late will allow for competitors to fill the demand.

Pre-existing infrastructure
A limiting factor to the utilization of renewable energy alternatives is the infrastructure in place. The pre-existing infrastructure can be divided in infrastructure outside of the industrial cluster and within the industrial cluster. Gasunie aims to create a H_2 infrastructure that will connect all industrial clusters in the Netherlands with external H_2 storages and nearby countries (Gasunie, 2022). For the electricity infrastructure, it has to be strengthened and upgraded to handle to increasing demand and to utilize the renewable electricity sources effectively. Large investments are being performed by the regional network operators combined with the government to realize this in the coming years (Netbeheernederland, 2022). Furthermore, existing infrastructures in industrial clusters also undergo the same problems faced as the national infrastructures. The infrastructures may be capped or need to be upgraded to utilize the new resources effectively or because of the location of industrial clusters, they may be limited in the resources they can receive. An example of this is in Chemelot: they are not situated near a large seaport, causing the majority of transportation of resources to Chemelot only be done through pipelines, railroads or by truck. The option of ships is available to Chemelot because they have a relatively small port, but unable to handle large quantities such as the Port of Rotterdam. This will not change in the near future towards 2050 and, therefore, may cause delivery problems in the future. the pre-existing infrastructure outside of the industrial is considered to be an exogenous factor, whereas, the pre-existing infrastructure within an industrial cluster is considered to be an internal factor.

Role of CO_2
Various things are going to happen with CO_2, first and foremost, the current CO_2 price is going to increase up to atleast $100/ton if a net zero emission future is to be reached (IEA, 2018). Furthermore, CO_2 is going to be stored into empty gas and oil fields (Hannis et al., 2017). The CO_2 captured using CCS can also be used to increase the CO_2 levels in greenhouses to promote growth for the fruits and vegetables (Ghiat et al., 2021). Furthermore, to accelerate the energy transition, a CO_2 cap is implemented. This cap fines companies that surpass the limit, or they need to buy CO_2 certificates to offset any excess CO_2 (Koelemeijer et al., 2019). Besides this, many roles exist and many roles can arise in the near future. The uncertainty of what the end role of CO_2 might be for industrial clusters and the lack of influence that industrial clusters have on this, makes the role of CO_2 both an internal and exogenous factor. Therefore, for this research, the price of CO_2 as well as the cap on CO_2 emissions will be considered exogenous. The system has no direct influence on the price or the cap set in place by the regulators.

Renewable energy alternatives As mentioned in chapter 2.4, various renewable energy alternatives exist. They will also be considered as a factor influencing industrial clusters since they allow clusters to become CO_2 neutral, depending on the amount available.

2.5.2 Categorizing the identified internal and exogenous factors

The multidisciplinary nature of the industrial clusters in the Netherlands forces the companies to act as a combined unity. However, mapping the factors that influence the investment behaviour as well as looking at their importance is difficult because they should not only be considered on an individual level. Because of the multidisciplinary nature and the broad array of factors coming from multiple institutions, this research shall make use of the simple contracting scheme developed by Williamson (1989) to categorize the factors, allowing the research to focus on the exogenous factors of most importance to the industrial clusters. Williamson categorizes institutions into four distinctive layers, where each layer interacts with others, provides feedback and each level operates at its individual pace (Groenewegen, 2006; Williamson, 1989).

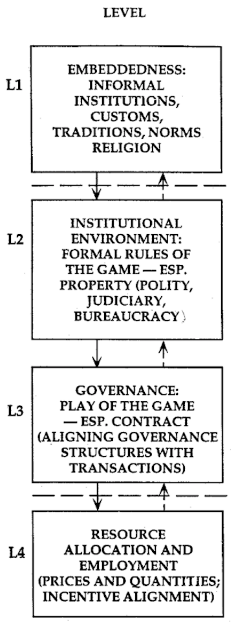

Figure 4: Contracting scheme by Williamson (1989)

First, Williamson looks at the first layer, **the social embeddedness** layer. This layer includes informal institutions of values and cultures, and moves at the lowest speed, taking over hundreds of years to change. This layer is of large influence to the other layers (Williamson, 1989). One layer below, is **the institutional environment**, a layer constituting of the political, legal and governmental arrangements. It looks at the formal arrangements that influence the activities in the remaining levels. The rate of change in this level is usually related to windows of opportunity such as a pandemic or a sustainable crisis. It can take from a decade up to a century for this change to occur (Groenewegen, 2006). The third layer is **the governance** layer. This layer analyses the organisations which are realized with contracts and agreements, and portray how the roles are divided and responsibilities are across stakeholders. The time horizon on this layer can take a single year, up to a decade (Williamson, 1989). The lowest layer is **the individual analysis**, this layer takes a look at the operation and management of the system. What is taken into consideration during the decision making and how is it executed? This layer changes at the highest speed, ranging from constantly changing up to a single year (Ghorbani et al., 2010).
Using the information gathered from expert interviews, literature and the framework by Williamson (1989) explained above, the factors influencing the industrial clusters can be categorized into four distinctive groups:

- Natural factors
- Political factors
- Individual invention factors
- Social factors

Having identified four distinctive groups for exogenous factors to be categorized in, the different layers and the influence they have on each other and on the system will be elaborated on below.

Layer 1 - Natural factors The natural factors are factor which are not controllable (anymore) such as the available amount of natural resources. Furthermore, the location of the industrial cluster can be a limiting factor, is it close to the sea? Or is it more inland and do they not benefit from the transportation possibilities of having a port. The natural factors are very rigid and do not quickly change over time. The availability of natural resources does not change overnight, nor does the location of a fully developed industrial cluster.

Layer 2 - Political and technological factors The political factors constitute the political, legal and governmental induced factors that influence the transition. Governmental induced factors can be emission reduction policies such as the Paris agreement. Other factors can be CO_2 taxes issued by the EU ETS. Subsidies and funding also do not change overnight. The technological factors constitute of the overarching technology change.

Technology as a whole does not change overnight or in a decade, it takes very large amounts of time for technology to change entirely. The main point in common is that these factors limit the possibilities for the industrial clusters and that they change at a more rapid speed than the natural factors, but still do not change that quickly. They create the 'rules' to which actors within the system have to adhere. These 'rules' have a slow changing rate, ranging from a decade to a century.

Layer 3 - Individual invention factors Because of the political factors, the current system has to change, however, the technology for this change may not exist yet or other developments hinder the implementation of the technology. The influence of emission reducing policies can cause other technologies or processes to be more profitable. However, the technology might be underdeveloped or not even in existence yet. Lack of technology becomes a limiting factor. In the case of H_2 for example, low efficiency of electrolysis is a limiting factor and H_2 carrying technologies are limited. The availability of renewable energy alternatives is a considered a limiting factor. Renewable electricity, green H_2, renewable naphtha, biomass and other renewable energy alternatives are needed to reduce emissions. Furthermore, the infrastructure outside of the industrial cluster is also considered a technological factor. If the infrastructure is not able to supply the demand of the industrial cluster, it limits the energy transition significantly. The infrastructure is closely related to the location of the industrial cluster, however, the rate in which the infrastructure can be adjusted is significantly higher than the rate in which you can change the entire location of an industrial cluster. The technological factors are largely influenced by the political factors, but change at a much higher rate. The rate of change is between 1 year and 10 years.

Layer 4 - Social factors On the bottom level, we find the level that looks at the operation and management of the system. It also takes into consideration the decision making of industrial clusters and how it is executed, on an individual level and the system as a whole. Relevant factors in this level are factors such as Economic interests of individual companies, Limited investment possibilities as a cluster, Scale and speed of change of the cluster, Misalignment of interests between individual companies, gas prices, return on investment and the Lack of social responsibility. This layer changes at the highest speed, ranging from constantly changing up to a single year.

2.5.3 Focus of the research on selected exogenous factors

Categorizing the identified factors using the simple contracting scheme by Williamson (1989) also shows the rate of change. The rate of change is important, it shows how controllable a factor is and to which degree they influence the investment behaviour of industrial clusters. The individual factors will remain of importance for every individual company, but are of less importance when looking at the macro-level. Added to that, investment options on the individual level are usually limited to a single option, whereas, on a macro-level, multiple investments could be implemented. The return on investment might be important for an individual company, but for the industrial cluster, it can be less important what the individual return is, and more important what the reduction of CO_2 will be with the use of CCS over the entire cluster for example. The political factors are far out of the control of the industrial clusters. The Paris agreement, CO_2 taxes and enablers such as subsidies cannot be influenced by the industrial clusters. They are clear rules to which they must adhere when making investment decisions on the macro level. They are both limiting and enabling, they demarcate the playing field for the industrial clusters. Furthermore, the natural factors are so far out of control of any party within the scope of this research, or even the entire world, that they will be considered as conditions, they are extremely rigid and the rate of change is so far beyond the 2030 and 2050 goals, that nothing will change these factors.

The third layer, individual invention factors, is of most importance to this research. This layer encompasses the factors with potentially large impacts on the emissions of the industrial clusters, require the participation of multiple companies and the rate of change are well within the goals of 2030 and 2050. From the identified and categorized factors, the following exogenous factors will function as input variables for the model developed later in this research. The considered exogenous factors are:

- Renewable energy alternatives availability
- Pre-existing infrastructure outside of the industrial cluster
- CO_2 price
- CO_2 cap

2.6 Concluding remarks

The theoretical lens of exogenous factors and investment behaviour are provided in this chapter and has placed the research in perspective. Looking at different types of multi-actor investments provides the research with insights such as how they are contractually structured in legal forms and financed. By further investigating the legal forms, insights were gained on the benefits of joint ventures and bilateral contracts. Using game theory, the cooperative and competitive strategies of actors in multi-actor investment decisions are defined, answering SQ1. Furthermore, the literature review also provided a list of factors and by applying the Williamson scheme to it, allows for the classification of the relevant exogenous factors for the next sections, answering SQ2. These factors are: renewable energy alternatives availability, pre-existing infrastructure outside of the industrial cluster, CO_2 price and CO_2 cap. Given the scope of this research and the focus on the influence that the identified exogenous factors have on the investment behaviour of industrial clusters, the contractual structures and the game theory will not be used in the development of the model used later on in this research.

3 Modelling

The goal of this chapter is to propose a form of conceptual representation of the potential investment options as well as the integration within the production processes in industrial clusters. First, the choice of modelling methodology is picked by making a comparison between the different modelling techniques usually applied in studying similar industrial systems. A solution following Mixed Integer Linear Programming (MILP) will be advanced on since it maximizes the cash flow of a cluster and incorporates the interactions existing among the different production units within an industrial cluster. It also provides the opportunity to include multiple actors to see how the different actors will behave when influenced by exogenous factors. Then, a problem description will be specified and here the relations between production units will also be stated. Secondly, insights are offered on how the investments and exogenous factors are included in Linny-R. Finally, the conceptual implementation of the investments and exogenous factors will be discussed for the remaining of the section, and the proposed model will be verified through testing of its functionality in various circumstances and conditions. This chapter will provide an answer to SQ3 and SQ4.

3.1 Model requirements

The aim of this research is to demonstrate the influences of multiple exogenous factors on the optimal investment trajectories for industrial clusters in the Netherlands with multiple investment options. To answer the main- and sub-questions stated in this research, a case study is executed. For this case study, a model will be designed with different input variables simulated over a certain time period and different outputs will be derived from the model. For the model to be designed correctly, the input and output variables need to be identified and clarified. Below is a model scheme provided with the input variables and the desired outputs.

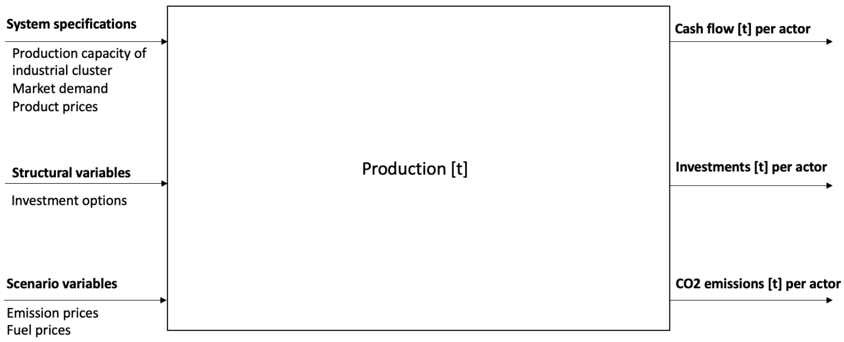

Figure 5: Model scheme

The model should be able to incorporate different input specifications like the production capacity of an industrial cluster, specified per actor. Other important specifications like the demand for the products to be produced, prices of those produced products and other specifications such as emissions should be used as input. For the model to decide on different investment trajectories, the model should be able to handle multiple investment options that potentially change the production route that the industrial cluster currently takes. Deciding what the optimal investment trajectory is, the model would require a function to compare a situation where it has full knowledge of every variable adjustment. By comparing this optimal investment trajectory with sub-optimal investment trajectories, insights can be gained on how industrial clusters should invest differently. Finally, testing the model for different scenarios will prove the robustness of the model, which requires variables such as emission prices and fuel prices to be entered in the model. As output, cash flow per actor is used for insights, the investments made per actor and when, and the amount of CO_2 that is emitted per actor. The following subsections will focus on how the requirements for the model are assessed in the methodology.

3.2 Methodology of the modelling

The Mixed Integer Linear Programming (MILP) methodology, supported by Linny-R, allows for representation of the networks within an industrial cluster and provides the options for analysis of the different investment decisions and interdependencies between different actors within that cluster. The model will provide the optimal investment path given the exogenous factors and investment options. The results derived from the model allow for assessing what the effect is of these exogenous factors on the investment behaviour.

3.2.1 Modelling methods assessment

The preferred modelling method is chosen to be MILP, after having performed a comparison with other frequently used modelling techniques for studying industrial clusters. Methods only capable of analysing a single production process have been excluded for this research as it increases the difficulty of optimizing a cluster consisting of multiple processes. Therefore, the MILP method was compared with two frequently used modelling techniques: System Dynamics (SD) and Agent-Based Modelling (ABM). These techniques were found during the literature review and are often used in studying industrial clusters from a systems engineering perspective (Demartini et al., 2018).
System Dynamics is useful in visualizing complex dynamic systems and analysing it. It uses a simulation to identify the changes in the system by looking at the system in terms of structural characteristics and changes, taking into account the influences of elements among relations within the subsystems and the influence of that between subsystems (Demartini et al., 2018). Implementing this for an industrial cluster, it starts of by developing a process flowchart, which then is translated using the system dynamics models using stock-flow diagrams and other diagrams such as causal loop diagrams. Allowing for quantitative modelling and conceptual understanding of the system (Cui et al., 2018). The downside of using system dynamics to model an industrial cluster is that the quantitative analysis derived from the model is on a relatively high level because it follows a top-down methodology, mainly used to gain more insights on large trends in the system that is modelled (Wirsch, 2014). This makes the approach potentially unsuitable for this research since the aim of this research is not to identify large trends among the industrial clusters, but to identify the effect exogenous factors have on the investment behaviour of industrial clusters. Looking at the Agent-based Modelling method, it is designed for simulation of different actions between multiple actors and their interactions according to a number of rules set, following a class of computational models. This allows for studying the aggregate level on a system (Demartini et al., 2018). Agent-based modelling makes it possible to analyse multi-actor perspectives of a system, making it suitable for this study. Through aggregation of multiple processes, it also allows for hierarchical modelling. But one of the biggest shortcomings of Agent-based modelling is that it does not perform the optimization of a model but rather using a bottom-up approach, it focuses on the different emergent behaviours. Agent-based modelling also requires programming code to use it, making it more difficult to perform actions as opposed to methods and models following a language based on graphical representation.
Having looked at the limitations of systems dynamics and agent-based modelling, MILP appears to be the most suitable method for modelling the industrial cluster. Especially because it looks for optimal investment trajectories by subjecting different constraints to the model and having it satisfy multiple objectives, instead of the model being heavily reliant on heuristics. The flexibility offered by MILP allows for developing an optimization model that optimizes the performance of the industrial cluster in terms of cash flow and includes all the actors and their dependencies within the cluster. Linny-R offers multiple opportunities for this research because it is not solely based on mathematical equations coded in the model, but it functions as a useful intermediary tool. This will be elaborated on later.

3.2.2 Problem description: Application of the MILP to industrial clusters

This research aims to demonstrate the influences of multiple exogenous factors on the optimal investment trajectories for industrial clusters in the Netherlands with multiple investment options.

Industrial clusters are made up of production units (PU's) in groups that are interconnected, where the outflow of a certain PU can be the inflow for another (Jamal & Montemanni, 2018). Maximization of cash flow for the total cluster can be the objective of a modelled cluster using the cash flows of the PU's situated in the cluster. The cash flow of such a PU is a combination of different variables such as cost of raw materials, cost of production, cost of waste disposal if applicable, selling price, and numbers of final product sold. In the case of a well integrated cluster, the waste disposal of a certain PU can actually be of use for another PU and thus increasing the efficiency and lowering costs. These waste streams, or from now on considered 'by-products', can be in the form of CO_2, energy, steam, water, heat and other forms of waste. Especially for by-product streams, contracts can be important in terms of allocating costs. Contracts regarding by-products state the exchange of these by-products, which reduces the risk for certain PU's in terms of uncertainty regarding inflow or outflow. The demand and supply in these by-products is extremely important for the continuous operating of an industrial cluster. If a certain innovation removes a certain by-product from a process, this can negatively affect a PU downstream reliant on said by-product. Interdependencies between PU's need to be taken into account when evaluating the optimal investment trajectories subject to multiple exogenous factors because they may lead to certain PU's having to import a by-product to adhere to the contractual agreement they have engaged in with another PU. These contract establish a price and a maximum and minimum quantity or volume of a certain product to be exchanged. In case of an innovation made that makes changes to the existing structure, costs for retrofitting or costs for new connections are included. However, as mentioned before, the contractual structures will not be modeled in this research, as it is outside of the scope of this research.

3.3 Representation in Linny-R

Linny-R has been chosen as a suitable MILP software tool to simulate the operations of an industrial cluster and to optimise those investments following the MILP approach, and allows for maximizing the cash flow of scheduled production processes. Linny-R is developed by Dr. P.W.G. Bots, and uses an executable graphical language whilst relying on an external solver to come up with solutions for MILP problems. This research uses Linny-R version 1.0.15. Linny-R allows for clustering of production processes, model those systems as a cluster and nested modelling, making it intrinsically suitable for this research. Added to that, the graphical language of Linny-R makes it user-friendly and visually appealing as well. The optimization for cash flows can be extended to that of the total cluster, but also for certain actors or to look at the position of a certain company within the cluster and determine the impact of multiple multi-actor investment strategies. In terms of evaluating interventions in the cluster, both institutional and technical, Linny-R is an ideal tool, especially also because of the performance measure being formed economically as well. The only shortcoming of Linny-R is that its solver time increases when the number of binary variables to be calculated increases, meaning that careful representation of the industrial cluster has to be considered.
The implementation of the Linny-R software to create the model aims to introduce a methodology allowing for the quantification of the effects of multiple exogenous factors on the optimal investment trajectories for industrial clusters in the Netherlands with multiple investment options. To develop this, accurate representation of investments and exogenous factors need to be conceptualized in Linny-R. First, investment options need to be represented using Linny-R. Following from that, extra options are added that can be 'switched on' if an investment is being introduced in the model. This will be elaborated on in the following subsection.

3.3.1 Investment representations in Linny-R

In normal MILP problems situated in industrial clusters, the goal is to optimise the production processes already existing in terms of cash flow, and not specifically identifying new optimal investment decisions. Therefore, a methodology has to be included in the model to be designed because Linny-R is not designed to identify such investment decisions.

To explain how the investment model looks like in Linny-R, first a simple model is developed involving a single-actor with a simple process. Apples are used as an input and processed into an output Apple juice. Furthermore, the process is extended by adding fixed and variable costs. Meaning that if the apples want to be processed into apple juice, a price needs to be payed to perform this action for every time step. The costs are then presented in the form of a data product, consisting of data that can be analysed to gain insights in the process. Linking a process to a data product creates a flow of '1', but a higher or lower multiplier can be added to the flow such that real life situations can be replicated. Such a link is called a data link. The data links also allow for different variations of flow, such as unitary flow, meaning that only a flow exists if the process is operational, or to give a certain value if nothing is happening for example. In the case of the figure given below, fixed costs only need to be payed if the process is activated, indicated by the + symbol, giving a value of 1 if flow is detected through the process and a value of 0 if no flow is detected. The value is not determined by the amount of products that pass through the process. Whereas for the variable costs, they are dependent on the amount of flow going through the process, meaning that the price to be payed is the multiplication of the amount of flow times the variable costs. Furthermore, a negative price is added to these products since it has a negative contribution to the model.

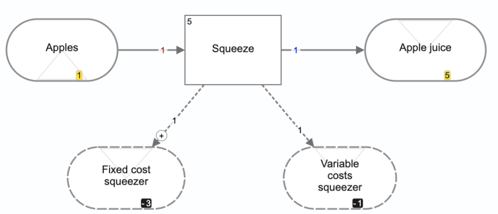

Figure 6: Simple Linny-R representation of a production process

This simple model will now be extended by adding three different investment options:

- A representation where first an investment has to be made before the system can start producing.
- A representation where the investment made increases the capacity of the system.
- A representation where the investment made replaces another technology.

Starting with the first investment representation, provided below is the adjusted simple model with an extra data product which represents the investment costs. The investment costs only need to be payed once upfront. This is implemented in the model by assigning the "first commit" symbol, represented by * to the data link connecting the 'squeeze' process to the 'investment costs squeezer' data product. The costs are incurred only once, when the process is activated. Through the use of a semi-continuous variable where the lower bound is higher than 0, the investment is realized. From then on, the investment has been made and the costs are not incurred in the rest of the time frame. Start-up costs can be implemented if desired through including a binary variable indicating whether the process is turned on or not, however, because of the time frame in which the model will be simulated (30 years) and start-up costs occurring mainly on an hourly/daily/weekly basis and not on a yearly basis, the costs can be integrated in the investment costs or in one of the other costs. For this research, the start-up costs are integrated with the investment costs to keep the model more simple and since it does not influence the outcome of the model or the results. Once again, the price of the investment costs are indicated as a negative price as it provides a negative contribution to the model. The figure below is one of many ways to represent an investment in Linny-R. This particular representation is used due to it being simple, when a production unit comes to the conclusion that it is not economically viable to produce anymore because of rising prices, the production can be stopped and resumed at any given time step without having to pay any new investment costs. This representation will be extended below, which shows the adaptability of the representation.

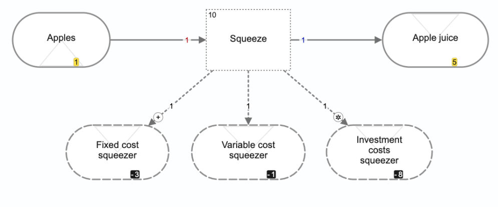

Figure 7: Simple Linny-R representation of an investment

The model above shows that the limiting factor in the amount of profit that can be made, is the capacity of the squeezer. By adding an extra squeezer, more capacity is added and the model can potentially make more profit depending on the costs related to the extra squeezer. The model is adjusted by introducing a second apple squeezer with investment costs, fixed costs and variable costs as well as a higher capacity than the current squeezer. Given below is the model with an extra investment possibility that increases the capacity of the system.

In some cases, it might be interesting to look at what might be a cheaper alternative on the long term if there are two (or more) process options, with different fixed, variable, and investment costs. Situations may occur where looking at a 10 year time frame might result in the process with higher variable costs but lower fixed and investment costs to be preferred, but looking at 30 years ahead, may result in the lower variable costs to be more profitable. This can be incorporated in the investment model by introducing an extra data product, which will be called in this representation 'one active'. Here, the data links will be given the same + value as with the fixed costs. This will give a value of 1 if a process is turned on. By giving the data product a lower and upper limit of 1, only a single process can be turned on. If both processes were turned on, a value of 2 would be registered in the 'one active' data product and the model would fail. A visual representation of the model can be found below. This structure is interesting when looking at the long-term cost benefits of introducing a new process into the model. This is especially applicable in this research since the time frame of the model is 30 years and deterioration of factories and processes causes clusters to constantly be aware of the lifespan and profitability of them. Given below is the model. Here it can be seen that because only one process can be active, Linny-R determines which process can produce the highest cash flow. In this case, squeezer 2 is more profitable and, therefore, turned on in the model.

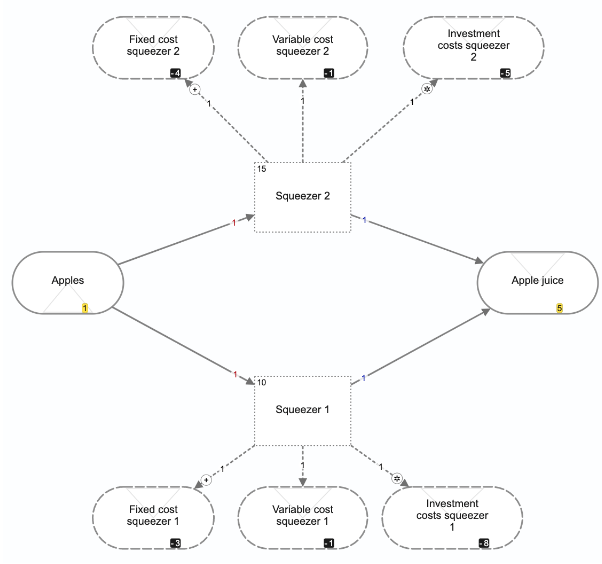

Figure 8: Simple Linny-R representation of an extra capacity investment

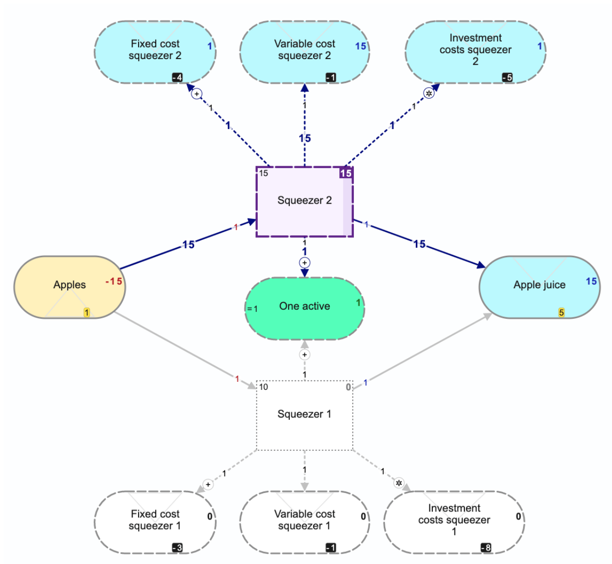

Figure 9: Simple Linny-R representation of an investment option with only one process allowed to be active

Linny-R has the option to include a stock level to a data product, making it possible to give a certain process a lifetime. So, if for example the new squeezer is able to squeeze apples for 15 years, the model can give an upper bound value of 15 to the data product, and once it reaches the upper bound, the process will be shut off. The investment representations given above can be adjusted and extended to represent numerous investment options and decisions. This can vary from choosing between multiple options but also represent an investment option for multiple actors.

Finally, Linny-R also possesses the power to assign processes to actors, making them owner of that particular process. When applied, the cash flow for the actors owning certain processes can be distinguished. This configuration can easily be added to the existing model by introducing two different actors into the model and by having them both be linked to a data product. This data product then forces them to share the costs, this can be done equally, but may also be performed in other ratio's. Below is an example of a simple investment structure as represented earlier, but with two different actors both responsible for coming up with 50% of the investment costs. By adding a data product which demands the actors to share the investment costs, this will be forced. Furthermore, the data product will have a constraint of having to be equal to 0. This is done such that the in-going data links have opposite rates of -1 and +1 resulting in both having to be activated to satisfy the constraint put on the data product. Meaning that the investment option only can occur if both parties provide funds for the shared investment costs. In certain situations, these investments can be fully shared, such as when a joint venture is created that co-invests in a certain innovation. In other situations, where an investment is made in a technology that also involves investing in an infrastructure, a different investment structure is implemented in the model. In the case of an investment made into an infrastructure, other companies can also benefit from using this infrastructure. An investment structure has been implemented in the model where multiple companies will invest in the infrastructure such that no free-riding will occur in the cluster. The free-riding has been eliminated from this model because it may cause a delay in innovations and CO_2 reducing technologies due to actors waiting until one succumbs and starts investing in the infrastructure and others benefiting from this.

3.3.2 Look ahead and investment payment forms in Linny-R

Having represented how investments are implemented in Linny-R, it is important to take a look at how the investments are payed. As mentioned in chapter 3.2.1, lack of available funds is a factor that influences the investment behaviour of actors within clusters. In this research, two forms of investment payments are identified. The first representation is used in the examples throughout chapter 4.2.1, where the investment costs are payed a single time upon activating the process. The second representation is an annual payment that is made starting when the process is activated and ending when the total costs have been fulfilled. To implement this form in the model, the model in figure 12 is adjusted. For this annual payment model to work correctly, the following requirements have been formulated:

- If the investment option is used at a certain time step, say t=1, then the payments will be performed 1 time step later, at t=2. The payments will then continue for a fixed amount of time steps
- If the investment option has been turned on, and then turned off but the loan has not been payed back yet, the payments continue until the full amount is payed back
- The annual payment does not change in size per year, every year until the loan has been payed back is the same payment size
- The model is not allowed to make a loan payment in the last time step

The first three points are implemented such that the solver has to evaluate whether the investment will be profitable or not. Calculations will be performed based on the objective function that the solver creates, determining which investment option will produce the largest cash flow. Including the second point restricts the solver from using the investment option only when the profits at that time step are higher than the investment costs. In real life, large investment options presented in chapter chapter 3.3.2, require years of planning and building. Simply deciding to invest in it for 1 year and then turn it off again for multiple years without payment is not an option in real life. The last point restricts the solver from investing in the last time step such that the investment option can be used, but no payment has to be made yet. This is implemented because the solver only simulates for a specified amount of years, whereas in the real world, life continues after the same amount of years. All this together, will provide the model with the possibility to invest in a technology by engaging in a loan, and pay it back over a specified amount of years, without the solver being able to evade payments.

For the payments to be made, an additional actor is introduced, the Bank actor. This bank will loan the money to the actor making the investment, and receives its money back through a fixed amount of payments which can include interest is desired (the interest has to be included with the investment capex to use it in the model). The layout of the model stays relatively the same, the same first commit is made when an investment option is used for the first time, and because the option has been engaged, apple juice can be made using apples. So, a flow is created from "Squeezer" to "investment costs". The flow will then be passed on from "investment costs" to the "Finance Loan" process, representing the loan that is engaged by the actor making the investment in the "Squeezer". Another product named "Funds" is made with a cost value, to represent that the bank provides the funds and then gets it payed back later on. Now, for the amount of money that has to be payed each time step to the Bank actor, a formula has been formulated. This formula determines the amount that flows from the "Squeezer" process to the "Investment costs" data product. To formulate this formula, first, an explanation is required on the actors investment behaviour within the model. When an actor has the possibility to invest, the solver will determine the price of the raw materials, the sales price of the product made, any other costs implemented in the model, and the investment costs. If the profits outweigh the costs, the solver will invest in the investment option, and if the costs outweigh the profits, it will not invest. The outweighing of the profits against the costs is based on how far the solver can look into the future. The solver can look into the future by adjusting the block length and look ahead. The block length represents the amount of optimizations it will perform, giving the following expression:

$$optimizations = \frac{T}{n}$$

where T represents the total amount of time steps and n represents the size of the block length. The look ahead is the amount of future steps that the model takes into account when optimizing one time step. By using these future steps, it will optimize its current step equal to the look ahead, giving the following expression:

$$optimizations = T * n$$

The profits resulting from the investment need to at least cover the costs that the actor can see in its (near) future. With this, the following formula has been formulated:

$$Ap = (\frac{(l+n)}{P} * C)$$

where Ap is the payment that is performed each year, l is the look ahead, n is the block length, P is the payback period and C is the capex of the investment to be made. This formula will be integrated in the arrow going from "squeezer" to "investment costs". The (l+n) combined equals the risk that actors take in deciding to invest. Changing the risk for individual actors can lead to interesting insights later on. With this formula, the aggregated redemption can now also be calculated according to an if statement that is integrated in the model as well. The if statement looks like the following:

$$R_t = \begin{cases} \frac{C}{P}, & \text{if} \sum_{i=t-P}^{t-1} C_{P,t} > 0 \\ 0, & \text{otherwise} \end{cases}$$

where Rt is the total amount of money invested, C is the capex of the investment to be made, P is the payback period and t is the time step.
This statement is used to calculate the redemption that each actor has made, which then in turn can be used to calculate the profits for each actor. Below is a representation of the annualized payment structure which will be used for the rest of this research. The representation looks simple, but its complexity lies in the flow rate formula and the aggregated redemption calculation.

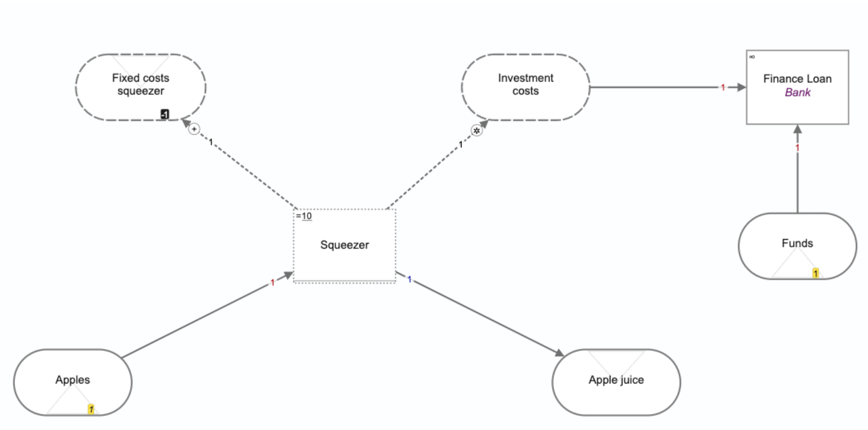

Figure 10: Simple Linny-R representation of an investment option with an annual payment

3.3.3 Actor weights in Linny-R

This research aims to determine the influence of exogenous factors on the investment behaviour of Chemelot, but also the investment behaviour of individual actors. Investing in a certain technology might be the obvious decision to make in terms of total cash flow for the entire cluster, but not for the individual actor. By creating a simple model that shows the total cash flows of individual actors but also the entire cluster can provide insights on the influence of certain investment behaviours. Furthermore, a difference will be made between the investment costs having to be paid up front, or if the costs will be spread out over a certain amount of years. A representation of the model is provided in Appendix B. First, the experiment is run where the solver does not look at individual gains, but maximizes the overall cash flow of the entire cluster. Below is a chart showing the cash flow for the individual actors and the cluster.

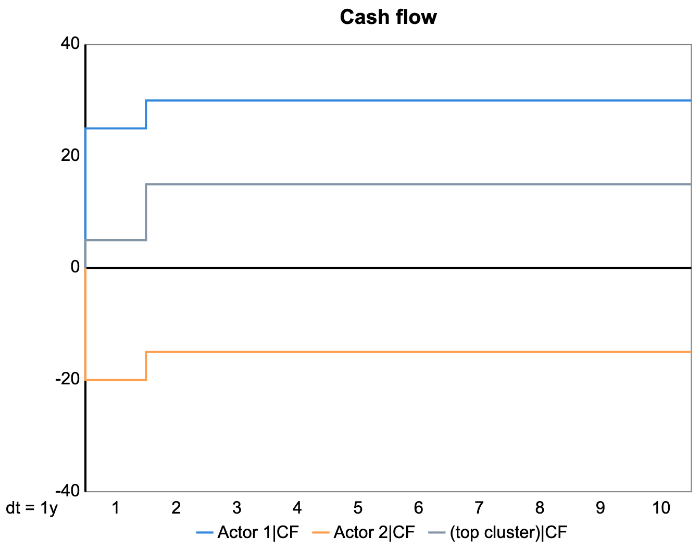

Figure 11: Cash flow for actors with different actor weights

What can be seen is that even with the investment costs and the intermediary price of the intermediate product, the cluster as a whole is profitable. But if we look at the individual actors, it can be seen that Actor 1 makes a very large profit compared to Actor 2, who makes a loss. In the real world, an investment decision might be profitable for the industrial cluster, but if it causes an individual company to lose money, the investment may not be made. Linny-R allows for managing actors within the model, weights (of importance) can be adjusted and changing production levels can be prohibited. By increasing the weight of Actor 2, or preventing Actor 2 from changing the production levels, the profits for Actor 2 cannot be optimized, resulting in no production taking place in the entire system. If we increase the weights of Actor 1 or the entire cluster, it can be seen that production does take place. So what this shows, is that some investments can be beneficial to a certain actor and the entire cluster, but it may come at the cost of other actors. Macro-level investment insights, may be irrelevant or infeasible on a micro-level. Furthermore, if we adjust the investment structure to having to pay a certain amount per year instead of total costs up front, it does not matter for the results of this model. By applying it to models later on in the research as well, conclusions can be made on the influence of the different investment payment forms.

3.3.4 Representing exogenous factors in Linny-R

Exogenous factors are factors acting on the system outside of the scope of this research. These factors can vary in how they affect the system, and do not follow a standard set of rules. As mentioned in chapter 2, a set of exogenous factors have been identified that influence industrial clusters. Because of the varying nature of these factors, the representation in Linny-R varies per exogenous factor.

The emission reduction policies can be implemented in multiple ways. Linny-R allows for putting a price on a product (in this case CO_2), but this price can also be part of a data set. Using a data set allows for adding a range of different values to a product corresponding to the time steps that the model is using. The price of CO_2 is dependent on the amount of EU ETS certificates issued each year and the demand for those certificates, making it difficult to predict the price in the coming 30 years. By making use of (grey) literature and market trends, a price range for CO_2 has been developed. Furthermore, to assess the effect that emission reduction policies have on industrial clusters, the price will be varied in a set of experiments presented later on. Implementing the price in this way will show the different pathways an industrial cluster can take and how it is influenced by the price of CO_2. Furthermore, emission reduction policies can also be translated in terms of restricting the amount of CO_2 allowed to emit. This can be represented in the model by adding a capacity to the CO_2 product, restricting the model from going over that value. Here, another data set can be used to slowly decrease the amount of CO_2 allowed to emit, with it finally being net zero in 2050.

Lacking infrastructure is an exogenous factor influencing multiple aspects of the system. The infrastructure to keep up with the increasing electricity demand of industrial cluster is an example of lacking infrastructure, but making use of hydrogen fueled steam cracking furnaces that requires a constant inflow of H_2 is another example of an infrastructure that is not present yet. Because this factor influences the system both upstream and downstream, it becomes more difficult to implement this into the model. Lacking electricity infrastructure can be represented in the model by adding a capacity on the electricity product, limiting the amount of products that can be made due to an energy capacity. This can also be applied to the other feedstock products such as naphtha and natural gas. Lacking infrastructure for H_2 needs to be represented in a different way in the model. If a certain technology cannot function without the appropriate infrastructure, an investment needs to be made into that infrastructure as well. By adding the costs of the infrastructure to be constructed to the investment costs of said technology, the exogenous factor can be represented in the model. This can cause companies to wait with investing in the technology and infrastructure until the price of CO_2 becomes so high or the price of H_2 reaches a low enough point for it to be profitable. Lacking CO_2 infrastructure representation in the model becomes difficult because it is heavily dependent on actors outside of the scope coming up with initiatives such as Porthos and Aramis, such that CO_2 can be transported and stored in gas fields on- and offshore. This can be represented in the model by adding a process to the model which represents the flow of CO_2 going from industrial cluster to the gas fields, but the amount that can be stored is highly uncertain. For this research, the existing infrastructure is represented and any additional technology investments that require additional capacity on the infrastructure are represented by including the costs in the technology investment.

Companies lacking available funds for large investments may make different decisions when knowing the future prices of everything. This will be represented in the model by creating two scenarios: One where the look ahead will be set to a high value such that the companies all know what the future prices will be, and one where the look ahead will be set to 0 ahead such that they do not know the prices in the later stages. This will allow for insights in the investment behaviour of actors when having absolute knowledge, or very little knowledge on the price of products, as well as giving insights on how they will invest when they know or do not know the prices and potential gains over time.

Availability of renewable energy alternatives can be represented by implementing capacity constraints on products. The utilization of renewable energy alternatives may require a certain investment to be made first, because a process needs to be altered. This is represented by an investment structure as mentioned in chapter 4.2.1. The new feedstock for the innovation will make use of a renewable energy alternative, but their availability may be restricted. By adding a capacity constraint on that energy alternative product, the model is restricted in the amounts of that product it can use. Such capacity constraints can influence actors to wait with using the renewable energy alternative if the CO_2 price is not high for example, or because with the constraints only a part of its former production capacity can be reached. The capacity constraint can be put on any renewable energy alternative, and also on multiple at the same time.

3.4 Experimental setup and formulation of hypotheses

From the insights attained earlier, several hypotheses have been constructed. These hypotheses will be tested by using Linny-R to perform different model simulations of a demarcated system of an industrial cluster. The industrial cluster will have multiple investment options and will be subject to different exogenous factors. The hypotheses are developed by varying the exogenous factors and stating the expected effects it will have on the investment behaviour and cash-flow of the industrial cluster. The system boundaries will be defined and presented later on in chapter 4. Testing the system under different exogenous factors through the optimization model will allow for individual and cluster results in terms of cash flow, investments made per time step and emission levels. The hypotheses that have been formulated are provided in the table below, along with the research question to be answered, the experiment and set-up and finally, the expected outcome of the experiments. By using the table below, SQ5 can be answered on how to the effects of different investment strategies can be tested in a structured manner.

Research question	Hypothesis	Setup & experiment	Expected outcome
Which form of CO_2 reducing policy generates more cash flow and how does it influence the investment behaviour in more sustainable options in industrial clusters?	Setting a price on CO_2 allows the model to produce more and, therefore, generate more cash flow. This makes it more preferable than a CO_2 cap since it may cause the model reduce its production levels	Two simulations with a simple model containing a single CCS investment will be performed, the only difference is that in the first simulation, the CO_2 that can be emitted is capped, the second simulation will have a price related to the CO_2	Putting a price on CO_2 allows the model to produce more and invest in the CCS. If a cap is imposed on the CO_2, the model will start producing less products since the CCS will be capped and no more CO_2 can be emitted. This will drastically reduce cash flow.
Which investment strategy stimulates actors to invest in sustainable options in industrial clusters?	Having to pay all costs up front results in actors being reluctant to invest, being able to pay a certain price per year reduces risk for the investor.	Each model has identical investments, with identical inputs and outputs. One model will have to pay all costs up front, the other model can pay per year. The model will evaluate which investment strategy stimulates investing more.	Investments will be made under the investment strategy where paying over time is possible. Only the costs for that year have to be covered for the investment to be profitable.
How does having full knowledge of future prices compare to not having full knowledge of future prices?	Having full knowledge of future prices will generate more cash and more investments	Two similar models will be made where the only difference is the investment strategy. Two simulations will be run per model, one with having full knowledge of future prices and one without having full knowledge of future prices.	Full knowledge gives the optimal investment trajectory. Here, investment strategy does not matter because the model knows if the investment is profitable. In a model with limited knowledge, investment strategy matters, paying over time reduces risk.

Table 1: Overview of experiments and hypotheses

3.5 Verification of the investment representations and actor weights

The representations of the investment structure and multi-actor involvement provided earlier require verification before implementing them into the case study. To verify those representations, the model will be tested for multiple actors with the options for multiple investments. From this, insights can be gained on the results which will provide knowledge on the robustness of the model. The results gained from the model should be in line with expectations on the robustness of the model. The model used is provided in Appendix B, and revolves around Actor 1 being able to invest in a CCS, which will reduce its CO_2 emissions drastically. With this model, the verification experiments will be performed.

3.5.1 Verification of the investment representation

For this verification step, the a simple model will be used. The model is a basic representation of an existing industrial cluster in the Netherlands and will be used to verify different investment options for different actors. The verification experiments were done through implementing the investment options with full payment upfront. For the experiments, investments are adjusted in their profitability to gain insights on the behaviour of the model. Only the investment was adjusted at the time, and the rest was left unchanged. This will test whether the model will show that actors have different behaviours. The table provided below shows a summary of the results from the experiments. Further details are presented in Appendix B, with extra information regarding behaviour and time step cash flow comparison.

Model addition	High profitability results	High loss-making results
Single investment	It can be seen that when an investment provides a large positive difference in cash flow, the model will opt this investment. Depending on its profitability, the model will invest in it at a certain time step. The more profitable the investment is, the earlier the investment will be made. In this case it can be seen that the investment is made at the first time step	When the investment would cause a decrease in cash flow, the model will not opt the investment. In this case, the extremely high costs of investment results in the model not opting the investment.

Table 2: Verification results for investment representation

The verification results show that the representation of the investment structures in the model influence the cash flow of an actor. It demonstrates that by making use of an investment that provides benefits over the existing structure, the model will opt the investment and that will result in a higher cash flow. Coincidentally, when the investment does not result in a higher cash flow, the model will not choose to opt the investment. Figure 15 shows a comparison between the cash flow of the base case model where no investment is added to the model, and the cash flow for when a single profitable investment is added to the model. In this case, Sabic was presented with an investment opportunity in CCS that would reduce the CO_2 they would emit. Because of the increasing price on CO_2, it appeared to be a profitable investment where the profits far outweigh the costs of the investment that would reduce the CO_2. If Actor 1 would not invest in the CCS, they would be left with a loss after 30 years. This verification experiment shows that the investment representation accurately models how actors behave when an investment arises within a cluster. It is especially demonstrated that the investment representation effectively responds when an investment is made extremely profitable, or if it would make large losses.

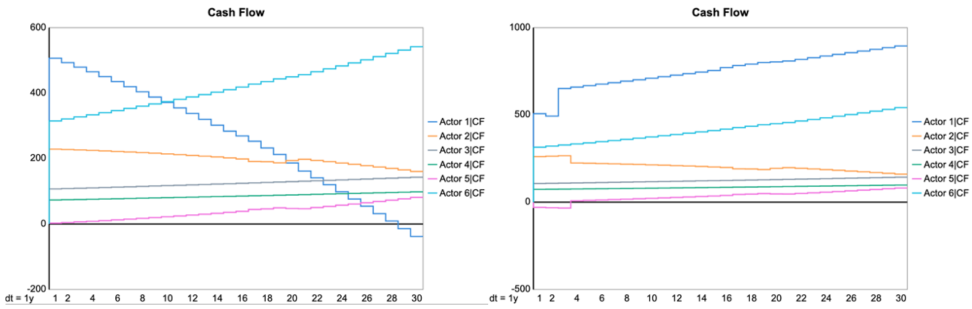

Figure 12: Cash flow of actors without an investment possibility (left) and a single investment possibility for Sabic (right)

In the case of an investment that would result in a large loss, the model does not choose for it. This will result in the same cash flow values as having a model without an investment possibility. Therefore, the cash flow will be similar to the cash flow figure on the left in figure 10.

3.5.2 Verification of the payment over time representation

This research tries to model the lack of available funds factor that influence the investment behaviour for actors within an industrial cluster. This factor is implemented by creating an invest-over-time structure to simulate loans/subsidies that companies may attract to still perform the investment. This representation requires verification before it can be implemented into the case study. First, the robustness of the representation will be tested by creating a simple model that will evaluate whether the risk integration works. This will be done by making an experiment consisting of two different actors, one actor with a payment over time structure and another actor with having to pay upfront. Both actors will be given the same risk value to see whether differences in investment behaviour occur. If both actors have the same risk value, but the actor with the payment over time structure invest, it will prove that the structure promotes investing. The model will then be adjusted that both actors have a payment over time structure, and the risk values will be adjusted to such a point that one actor will not invest, whereas the other actor will invest. This will show that the integrated risk factor also works accordingly. After this has been tested, a small adjustment from the verification experiment in chapter 4.3.1 will be made to test the representation in a larger model with more actors.

Model addition	Risk value	Results
Actor 1 payment over time structure, actor 2 direct invest. Same risk values	Both actors have a risk value of **3**	Actor 2 requires to earn its total investment back in the years it can see ahead, whereas actor 1 only needs to earn a part of the investment back. The risk values are the same, meaning they can both look the same amount of years ahead. This results in actor 1 making the investment and actor 2 not making the investment.
Actor 1 & actor 2 payment over time structure. Different risk values	Risk value of actor 1 is **3**, risk value of actor 2 is **6**.	With similar payment structures, the amount of investment that has to be earned back is now only related to the risk values. Since actor 1 has a lower risk value than actor 2, it needs to earn back less of the investment before it will take the chance to invest. This results in actor 1 investing and actor 2 not investing.

Table 3: Verification results for payment over time structure

The adjustment made is the implementation of the payment over time representation provided in chapter 4.2.2, such that the cost of the investment are spread out over multiple years. For the second verification experiment, the same investment options for the actor is implemented, a CCS structure for Sabic to reduce CO_2 emissions and cut costs in paying for those emissions, the only difference is the payment structure. The implementation of the payment structure will prove that the model can allocate costs over time in an environment with multiple actors, where one is presented with the a certain investment option. Provided below is a table with the summary of the results from the experiment. Further details are presented in Appendix B, with extra information regarding behaviour and time step cash flow comparison.

Model addition	All costs upfront	Payment over time structure
Profitable investment	Because of the total costs of the investment having to be paid at once and the model not being able to look ahead, it did not opt for the investment because at no point in time, was the costs of emitting CO_2 higher than investing in the CCS to reduce the emissions.	Since the investment is profitable from the first moment, the model will invest in the CCS immediately, resulting in large amounts of money to be made due to saving costs on the CO_2 emission costs. Even when the model is not able to look ahead, it compares the prices and chooses the option with the highest cash flow.
Loss making investment	The total costs of the investment outweigh the returns it can provide by a large amount. Meaning that even though the model cannot look ahead, it will not opt the investment because of the reduced cash flow.	With the ability to compare the price of the investment on a yearly basis with the price of CO_2, the model still chooses to keep on emitting CO_2 since the costs related to those emissions are lower than the yearly payment plans for the CCS investment.

Table 4: Verification results for payment over time structure

The verification results show that the representation of the investment over time structure in the model influences the cash flow of an actor. just like the regular investment structure, It demonstrates that by making use of an investment that provides benefits over the existing structure, the model will opt the investment and that will result in a higher cash flow. Figure 16 shows a comparison between the cash flow of the investment representation with the investment costs having to be paid all in once, and the cash flow for when the investment is paid over time. Because of the increasing price on CO_2, it appeared to be a profitable investment where the profits far outweigh the costs of the investment that would reduce the CO_2. If Sabic had to pay for the investment all in once, they would not invest in it and make only a small profit after 30 years. This verification experiment shows that the investment over time representation accurately models how actors behave under different payment structures. It is especially demonstrated that the investment over time representation effectively responds when an investment is made extremely profitable, even if it does not seem profitable at first.

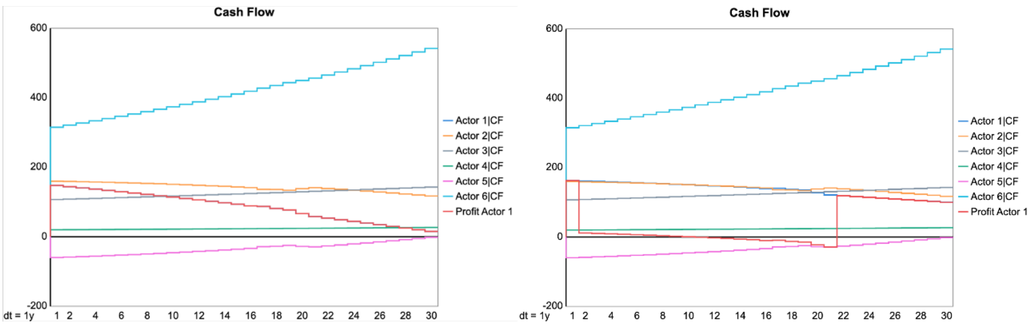

Figure 13: Cash flow of actors with payment upfront structure (left) and a payment structure over time (right)

3.5.3 Verification of the actor weights

Because the actor weights highlighted in chapter 4.2.3. can heavily influence the outcome of the cluster, they will be verified by using the same model. The verification experiments were performed by assigning a high actor weight and a low actor weight to a certain actor to gain insights on the behaviour of the model. For the experiment, only 1 actor weight will be adjusted, and the rest will remain unchanged. The investments are implemented with values such that the investment is more profitable. This will prove that the model will cause certain actors not to invest into a more profitable option, or cause certain actors to make losses because of the actor weights assigned. The table below shows a summary of the results from the experiments.

Actor	OCI weight 1	OCI weight 0
Actor 1 weight 1	If both actors have an actor weight of 1, their importance is equal. The objective function is to maximize cash flow for both. Actor 1 is expected to make the most amount of money due to its size	Actor 1 is more important than Actor 2, meaning that the objective function for the model is to maximize the cash flow of Actor 1, which will earn more than Actor 2.
Actor 1 weight 0	Because Actor 2 is more important than Actor 1, the objective function for the model is to optimize cash flow for Actor 2. Actor 2 will earn more profits than Actor 1	Because both Actor 1 and Actor 2 have an actor weight of 0, and the other actors have a value of 1 (not included in the table or figure), the objective function will not optimize the cash flow of Actor 2 and Actor 1, but rather of the other actors. This will result in Actor 1 making more money than Actor 2 because more actors depend on Actor 1 for the feedstock.

Table 5: Verification results for actor weight representation

What becomes evident from this experiment, is that when certain actor weights are assigned, the model will remove or prioritize the cash flow of that particular actor in the objective function. Here it can be seen that that the verification results show that the representation of the actor weights in the investment model influence the investment behaviour and the cash flow of actors. It demonstrates that even when an investment is profitable, if the actor weight is set to 0 such that its cash flow is removed from the objective function in the model, the investment shall not be opted for. Even if the investment would create a very large increase in cash flow, the model will still not choose to invest into it. The bar chart below displays the cash flows of two actors in the model with varying actor weights and the cash flow of the total cluster. It can be seen clearly that when the actor weight of 0 is assigned to Actor 2, it will not invest in a very profitable investment, whilst in the cases where an actor weight of 1 is assigned to Actor 2, the total cash flow is increased massively.

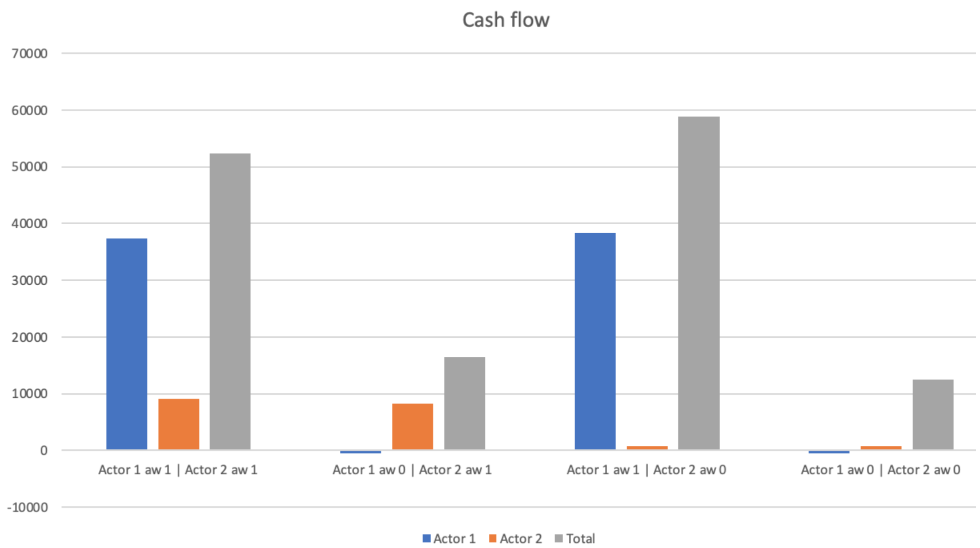

Figure 14: Cash flow of Actor 1, Actor 2 and of the entire cluster under varying actor weights (aw)

3.6 Verification of the exogenous factors and validation

The representations of the investment structure and exogenous factors provided earlier require verification before implementing them into the case study. To verify those representations, the model will be tested for multiple actors under various extreme conditions. From this, insights can be gained on the results which will provide knowledge on the robustness of the model. The results gained from the model should be in line with expectations on the robustness of the model. For this verification step, the model provided below will be used. The model is a basic representation of Chemelot and will be used to verify the exogenous factors described in chapter 3.2.1. The verification experiments were done through implementing extreme values on variables within the model. Variables such as product price and availability of products are variables with large influences on the profitability of the cluster. For the experiments, one extreme value manipulation was implemented and the rest was left unchanged. The table provided below shows a summary of the results from the experiments. Further details are presented in Appendix B, with extra information regarding behaviour and time step cash flow comparison.

Variable changed	Low value results	High value results
Naphtha price	With the naphtha price being very low, producing at full capacity becomes very profitable for the naphtha chain. It can be seen in the graph that an extremely large amount of profit is made	With the naphtha price being very high, producing at full capacity results in losses for the naphtha chain, it is shut off. The model still produces in the NH_3 chain, but only to sell NH_3, no other products are being made with NH_3 because of the high price of naphtha.
CO_2 price	With the CO_2 price being very low, both the naphtha chain and the NH_3 chain will produce at full capacity, since their emissions will not be penalized. Because CO_2 is quite a cost item in the base case, a large profit will be realized in this scenario	With the CO_2 price being very high, both the naphtha chain and the NH_3 will not produce at all. Because CO_2 is quite a cost item in the base case, and in this scenario it is increased extremely, the cluster will not produce at all to minimize losses.
Natural gas price	With the natural gas price being very low, both the naphtha chain and the NH_3 chain will produce at full capacity. Natural gas is a feedstock for both chains and a large cost item, resulting in a large profit if the price is low.	With the natural gas price being very high, both the naphtha chain and the NH_3 chain will be shut off. Natural gas is a feedstock for both chains and a large cost item, resulting in large losses if the price is high if the system is not turned off.
Final product price	With the price of final products being very high, large profits are made when both chains operate at full capacity.	With the price of final products being very low, large losses are made when both chains operate at full capacity because the material price is higher than the revenue of the final products.

Table 6: Verification results for exogenous factors representation

The verification results show that the representation of the exogenous factors in the model influence how the actors behave within the cluster. It demonstrates that by implementing extreme values in the model, it will avoid producing in a certain chain when the values cause large negative cash flows, and will start producing if it produces a positive cash flow. These results are in line with the expectations of what would have happened if such extreme values were implemented in the model.

An interesting notation is that with an increasing CO_2 price, companies that have large amounts of emissions tend to make a larger profit. Furthermore, actors that are dependent on selling CO_2 to other actors see their profits reduced due to the lower price. So, the model maximizes the cash flow of the total cluster favoring the

companies that normally have large amounts of CO_2 emissions.
Other interesting insights obtained from other verification experiments was how the increase of raw materials price such as naphtha can cause an entire chain to shut down being in the best interest of the entire cluster. In the model, when the naphtha price was increased to a very high value, the NH_3 chain would still operate, but only to produce and sell the NH_3. No other products were produced because of the need for products that are created as a result of cracking the naphtha. This demonstrates that implementing extreme values on exogenous factors can cause the model to partly shut down the processes that are sensitive to those price fluctuations. OCI mainly dictates the cash flow of the entire cluster because a large part of the chain is not reliant on naphtha or products derived from naphtha.

3.7 Concluding remarks

In this section, an extensive discussion has been performed of the conceptual representations for exogenous factors and for investments in Linny-R. The methodology provided in this research to optimize the processes within an industrial cluster have allowed to see how the exogenous factors should be implemented as variables and how the investments should be represented in the model as structural variables. Having performed the verification experiments and validating the model to determine the robustness of the methodology that is proposed, the experiments have shown that the exogenous factors play crucial roles in the investment behaviour of actors. The methodology allows for the optimization of the cash flow all individual actors situated in the cluster, but also of the total cluster. Through the experiments and proving the robustness, the proposed methodology is considered to be a solid method to represent any exogenous factor and investment decision, such that cash flow is optimized and the investment behaviour of actors can be analyzed. Through this, SQ3 and SQ4 have been answered. The following chapter will provide a real-life application of the conceptual efforts performed in an attempt to understand the influence that the selected exogenous factors have on the investment behaviour in a real life example. This will be done by first assessing the different investments for that industrial cluster. The proposed modeling methodology combined with Linny-R will be used to represent the parts of the industrial cluster that will be considered. For this case study, the model that will be developed allows for insights to be gained on the evaluation of different influences the exogenous factors have on the optimal investment trajectories for industrial clusters. Furthermore, these results can then be quantified to gain more in-depth insights.

4 Exogenous factors influencing investment behaviour in practice

This chapter will look at a specific industrial cluster and the energy transition its currently facing. The goal of this chapter is to apply the proposed modeling methodology from the previous chapter to an existing industrial cluster in the Netherlands.

4.1 Case study requirements

As mentioned in chapter 3.1, the model to be developed should be able to handle input specifications such as production capacity, product demand, product prices, fuel prices, raw material prices, the exogenous factors identified in chapter 2, the model should include multiple actors that are interconnected and multiple investment options should be present throughout the cluster. The model will be tested by applying it to a real life case, which must adhere to the requirements above. The case study will be focused on Chemelot, because of the available literature and its unique specifications.

4.2 Emissions, throughput and challenge faced by Chemelot

Chemelot is a large industrial cluster in Geleen, with a large focus on producing hydrocarbons and ammonia-related products. Throughout the years, they have been focusing on becoming more sustainable and have done this through a high level of interconnectivity and hubs to develop more sustainable practices (Chemelot, 2021), which aligns with the literature from chapter 2. However, with the regulations to become CO_2 neutral in 2050, they still need to make large steps within the energy transition. In 2020, Chemelot used 1.5 billion cubic meter natural gas and 4 Megaton naphtha. Furthermore, its electricity use in 2020 was around 2 Terawatthour (Chemelot, 2021; Bruijns, 2020), and the CO_2 emissions were roughly 6 megaton.

In order to reach the 2030 goals of reducing CO_2 by 50% and CO_2 neutral by 2050, it is necessary to move away from the fossil-fuels and use renewable sources. Becoming more sustainable for Chemelot is not an easy task. They need to maintain its current output to stay competitive with competitors, or else they will lose revenue (Kwaak et al., 2021). Moving away from fossil-fuels such as gas to heat up certain processes, requires more electricity to reach the required temperatures (Chemelot, 2021). One of the problems is that the current electricity infrastructure cannot supply the required future electricity demand, requiring investments to be made into the infrastructure (ANP, 2022). This also goes for other energy alternatives.

Such problems are faced by multiple industrial clusters in the Netherlands, they all require large amounts of fossil-fuels, raw materials and electricity to produce the (half)products and export them. Without the proper sustainable investments being made, the targets of 2030 and 2050 will be difficult to reach. An option to lower emissions would be to lower the production output of an industrial cluster such that less fossil-fuels will be used. But, applying this to all industrial clusters would lose the competitive position that the Dutch industrial clusters have over other countries and significant amounts of revenue will be lost (Janipour et al., 2020).

4.3 Chemelot in the energy transition

4.3.1 Layout, processes and operations in Chemelot

Chemelot is regarded as one of the leaders in chemical processing in Europe, covering around 20% of all chemical processing of the Netherlands and generates a revenue of 10 billion per year. The geographical position of Chemelot is challenging due to not being near a large seaport, it does, however, have access to a small port. All resources are transported to Chemelot by pipeline, truck, railroad or through the small port. The petrochemical department of Chemelot can be divided into two large streams: Natural gas and naphtha. Natural gas is used for the production of NH_3 and naphtha is used for the production of Ethylene and Propylene. The yearly throughput of natural gas is 1.5 billion cubic meter 4 Megaton naphtha. Chemelot processes these raw materials into products such as Urea, Melamine, Acrylonitrill, PVC and Polyethylene. Chemelot has a strong position in the chemical industry, but is also a large emitter of CO_2, and reducing their emissions has become a challenge. Maintaining its competitive position in Europe requires Chemelot to move away from its current processes and move towards sustainable technologies and materials.
The image shows the two petrochemical streams of Chemelot. The first stream is focused on making NH_3 or NH_3 related products. OCI uses natural gas as a feedstock, combined with water and air to produce NH_3. The NH_3 is then further used by OCI to make products such as calcium ammonium nitrate and nitric acid. Another large part of the NH_3 produced will be sold to other companies on the Chemelot site, for them to process it

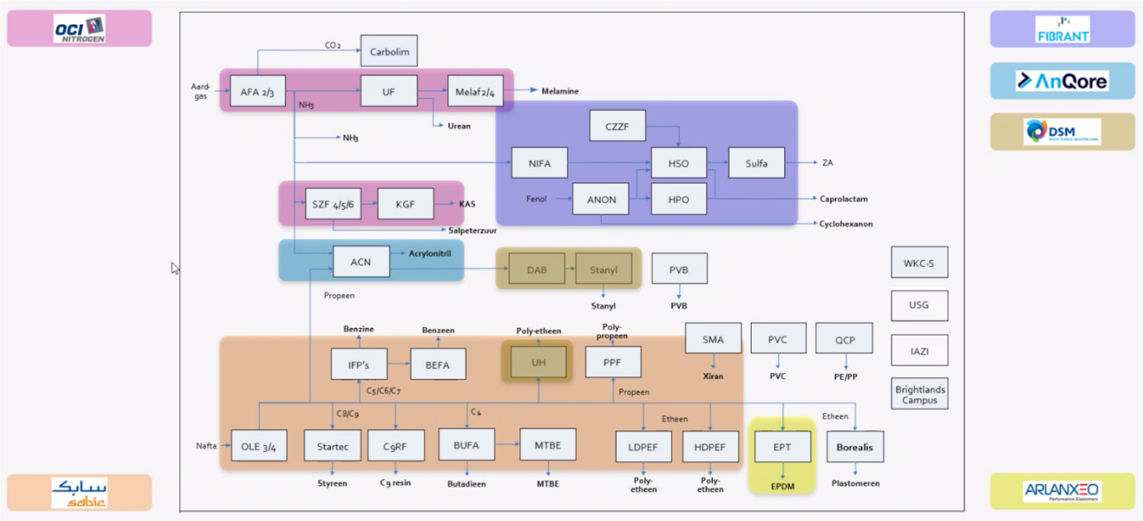

Figure 15: Raw material streams in Chemelot

further into other products such as acrylonitrill, caprolactam and stanyl. What is also interesting to see is that the CO_2 that is released when making NH_3 from natural gas, is sold to another company on site. This is an example of the integrated structure that an industrial cluster can have. Looking at the naphtha chain, it can be seen that it is largely owned by Sabic. They use naphtha to produce ethylene and propylene, as well as making other products such as benzene and styrene. A part of the ethylene and propylene is sold to other companies, which process it into products such as stanyl, poly-ethylene and plastomers.

For the model that will be developed in this research, the NH_3 and naphtha stream will be partly considered. The figure below shows what part of the streams are considered for the model. The demarcation is made based on the availability of data, CO_2 emissions, amount of time available and number of different actors. With the demarcation, the exogenous factors that influence the actors and processes can be assessed as well as the impact they have on the investment behaviour. The two main processes included are AFA 2/3 and OLE 3/4. Furthermore, the associated CO_2 emissions, NH_3 stream, products produced from NH_3, ethylene and propylene are considered.

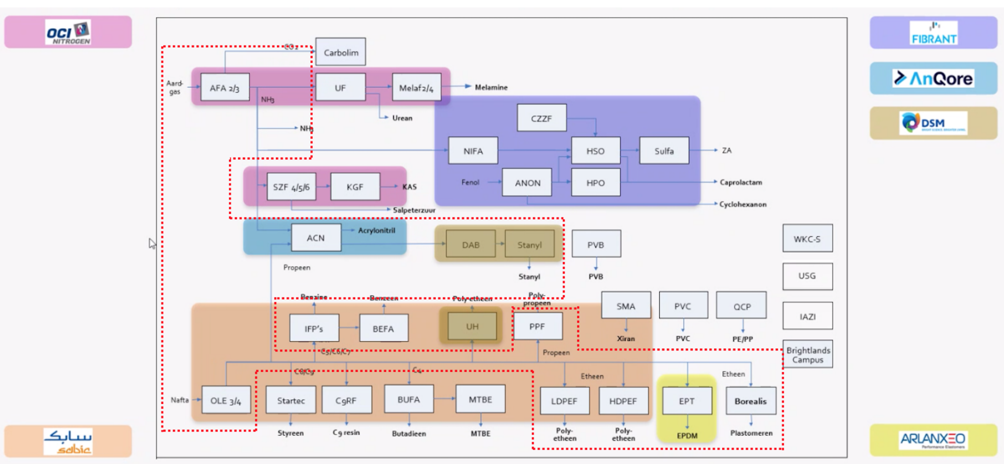

Figure 16: Considered streams for the model

4.4 Exogenous factor influencing Chemelot

Chemelot has multiple plans to move away from fossil fuels and feedstock and become more sustainable, with the aim to reach the 2030 and 2050 goals. However, certain conditions must be in effect for Chemelot to really achieve those goals. The exogenous factors identified in chapter 2 are applied to Chemelot and the effects to the goals of Chemelot are elaborated on. Later on, possible solutions to the exogenous factors will be provided.

4.4.1 Exogenous factors in practice

Lacking infrastructure
The infrastructure required for the supply of the renewable energy alternatives and the transportation of CO_2 is a large enabler for Chemelot to reach its goals. The infrastructure can be divided into three categories: electricity infrastructure, H_2 infrastructure and CO_2 infrastructure. The exogenous factors provided in this chapter will form the basis of the scenario analysis that will be performed later on in this research.

- The electricity demand of Chemelot is expected to quadruple in 2050 (Chemelot, 2022), meaning that the current electricity infrastructure in and around Chemelot needs to be strong enough to handle these amounts. Unfortunately, TenneT (the network operator in Limburg) has announced that its network is at max capacity, and no new (large) customers can be connected to the network (ANP, 2022). Meaning that on the short term, Chemelot may be unable to increase its electricity demand, resulting in processes such as the Ole 3/4 which are high in heat demand currently heated through fossil fuels, not being able to be electrified, slowing down the transition of Chemelot.

- The H_2 infrastructure in the Netherlands will be built and monitored by Gasunie. This entails the H_2 infrastructure throughout the Netherlands, but not on-site infrastructure such as the H_2 infrastructure on Chemelot. Individual companies are responsible for the development of this infrastructure, but they can make use of the expertise Gasunie has. The H_2 network will consist of newly constructed pipelines and old gas pipelines transformed into H_2 pipelines. It is expected that this network will be partially in use per 2025, mainly consisting of the old gas pipelines. By 2028, all the industrial clusters should be connected to the network and able to provide them with H_2 transportation possibilities (Aramis, 2021). It is the responsibility of Chemelot to develop the internal infrastructure for H_2.

- the CO_2 infrastructure projects in the Netherlands are currently in progress to provide transportation possibilities for excess CO_2. The current reserved customers already exceed the maximum capacity of the CO_2 network, resulting in Chemelot not being able to connect to this network at least in the early stages. Meaning that Chemelot either has to wait for a new CO_2 transportation project such as Aramis to see whether they can connect to it, pay for the excess CO_2 they currently produce or start investing in its own CO_2 infrastructure. The lack of CO_2 transportation possibilities can slow down the path to the goals of 2030 and 2050.

Availability of renewable energy alternatives
One of the biggest limiting factors for Chemelot in reaching the 2030 and 2050 goals is the availability of renewable energy alternatives. The electricity requirements for the industrial sector and also Chemelot, is expected to be four times higher due to decarbonization options such as electrification of processes and utilization of electrolyzers (Scheepers et al., 2022). As mentioned earlier, it is expected that the biomass demand for Chemelot cannot be supplied (Spijker et al., 2020). Renwable electricity is also a limiting factor in Chemelot's goals for 2030 and 2050. Since the electricity network of Limburg is already at its max (ANP, 2022) and transportation of offshore renewable electricity can only be performed with substantial losses (Kucuksari et al., 2019), or carriers such as ammonia need to be used, means that for Chemelot being able to be supplied with its future electricity demand in renewable electricity, numerous innovations need to take place outside of the boundaries of Chemelot and resulting in the current demand for electricity mainly being generated through fossil fuels. An even more disturbing recent development is that because of the war in Ukraine, and the need to maintain a certain natural gas reserve, the Dutch government has allowed electricity generation through coal to fully operate until 2024, meaning that electricity received from the net will be even more CO_2 emitting (Telegraaf, 2022). Furthermore, H_2 is expected to become more and more relevant from 2040 onward (Detz et al., 2019), both for heating processes instead of natural gas, but also as feedstock for synthesis of base chemicals. However, the supply of green H_2 is nowhere near the demand, therefore, blue H_2 will be needed to reduce the emissions on the short term and because of its reduced costs compared to green H_2 (Detz et al., 2019). This is only a short term solution and still does not solve the long term demand for green H_2. This shows that the dependency of

Chemelot on innovations in energy carrying techniques and availability of the renewable energy alternatives is large, and negatively impacts the rate of progress for Chemelot working towards 2030 and 2050.

Emission reduction policies
The emission reduction policies have been highlighted throughout this research, mainly focusing on the regulations of 2030 and 2050. In short, the 2030 regulations obliges companies to reduce their CO_2 emissions by 49% compared to the 1990 emissions. The 2050 regulations obliges companies to reduce their CO_2 emissions by 95% compared to the 1990 emissions, but CO_2 neutrality is also often used as an indicator for the amount of emissions to be reduced (Agreement, 2015). However, parallel to the emission reduction policies, the European Union Emissions Trading System (EU ETS) has been established which issues certificates, putting a price on CO_2 emitted from installations that fall under the jurisdiction of the EU ETS. With the goal to reduce CO_2 emissions, the number of issued certificates will be reduced towards 2050 (Y.-J. Zhang & Wei, 2010). Reducing the supply will cause for an increase in demand and this will increase the price of CO_2. For Chemelot, this is a difficult case. With the dependency on innovations and infrastructures outside of the scope of Chemelot to reduce its CO_2 emissions, a large increase in the price on a short term can become large costs for Chemelot. So combined with the lack of enabling technologies, increasing price can also cause Chemelot to further slow down in its transition.

Lack of available funds
Although lack of available funds may seem like an internal factor, having no available funds for sustainable innovations within the Chemelot site slows down the implementation and reducing the CO_2 emissions. Nowadays, companies do not often have large sums of money (more than a billion) ready in cash to start developing an electrifier for example. If they do have cash, quite often it is not the total sum of the investment to be made (H. Zhu et al., 2016). To cover this gap in cash, subsidies are used as enablers. The Dutch government has quite some subsidies that allow for companies within the industrial sector to be granted large sums of money to make CO_2 reducing investments. One of the biggest subsidies is the SDE++ which covers topics from renewable energy to low CO_2 production techniques such as CCS. The entire SDE++ budget for 2022 is 13 billion, with the amount of subsidy gained being dependent on the amount of CO_2 reduced by the investment (RVO, 2022). The subsidies in the Netherlands function as a large enabler for innovations that speed up the transition for Chemelot. Therefore, lack of available funds is translated to the possibility for actors within industrial clusters to still invest in sustainable innovations, through engaging in a loan with very low interest (<1%) or through subsidies.

4.4.2 Renewable investment options Chemelot

With the influences of the exogenous factors provided, the path towards CO_2 neutrality for Chemelot will be assessed. Certain transition options for Chemelot might be more easier implemented, such as using renewable energy sources to reduce CO_2 emissions. Other transition options require more planning and funds to be realized such as the electrification of processes or capturing CO_2 emissions. The renewable investment options can be categorized in the following:

- Carbon capture
- Alternative energy supply
- Alternative feedstock
- Alternative process

Provided below is an in-depth elaboration on different renewable investment options for Chemelot. The investment costs related to the provided investment options consist of two types of cost: *capital expenditure costs* (CAPEX) and *operational expenditure costs* (OPEX). CAPEX refers to the costs related to buy or upgrade a certain physical process and OPEX refers to the costs related to operating said physical process.

Carbon capture and storage or utilization
Currently, three CCS technologies are in development: Oxyfuel combustion capture, pre-combustion capture and post-combustion capture. Because oxyfuel combustion capture is not relevant for the Olefin 3/4 on the Chemelot site (Y. Zhang et al., 2021), only pre-combustion capture and post-combustion capture will be assessed.

Post-combustion capture
This technology captures CO_2 after the combustion of the fuel gas required to operate the Olefin 3/4. The CO_2 is chemically captured using a solvent, and then is rapidly cooled and lowered in pressure to desorpt the CO_2. Following, compression of the released CO_2 follows to prepare it for transportation for utilization somewhere else or for storage. The solvent used for the capturing can be cleaned and reused for another cycle of CO_2 capture. The integration of such a capturing system after the combustion process is site dependent, making it difficult to estimate the costs associated for the implementation, especially the costs of integrating the capturing unit into the already existing installations. Furthermore, large installations may require a capturing unit per process, but also potentially multiple capturing units per process. The benefits of the capturing system is that the solvent most suitable for the absorption (amines or ammonia) are already largely used within the chemical industry, and that the purity levels of CO_2 they reach are very high (99.99%). Compared to other CCS technologies, this is very high (Markewitz & Bongartz, 2015). Research is currently being committed to other solvents to increase the capturing efficiency of the post-combustion capture technique, as it is currently 90%.

Because of the cost being dependent on the location of a site, a wide range of costs has been found in the literature, ranging from €45/ton CO_2 to €245/ton CO_2 (Ho et al., 2011; Sannan et al., 2017). The differences in price may also be due to varying CO_2 concentrations of the flue gas, configurations of the combustion systems, other assumptions made and the location of the site. Assessing how specific the price is for the site is important to achieve a realistic cost indication for the installation of CCS on Chemelot. Offshore storage is currently the preferred form of storing CO_2, especially in terms of the public perception but also the availability of storage possibilities. Since Chemelot is located over 100km away from Rotterdam, and as mentioned earlier, the contracts for the Porthos initiative have already been issued, the CCS price assessment is very important, and may require CO_2 transportation infrastructure between the two locations in the future. The determination of the costs of a post-combustion CCS in steam cracker furnace is based on a study committed by Sherif (2010). The site studied differs from Chemelot, but the costs presented in this study are used to approximate the costs for implementing post-combustion capture in a steam cracker. The CAPEX covers all the equipment costs for capturing the CO_2, such as the absorption to compression chain but also the costs associated with integrating it into the existing installation. The fixed OPEX value is considered to be around 4% of the CAPEX costs, excluding the costs for energy. Below is an estimation of the costs:

Sort	Value	Unit
CAPEX	156	EUR/t CO_2 captured/yr
Fixed OPEX	6.8	EUR/t CO_2 captured
Capacity	428	kt CO_2 captured/yr

Table 7: CAPEX, OPEX and capacity for post-combustion CCS

Furthermore, the electricity consumption of the post-combustion capturing unit is estimated to be between 156 and 172 kWh/t CO_2 captured (Kuramochi et al., 2012; Sannan et al., 2017).

Pre-combustion capture
This technology requires a different form of fuel to be used for the process, a hydrocarbon-rich fuel. Here, the fuel is first fed to a gasifier or reformer to produce syngas (CO_2 and H_2). Using a shift-reactor, the concentration of the syngas is increased and then rapidly cooled to capture the CO_2 using a solvent for the chemical absorption. The new syngas is high in pressure, allowing for the CO_2 to be captured using physical absorption instead of chemical absorption through dimethyl ether/polyethylene glycol or methanol. This results in a CO_2 stream which can be compressed, transported and utilized or stored similar to the post-combustion capture. Furthermore, it also results in a H_2 stream of high quality which can be used to replace the fuel used for cracking furnaces (Markewitz & Bongartz, 2015; C. Oliveira & Schure, 2020).

Cost estimation of implementing a pre-combustion system has been performed using Kuramochi et al. (2012), who investigates the option in the refining but also petrochemical sectors. The table below summarizes the CAPEX, Fixed OPEX and Capacity of a pre-combustion carbon capture system.

Sort	Value	Unit
CAPEX	150	EUR/t CO_2 captured/yr
Fixed OPEX	7.5	EUR/t CO_2 captured
Capacity	770	kt CO_2 captured/yr

Table 8: CAPEX, OPEX and capacity for pre-combustion CCS

Furthermore, the electricity consumption of a post-combustion carbon capture system according to Kuramochi et al. (2012) is -0.1 GJ/t CO_2 captured, meaning that energy is generated. Additionally, the heat consumption of the system is estimated to be around 4.8 GJ/t CO_2 captured.

Electrification

This entails replacing technologies using fossil fuel as their main fuel with a technology that uses electricity as its fuel. Electrical heating methods such as furnaces or boilers have already proven to be effective using resistance heating or electromagnetic fields such as induction. Electric heating can be divided in direct heating technologies that generate the heat inside the material with the absence of a heat transfer medium, and indirect heating, where the heat is generated outside of the material and is transferred with the help of a heat transfer medium (Schüwer & Schneider, 2018). Although it has been proven to also be useful in the industry, it has not been applied yet for replacing the current fuels used for the steam cracking process. Arc heating (1200-3000 degrees) is currently being applied to high temperature range processes, exceeding the pyrolysis window (850 degrees) (Lu et al., 2021). Other technologies such as infrared heating has shown rapid heating capacities and high energy densities as opposed to gas furnaces. Resistance (indirect) heating has shown ease of automation and low maintenance rates, whereas also providing a steady state level of energy supply whilst processing and in the level of installation flexibility (Atkinson & Steel, n.d.). Showing that gas-fired furnaces on an industrial level, using electrical resistance heating is the best substitution (Lu et al., 2021). However, indirect resistance heating for electric furnaces is currently not available on an industrial scale yet for steam cracking processes, because of the importance of the temperature gradient in steam cracker furnaces for the value of the chemical yields. Developments regarding the industrial application are in progress currently, but not ready yet (C. Oliveira & Van Dril, 2021).

The integrated nature of Chemelot can cause other processes downstream to implement modifications due to electrification of the cracking furnaces reducing the demand for fuel gas for Chemelot. This by-product, however, can be used in other processes such as using it as a feedstock to generate blue hydrogen using methane reforming and a carbon capturing system. It could also cause problems downstream in the availability of steam due to heat recovery of by-products not being present and in turn causing an imbalance in the steam level. A different option for electrification might be implementing electrical driven compressors instead of the steam driven compressors. Doing this, the steam demand goes down in Chemelot, solving the issue partially (C. Oliveira & Van Dril, 2021).

For the cost analysis, it is assumed that Olefin 3/4 is electrified, without the electrification of the compressors, meaning that steam is still required. The estimated costs and potential are according to C. Oliveira & Van Dril (2021). Here it is shown that the electricity price is a very determinant factor in the investment potential of this technology, since the electricity demand for Chemelot increases, as well as its need for security of supply. Renewable electricity is especially required if significant amounts of CO_2 emission reductions are the goal. Generic electric furnaces in refinery sites have around 10MWth output. The table provided below provides the estimated costs if electric furnaces are implemented on Chemelot using a conversion rate of 0.7 of the output (919 MWth and 933 MWe input). Furthermore, the fixed Opex costs do not include the cost of electricity.

Chemelot imports around 7 PJ per year, or 2000 kt per year of high pressure steam. As mentioned above, it is possible to obtain this amount of steam through electrical boilers. The steam currently used has a temperature of 500 degrees, whereas the steam generated using electrical resistance does not exceed 350 degrees (Berenschot, 2017), meaning that new developments are required to reach this temperature. Furthermore, Lu et al. (2021) states that because of the fast response time of electrical boilers, its economic feasibility is heavily dependent on the availability of renewable electricity and the price of (renewable) electricity. Furthermore, steam turbines on the Chemelot site use the steam that is currently being imported to run compressors, and they have a key function for the entire steam chain. If Chemelot were to substitute these steam turbines for electrical turbines,

Sort	Value	Unit
CAPEX	3.5-5	$MEUR_{2018}$/MWth
Fixed OPEX	2	% CAPEX
CAPEX for SABIC	800-1200	$MEUR_{2018}$
Fixed OPEX for SABIC	17-24	$MEUR_{2018}$/yr

Table 9: CAPEX, OPEX and capacity for electrification of Olefin 3/4

the steam demand would decrease, but the supply would also be affected. The 7 PJ/y should be able to be delivered using electrical boilers, since they have a very high efficiency (nearly 99.9%) Berenschot (2017). The capacity of the electric boiler is estimated to be 222 MWe.

For the cost analysis of the implementation of the electric boiler, literature regarding an electrical boiler with a 70 MWe capacity and 99.9% efficiency is used and adjusted for a capacity of 222 MWe. The same 0.7 scaling factor has been used as previously and the electrical costs are not included in calculating the fixed OPEX. For the CAPEX, the equipment and costs of connecting the electricity are included. However, due to the costs being site dependent, they may vary.

Sort	Value	Unit
CAPEX	150-190	$kEUR_{2017}$/MWe
Fixed OPEX	1.1	$kEUR_{2017}$/MWe/yr
CAPEX for SABIC	24-30	$MEUR_{2017}$
Fixed OPEX for SABIC	0.17	$MEUR_{2017}$/yr

Table 10: CAPEX, OPEX and capacity for electric boilers

Bio-naphtha

This alternative fuel can be used as a fuel for the steam crackers if the bio-naphtha reaches certain specifications in terms of quality compared to normal naphtha using an upgrading process. For the steam crackers, little changes are expected, meaning that costs related to implementing bio-naphtha is mainly determined by the price of the feedstock (De Jong et al., 2015). The costs for implementing bio-naphtha are largely related to the price of feedstock, which changes per year and per scenario.

Methanol to olefin

This technology has appliances on an industrial scale in China on several locations , but not yet in Europe (A. M. Bazzanella & Ausfelder, 2017). Where normally fossil-based methanol is being used, research is being committed to developing sustainable methods for making methanol. One of the possible technologies is producing ethylene and propylene using methanol synthesized using captured CO_2 and green H_2. The H_2 would be produced using water electrolysis and coupled with the CO_2 and undergoing a methanol synthesis, ethylene and propylene can be produced. The heat demand for the methanol synthesis can be covered by the steam that is produced internally, making electricity the only external source required (Pérez-Fortes et al., 2016). However, following the methanol synthesis, producing ethylene and propylene requires additional heat which is supplied through importing steam (Jasper & El-Halwagi, 2015). So, for the implementation of this technique for Chemelot, a water electrolyzer and a methanol synthesizer are required, as well as a methanol to olefin processor.

The costs regarding these two investments are estimated using Pérez-Fortes et al. (2016) and Jasper & El-Halwagi (2015) where the fixed Opex value is the base for the CAPEX value and the costs do not include the energy costs or the cost of the feedstock.

Sort	Value	Unit
CAPEX	1.28	$MEUR_{2016}$/kt MeOH/yr
Fixed OPEX	0.07	$MEUR_{2016}$/kt MeOH/
Capacity	440	kt MeOH/yr

Table 11: CAPEX, OPEX and capacity for water electrolysis and methanol synthesis

Sort	Value	Unit
CAPEX	0.19	$MEUR_{2016}$/kt MeOH
Fixed OPEX	0.01	$MEUR_{2016}$/kt MeOH/yr
Capacity	1523	kt MeOH/yr

Table 12: CAPEX, OPEX and capacity for for methanol to olefins process

Hydrogen fueled steam cracking furnaces
This technology uses green H_2 instead of fuel gas as a fuel for the cracking process. Substituting natural gas or fuel gas with H_2 causes only water to be generated and thus reducing the CO_2 emitted. However, this is only if the H_2 is produced in a sustainable way, and thus it being green H_2. Some changes in the operations would be required in terms of the combustion and the burners to be capable of burning the H_2. Currently, barriers do exist in terms of efficiency of H_2 production using electrolysis (roughly 70% efficiency (Gil et al., 2015)) and the cost of electricity. Especially with the limited supply of renewable energy, which is required to produce the green H_2, prices might be even higher (Q. Zhu et al., 2022). In terms of properties, H_2 burns with a lower radiation heat transfer, has higher NOx concentration so technology is required for the abatement and replacing the steam cracking furnaces fuel with H_2 might cause a surplus of fuel gas on the Chemelot site. So, finding different applications for the surplus of the fuel gas also becomes an interesting part of this option. If combined with other technologies, pre-combustion carbon capture plus steam reforming of the fuel gas may result in enough supply of the H_2 required for this process.

The costs regarding this investment are estimated for a standard heating system using H_2 fuel combustion with a 10 MWth capacity as output. Within these costs, H_2 pipelines are included as well as compressors, adjustments needed to be made to the original installation, but does not include the costs for removing the excess NOx from the process. Furthermore, the costs only serve as a reference point. A similar thermal efficiency for the H_2 furnaces has been assumed compared to the conventional furnaces. So, as previously done, a scaling factor of 0.7 has been included for the calculations.

Sort	Value	Unit
CAPEX	0.5-1.5	$MEUR_{2017}$/MWth
Fixed OPEX	1	% CAPEX
CAPEX for Sabic	150-460	$MEUR_{2018}$
Fixed OPEX for Sabic	1.5-4.6	$MEUR_{2018}$/yr

Table 13: CAPEX, OPEX and capacity for hydrogen fueled steam cracking furnaces

Green hydrogen for ammonia production
This technology uses green H_2 produced by electrolysis of water instead of normal H_2. Here, the electrolyzer splits the water into H_2 and O_2. To implement this technology, compressors are required that compress the N and H_2 in a pressure area of 100-250 bar (A. Bazzanella & Ausfelder, 2017) and air separation units are needed. The emissions coming from producing the grey H_2 will be reduced when this technology is implemented. However, no large plants have used electrolysis to produce ammonia currently (Batool & Wetzels, 2019). This is mainly due to the efficiency rates of electrolysers and the higher energy consumption per mole of H_2 compared to steam reforming. Current ammonia synthesis installations can be used, but do require some adjustments to implement the new feed-ins coming from the compressor and the air separation unit before synthesis. OCI would require roughly 192 kt H_2 per year to produce the ammonia. The electricity demand in total (including compressors and air separation units) would be roughly 40.2 GJ/t ammonia. The ammonia production of the ammonia production units AFA 2/3 was combined 1081 kt in 2020. The OPEX costs exclude feedstock costs and is assumed to be 3% of the CAPEX (Batool & Wetzels, 2019).

Sort	Value	Unit
CAPEX for OCI	1438	$MEUR_{2017}$
Fixed OPEX for OCI	43	$MEUR_{2017}$/yr

Table 14: CAPEX, OPEX and capacity for green hydrogen for ammonia production

4.5 Concluding remarks

In conclusion, this chapter has first presented requirements for the case study, and then introduced the petrochemical site of Chemelot and the streams on site. After demarcating the area of Chemelot that will be considered for the model based on available data, CO_2 emissions and number of actors present, the exogenous factors that impact Chemelot were elaborated on. Furthermore, examples of large decarbonization projects for Chemelot were presented with the related CAPEX and OPEX. Furthermore, the configurations regarding these exogenous factors and the decarbonizing options have been highlighted.

Looking back at the requirements for the case study, it can be confirmed that Chemelot is a right fit for a case study. Firstly, Chemelot has multiple actors on site that all function with a high level of interconnectivity. Secondly, multiple decarbonizing investment options are available for Chemelot and can be implemented in the future. Thirdly, data is available regarding required input specifications and allows for effective modelling of Chemelot. The investment options presented will be used as structural variables in the upcoming model, whereas the exogenous factors will be implemented to first serve as the base for the scenario analysis performed later on. It is important to note that the investment options identified are not considered to be exogenous factors. By taking the identified exogenous factors from this chapter and their impact on Chemelot, the basis for SQ5 and SQ7 have been made.

The exogenous factors and the investment options presented and discussed in this chapter will be incorporated in the upcoming model. The investment options will serve as structural variables to guide as decarbonizing options for Chemelot, whereas the exogenous factors will be included to investigate how they change the investment behaviour of actors within Chemelot. The translation of those investment plans with the investment structures will be evaluated through the use of an optimization model.

5 Case study implementation

In this chapter the proposed method from earlier sections will be applied to demonstrate the influences of multiple exogenous factors on the optimal investment trajectories for Chemelot. The model that is used for this has been developed in Linny-R. This model will provide a proof of concept on the assessment of how exogenous factors and multiple investment options are influenced. chapter 5.1 will describe the Linny-R model that will be used and how it will be used. chapter 5.2 elaborates on the different modelling choices that have been made by providing the model of the industrial system of Chemelot. The assumptions that have been made and rationale are described here. In chapter 5.3, the modelling approach is presented, where the set-up of the experiment is explained and the different scenario approaches will be assessed to determine the influence on the system. Finally, chapter 5.4 will look at how the model is validated and verified.

5.1 Linny-R model and requirements

This chapter aims to create a model that allows for the evaluation of the investment trajectories of the system and the influence of exogenous factors on the investment behaviour using Linny-R. The model created is not a complete model of Chemelot with all real-time data, where the aim is to come up with new investments to decarbonize the cluster. Instead, the aim of the model is to serve as an example on how new insights can be gained on the effects of exogenous factors on the investment behaviour. Linny-R should not be used as a tool to predict investment decisions, but rather as a tool to test what the effect is of certain decisions or exogenous factors. The parts that are modeled in Linny-R have been showcased in figure 8. A description below is given on the data that is required for the model to operate correctly and what inputs are needed for the experiment. Furthermore, the relevant outputs and the overall process outline are also given.

The data requirements regarding the capacity and flow rates of different processes and financial parameters are necessary for the functioning of the Linny-R model to optimize the overall cash flow. The data has been derived from publicly published reports and other (grey) literature. Furthermore, regarding input concerning the exogenous factors and investment options, data is needed on the Capex and Opex of investments, costs of raw materials and profit margins. Products produced on Chemelot are mostly sold in mature markets, meaning that the market price is based on the supply and demand in said product. However, in reality, some products may not function in a mature market yet and the price is based on the price of the raw materials plus the fixed and variable costs plus a profit margin. This is mainly the case for H_2. Because H_2 follows such a price structure, the same methodology will be adopted to derive relevant H_2 prices when Chemelot would import it. This methodology is currently for grey H_2, however, as long as there is no benchmark price for H_2, it is argued by Martin (2021) that green and blue H_2 will follow this price structure at least early on. Furthermore, scenario parameters are required to create a final evaluation on the results of the model through iterations. It tests the robustness of the model and how credible the results and its conclusions are. All this data is used in Linny-R to maximize the cash flow of the total cluster. Linny-R will determine the maximum profitability of the system through optimal allocation of materials and by investing in the best options. The model will provide the optimal investment path given the exogenous factors and investment options. From these results, it can be assessed what the effect is of these exogenous factors on the investment behaviour.

5.2 Model input values

5.2.1 Data points of investment options

In chapter 3, the CAPEX and OPEX for several sustainable innovations for Chemelot are presented. Some simplifications are made to the different investment projects to include them into the model according to the literature from which they are retrieved. Here, an overview will be provided with the prices that will be used in the model for these innovations. Because some technologies have not reached technological maturity yet, the prices in this research are only an estimation of the real world. Significant cost reductions may occur in the future if they reach technological maturity.

Large processes such as processing Naptha into Ethylene and Propylene or making NH_3 are very complex and require multiple intermediary steps. These processes also differ per site in the configurations and how integrated they are per site. Calculating the mass balance and output for every individual step would cost large amounts of time, and the more detailed representation could impose complications due to its complexity. This would all result in only a more specific representation of the cash flows. Therefore, this over-complication of the model is considered unnecessary and a simplified representation of large processes is used for the model.

Technology	Capacity	CAPEX (MEUR)	OPEX (MEUR/year)
Post-CC	428 kt CO2/year	2003	2.9
Pre-CC	770 kt CO2/year	3465	5.8
Electrification of Olefin3/4	933 MWe	1000	20.5
Electric Boiler for steam	222 MWe	27	0.17
Water electrolyzer and methanol synthesis	440 kt MeOH/year	563	30.8
Methanol to olefin	1523 kt MeOH/year	289	15.23
Hydrogen fueled steam cracking furnace	300 MWth	305	3.05
Green hydrogen for ammonia production	1081 kt NH3/year	1438	43

Table 15: Total capacity, CAPEX and OPEX for investment options

Olefin 3/4

The Olefin 3/4 has been modelled as a single process using naphtha as input among others, from which Ethylene and Propylene is produced. Natural gas is used to power the Olefin 3/4, CO_2 is emitted and CH_4 is captured and reused. Integrating H_2 could allow Sabic to avoid emission costs, but it depends on the price of H_2 at that moment in time. The Ethylene and Propylene are not represented as a single output, because both products are further processed by the same or other actors into other products. This was possible due to provided data regarding the mass balances of each product. The processing of Ethylene and Propylene are represented in a simple way, since increasing the details on those processes would increase the complexity of the model without providing much more added value. The pricing of the intermediary and final products were established based on data points from (grey) literature. The inlet and outlet for the Olefin 3/4 are summarized in the table below:

Inlet	Upper bound value	Outlet	Upper bound value
Naphtha (ktons/y)	4000	Methane captured (ktons/y)	600
Electricity (PJ/y)	1	CO_2 emissions (ktons/y)	1700
Natural gas (ktons/y)	545	Ethylene (ktons/y)	1200
		Propylene (ktons/y)	700

Table 16: Inlet, outlet and upper bound values for Olefin 3/4 from C. Oliveira & Van Dril (2021)

Electrified Olefin 3/4

If the model chooses to invest in the electrification of the Olefin 3/4, the table changes. As elaborately explained in chapter 3.3.2, replacing the Olefin 3/4 technology to be able to produce without using fossil fuel as their main fuel results in an increase in electricity demand. Furthermore, it has been assumed that the ethylene and propylene production of the electrification technology is similar to the existing Olefin 3/4 production. As with the existing Olefin 3/4, simplifications to the process have been applied because of the scope of this research and because the importance of intermediary steps are of no influence to the overall investment behaviour of actors. Finally, it is also assumed that the electricity used to power the electrified Olefin 3/4 is renewable electricity, resulting in no CO_2 emissions coming from operating the technology. The inlet and outlet for the electrified Olefin 3/4 are summarized in the following table:

Inlet	Upper bound value	Outlet	Upper bound value
Naphtha (ktons/y)	4000	Methane captured (ktons/y)	600
Electricity (PJ/y)	7	Ethylene (ktons/y)	1200
		Propylene (ktons/y)	700

Table 17: Inlet, outlet and upper bound values for electrified Olefin 3/4 from C. Oliveira & Van Dril (2021)

Methanol to Olefin

A third option to replace the current capacity of the Olefin 3/4, or to expand it, is to introduce the Methanol to Olefin producing technology. Although it is a young technology, it is interesting to look at how and when the technology will become interesting for industrial clusters to invest in. The largest difference is that it uses CO_2 and H_2 to produce the ethylene and propylene, without using any fossil fuels or naphtha as a raw material. The required investments for this technology have been combined and simplified to ease the implementation in the model without compromising any useful information output. The inlet and outlet for the methanol to olefin investment are summarized in the following table:

Inlet	Upper bound value	Outlet	Upper bound value
Electricity (PJ/y)	6,5	Ethylene (ktons/y)	213.22
Hydrogen (ktons/y)	3046	Propylene (ktons/y)	380.75
CO_2 (ktons/y)	2224		

Table 18: Inlet, outlet and upper bound values for methanol to olefin from C. Oliveira & Van Dril (2021)

Hydrogen fueled steam cracking furnace

Instead of trying to remove CO_2 from the production process, efforts can be put into removing CO_2 by moving towards more sustainable fuel sources. The hydrogen fueled steam cracking furnace allows for the energy demand of the Olefin 3/4 to be covered by making use of green H_2 as a source to get the steam up to temperature. With this technology, the naphtha and electricity demand stay the same, only the natural gas demand changes. The inlet and outlet for the hydrogen fueled steam cracking furnace investment are summarized in the following table:

Inlet	Upper bound value	Outlet	Upper bound value
Hydrogen (ktons/y)	259	Energy demand	Total

Table 19: Inlet, outlet and upper bound values for the hydrogen fueled steam cracking furnace from C. Oliveira & Van Dril (2021)

AFA 2/3

Producing NH_3 requires natural gas, air and water, and CO_2 is emitted into the air. In reality, this process requires intermediary steps and differs per site in its configurations and its level of integration. Calculating the mass balance and output for every individual step would cost large amounts of time, but the more detailed representation would not add value to the outcome of the model, it would only increase the complexity and the chance for errors to occur. Therefore, a simplified representation of this large process is used in this model, where the AFA 2/3 is represented as a single process using natural gas, air and water as an input to produce NH_3. The NH_3 is then either sold as NH_3, or further processed into either Acrylonitrile or Stanyl through the addition of Propylene. The pricing of CO_2, NH_3, Acrylonitrile and Stanyl have been established based on data points from (grey) literature. The inlet and outlet for the AFA 2/3 are summarized in the table below:

Inlet	Upper bound value	Outlet	Upper bound value
Natural gas (ktons/y)	827.4	NH_3 (ktons/y)	1184
Electricity (PJ/y)	0.3	high purity CO_2 emissions (ktons/y)	1400
Water (ktons/y)	1468	low purity CO_2 emissions (ktons/y)	800
Air (ktons/y)	1492		

Table 20: Inlet, outlet and upper bound values for AFA 2/3

Green hydrogen for ammonia production

The model can choose to start producing NH_3 by making use of green H_2 as described in chapter 3.3.2, if prices of fuel and feedstock rise in the future. By using an electrolyzer to produce green H_2, the only inlets for this technique would be water and electricity. With no emissions coming from this technology, it becomes an interesting investment in certain scenarios. Simplifications have been applied to this process because of the scope of this research and because the importance of intermediary steps are of no influence to the overall investment behaviour of actors. Finally, it is also assumed that the electricity used to power the electrolyzer and green H_2 to NH_3 plant is renewable electricity. The inlet and outlet for the green hydrogen for ammonia production are summarized in the following table:

Inlet	Upper bound value	Outlet	Upper bound value
Water (ktons/y)	1852	NH_3 (ktons/y)	1184
Electricity (PJ/y)	4.6		

Table 21: Inlet, outlet and upper bound values for green hydrogen for ammonia production

5.2.2 Data points of commodities and finished products

Predicting how 2050 will look like is impossible, even educated guesses based on historical trends have been proven to be inaccurate in cases such as with the gas price increase due to the war in Ukraine. The uncertainty regarding the developments of commodity prices, fuel prices and raw materials heavily influence the potential investment behaviour of companies. For the model, base values for commodities will be used as well as for intermediary and finished products. By adjusting the price of a single commodity at a time, or an identified exogenous factor from the previous sections, to either a low, medium or high value, new scenarios will arise. From these scenarios, the effect of a single exogenous factor on the investment behaviour of the cluster can be quantified and analyzed. From this, insights can be derived as well on how actors within Chemelot should react when such exogenous factors would occur.
The prices of commodities like electricity, naphtha, CO_2 and natural gas are derived from reports by the International Energy Agency, literature such as Zhou et al. (2022) and other public reports and (grey) literature. Factors such as availability, geopolitical issues and other large fluctuations may influence the price of commodities (Zhou et al., 2022; IEA, 2019), but since the time span in which the model will be simulated is 30 years, large fluctuations will be not taken into consideration. Below is a table provided with an overview of the commodity prices going from 2020 to 2050. In the model, the price range is integrated per year instead of per 10 years as shown in the table. Because the model uses an input of Kiloton (kt), the prices will be adjusted to €/kt instead of their original form. This can lead to small variations in the price used in this research compared to the actual price, but this should have little influence on the outcome of the model.

Commodity	unit	2020	2030	2040	2050
Natural Gas	MEUR/kton	€0.264	€0.270	€0.277	€0.283
Electricity	MEUR/PJ	€18.3	€21.9	€25.5	€29.1
Naphtha	MEUR/kton	€0.442	€0.588	€0.734	€0.88
Hydrogen	MEUR/kton	€0.6	€0.43	€0.27	€0.11
CO_2 emissions	MEUR/kton	€0,03	€0.073	€0.117	€0.16
CO_2 transport and storage	MEUR/kton	€0.0225	€0.0225	€0.0225	€0.0225
NH_3	MEUR/kton	€1.3	€1.083	€0.87	€0.65
Water	MEUR/kt	€0.000391	€0.000461	€0.00054	€0.00064

Table 22: Table with base values of commodities. Data derived from (Consortium, 2019; IEA, 2019, 2018; Zhou et al., 2022; Kleefkens, 2017; Energie-Nederland, 2022)

The price of the finished products is difficult to predict as well. Because the price of the products depends on the price of raw materials, fossil-fuels and the willingness of customers to pay. Therefore, the price of the finished products have been determined using the current price, taking a linear increase in the price until 2050. The linear increase is based on historical price data combined with historical data on inflation to make it as realistic as possible. Furthermore, small adjustments may be applied to ensure good working of the model. Given below is a table with the prices for 2020 to 2050 with the linear increase as formulated. Variations in these prices may occur due to unforeseen circumstances such as the impact of the war in Ukraine has on the price of fossil-fuels. However, these kind of outliers have always been present in the past and most likely do not influence the investment behaviour of companies on a long term.

Finished product	unit	Price 2020	Price 2030	Price 2040	Price 2050
Ethylene export	MEUR/kt	€1.5	€1.77	€2.08	€2.46
LDPE	MEUR/kt	€1.2	€1.41	€1.67	€1.97
HDPE	MEUR/kt	€1.21	€1.43	€1.69	€1.99
UHMWPE	MEUR/kt	€1.75	€2.06	€2.43	€2.87
Plastomers	MEUR/kt	€2.5	€2.95	€3.47	€4.09
Elastomers	MEUR/kt	€1.2	€1.42	€1.67	€1.97
Polypropene	MEUR/kt	€1.49	€1.71	€1.98	€2.30
Acrylonitrile	MEUR/kt	€2	€2.36	€2.78	€3.28
Stanyl	MEUR/kt	€1.5	€1.77	€2.08	€2.46

Table 23: Table with data finished products produced on Chemelot site

5.2.3 Model and setup of the experiments

In this section, six experiments will be performed with the model to test the hypotheses formulated in chapter 3.4, and to gain insights on the effects of exogenous factors on the investment behaviours. The first two experiments will have a similar model, but differ in the costs of investments having to be paid upfront or paid over time, as discussed in chapter 4.2.2. The second two experiments will analyze the effect of having full knowledge of future prices has compared to only having limited knowledge, where having limited knowledge is defined in this research as giving the model a look ahead of 4. The last two experiments will determine which form of Co_2 reducing policy stimulates investing more and generates more cash flow. The model is set to analyse the influence of the exogenous factors over a time horizon of 30 years, therefore, a time step of 1 year per step is implemented into the model. Smaller time steps would increase the complexity of the model and thus also the computation time, as well as extra input variables being needed such as start-up and shut-down of processes to become more accurate. This choice is further reflected on in chapter 6. By performing the experiments, the hypotheses that allowing to pay for an investment over time promotes investment behaviour will be tested, that the data points are integrated correctly and that the model works accordingly. Furthermore, preliminary insights on the effect of having full knowledge of future prices are gained. Having proven that the model works accordingly, it can serve as a representation of Chemelot to perform other analyses in chapter 6. With the final model, two objectives will be achieved: The model will provide as a proof of concept for the methodology created to represent exogenous factors in MILP models and to provide insights on the influence of exogenous factors on the investment behaviour of multiple actors in an industrial cluster under different scenarios. Below is the model that is used for both the experiments and for the results in chapter 6.

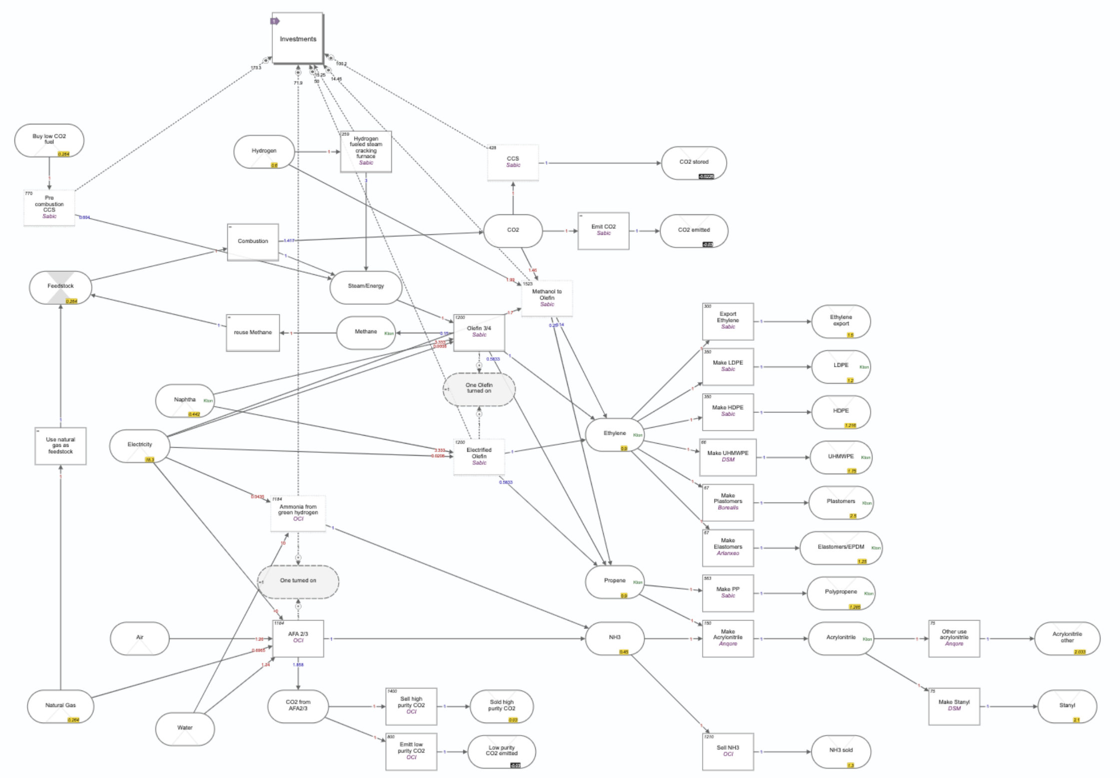

Figure 17: Linny-R model of Chemelot

After having performed the experiments, two forms of analysis will be carried out in chapter 6 to identify the effects of exogenous factors on the investment behaviour and to generate optimal investment trajectories. These will be carried out by adjusting the model and simulating the 30 years again. First, prices of commodities will be adjusted to a very high and very low value to determine the impact it has on the system. This sensitivity analysis will allow for identification of how the exogenous factors influence Chemelot. Then, three scenarios will be established. The scenarios that have been established, are realistic in terms of price increase and decrease of various commodities and will function as a proof of concept for the methodology to not only investigate the effect of exogenous factors on the investment behaviour, but also determine optimal investment trajectories given the demarcated system and data input. This excludes extreme values from the scenarios such as free electricity, the demand for the finished goods plummeting suddenly or CO_2 price becoming cheaper. The table below gives the price increases that have been implemented per commodity to determine the effect they have on Chemelot. Only 1 variable is changed per simulation, the rest of the variables stay the same.

Commodity changed	**First simulation price change**	**Second simulation price change**
CO_2 price	Multiplied by 100	Divided by 100
Naphtha price	Multiplied by 100	Divided by 100
Electricity price	Multiplied by 100	Divided by 100
Natural gas	Multiplied by 100	Divided by 100
Finished products price	Multiplied by 100	Divided by 100

Table 24: Data input changes per scenario

The results coming from the experiments are unrealistic in terms of cash flow, but they magnify the effects changing a single commodity has on Chemelot. This allows to identify and quantify the effects of these changes, and also insights can be gained on how resilient Chemelot is to certain changes. After having performed this analysis, it is now important to determine optimal investment trajectories for Chemelot in realistic scenarios. The scenarios that have been established, are realistic in terms of price increase and decrease of various commodities and will function as a proof of concept for the methodology to not only investigate the effect of exogenous factors on the investment behaviour, but also determine optimal investment trajectories given the demarcated system and data input. This excludes extreme values from the scenarios such as free electricity, the demand for the finished goods plummeting suddenly or CO_2 price becoming cheaper. The first scenario focuses on an increase in the commodities, mainly to reduce the emissions, but also to represent inflation in the coming years. The second scenario represent a scenario where the focus is on decarbonization by making electricity cheaper and increasing the prices of other commodities. The third scenario is focused on economic profit, where the prices of all commodities are lowered to create more cash. Below is a table given with the increase or decrease per commodity.

Commodity	**Scenario 1**	**Scenario 2**	**Scenario 3**
CO_2 price	+50%	+100%	+20%
Naphtha price	+15%	+30%	-5%
Electricity price	+20%	-20%	-15%
Natural gas	+30%	+60%	-10%
Finished products price	+5%	+10%	-10%

Table 25: Data input changes per scenario

5.3 Influence of investment strategy and knowledge of future prices

Lack of available funds is an exogenous factor influencing innovation possibilities. It is a very broad term and can relate to not having enough cash at the moment, but also not being able to liquidate certain assets to generate the cash in a fast enough way. To overcome this and to implement it in the model, a representation has been developed in chapter 3.2.2 which allows for paying for an investment over time. This will allow for the model to invest in a certain investment without having to pay all of the costs at once. Two separate experiments will be performed using the final model, to quantify and compare the effects of direct-pay investments and pay-over-time investments. The first experiment will force actors to pay all costs immediately if they want to make an investment, both with and without knowledge of future prices. The second experiment allows actors to pay for the investment over a time span of 20 years, also both with and without knowledge of future prices. In total, there will be 4 simulations that will be run. By implementing all investment options provided in chapter 3.2.2, and making a comparison between the two experiments, the effects can be quantified. Furthermore, for the analysis, the following parameters will serve as the basis: cash flow, investment curve and CO_2 levels. Both simulations will have the same prices, same investment options and same model configurations.

5.3.1 Effects of direct-pay and pay-over-time

By using the model represented in figure 18 and the data points from table 22 and 23, the two different simulations have been performed to show the effects of direct-pay and pay-over-time. The results of the simulations are provided in the figures below.

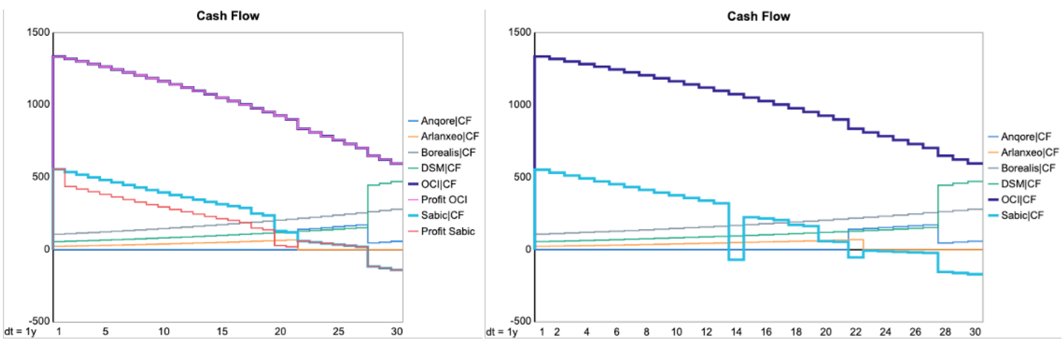

Figure 18: Cash flow per actor of the pay-over-time structure (left) and direct pay (right)

Looking at the individual cash flows and comparing them, it can be seen that Sabic makes an investment in a very early time step. Having the possibility to pay for investments over time opens up the possibility to invest in more expensive technologies that can reduce emissions more drastically and increase profits. The difference in profits are shown in the figure below.

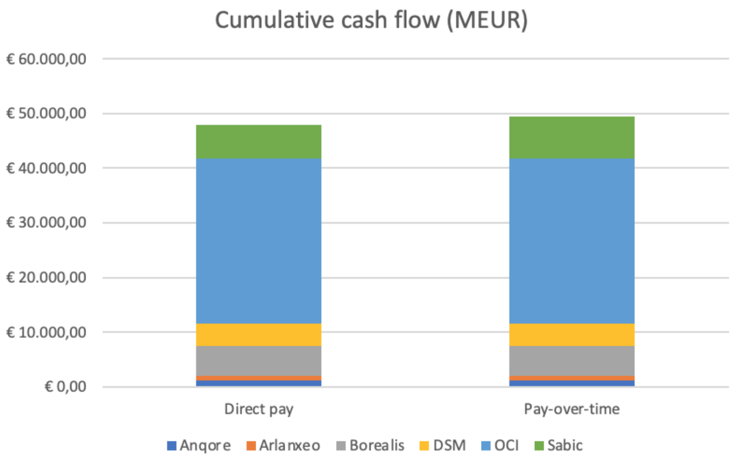

Figure 19: Cumulative cash flow of the direct pay and pay-over-time investment structure

The pay-over-time investment structure has a higher cumulative cash flow of €1533 MEUR, which is quite the difference, even on a 30 year basis. This aligns with the previous statement made that the pay-over-time investment structure increases profits. The increase of the profits is caused because an investment can be made in a more superior technology to cut costs for individual actors, but also for the total cluster. By looking at the investment curve in the figure below, more can be learned on the investments that have been made.

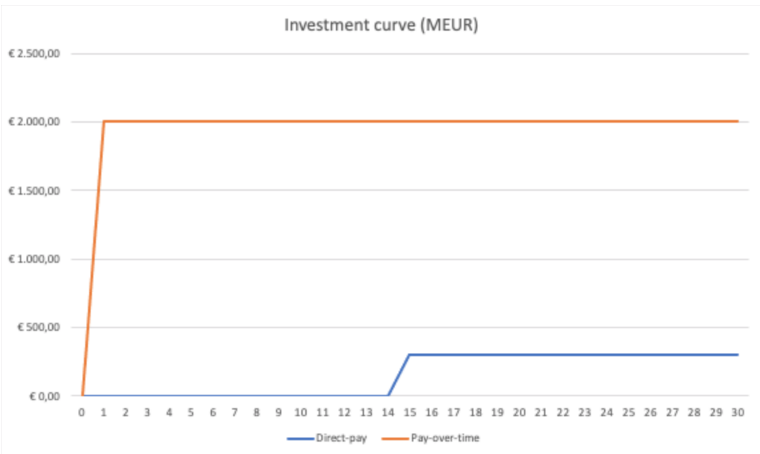

Figure 20: Investment curve over time

The investment curve shows that the pay-over-time investment strategy not only accelerates investments, but also increases the amount of money invested. If we compare the money spent with the investment technologies provided in chapter 5.2.1, it can be seen that the pay-over-time structure invests in Post-CCS in the first time step, whereas, the direct-pay structure invests in the hydrogen fueled steam cracking furnace at time step 15. So, not only is the investment made far later, but also the amount invested is significantly lower and a different investment has been made. The different investment structures also have an impact on the amount of CO_2 emitted. The different investments made reduce the CO_2 emissions by a different level, the Post-CCS is able to reduce the CO_2 emissions more than the hydrogen fueled steam cracking furnace. This means that the simulation that invests in this technology will have a lower total emitted. This can also be seen in the figure below.

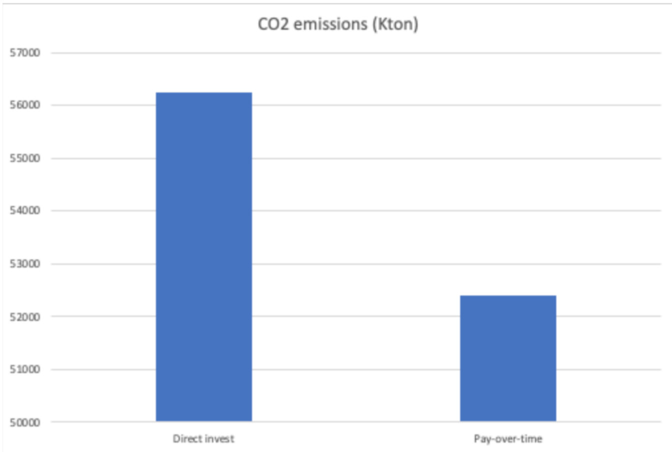

Figure 21: CO_2 emissions comparison of the pay-over-time structure and direct pay

By looking at all the results, an interesting trend can be spotted. If actors are allowed to pay for their investments over time, more money is invested in more sustainable options. This is in line with literature found and interviews held that few companies have the available assets to make an investment of a few hundred million euros. In the real world, investments are often performed by making use of subsidies and loans, meaning that actors and clusters that have more available assets allows them to invest more and in better technologies. So, the investment strategy makes a difference in when an investment will be made, how much money invested, the type of technology, the amount of CO_2 emitted and the amount of profit made.
Now, the second experiment to determine the effect of having full knowledge of prices versus only limited knowledge of prices on the investment behaviour of actors and clusters.

5.3.2 Effects of full knowledge versus limited knowledge

Having full knowledge of what the prices will do in the future is not a realistic scenario for industrial clusters, but it does allow for interesting insights to be gained, such as the effect it has on cash flow, emissions and investments made. Here, the remaining two experiments will be performed using the model provided in figure 18, where the only difference between the two experiments is the amount of knowledge they have of future prices. The first experiment will have full knowledge of the future prices, whereas the second experiment will have a look ahead of 4, meaning that it can look 4 years into the future in terms of prices and capacity. In reality, large amounts of resources and efforts are put into the forecasting of future prices, and for this research it has been determined that the look ahead will be set on 4. This value does give new and interesting figures compared to having no knowledge, and it still remains realistic because some companies do have very good predicting capabilities. The results of the two experiments are compared with the results of the investment strategies as well to show the full effect of having full knowledge versus limited knowledge under different investment strategies. The results of the two simulations are provided in the figures below.
By looking at the overall cash flow, for both investment strategies, two things stand out. Firstly, the previous statement that the pay-over-time investment strategy generates more cash flow is confirmed again. For both the pay-over-time simulations, a higher cash flow is generated than the direct pay simulations. Secondly, under both investment strategies, the simulation with full knowledge generated a higher cash flow. The increase in cash flow is caused because the model can better determine the amount of products to be produced in the long term. This can also be seen in the figure below.
Where the pay-over-time with full knowledge of future prices does produce substantially more than the other

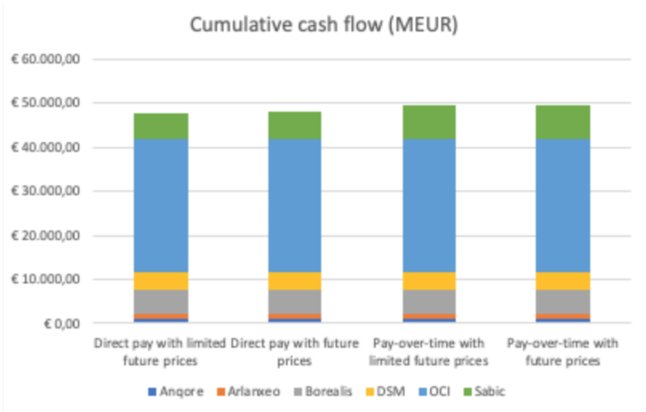

Figure 22: Cash flow comparison of the pay-over-time structure and direct pay with and without future knowledge of prices

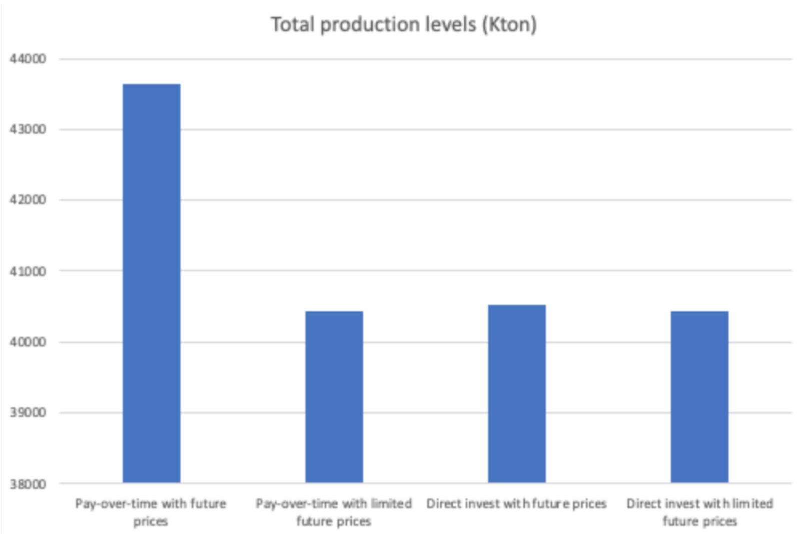

Figure 23: Production levels comparison of the pay-over-time structure and direct pay with and without future knowledge of prices

simulations, nearly 10% more, it does also show that the direct pay with full knowledge of future prices produces a small amount more than the simulations with limited knowledge. What is interesting to see, is that the investment strategy does not influence the production levels, since the pay-over-time and direct pay both with a look ahead of 4 produce the exact same amount. In trying to analyze the difference in cash flow, the investment curve must be investigated. This is presented in the figure below.

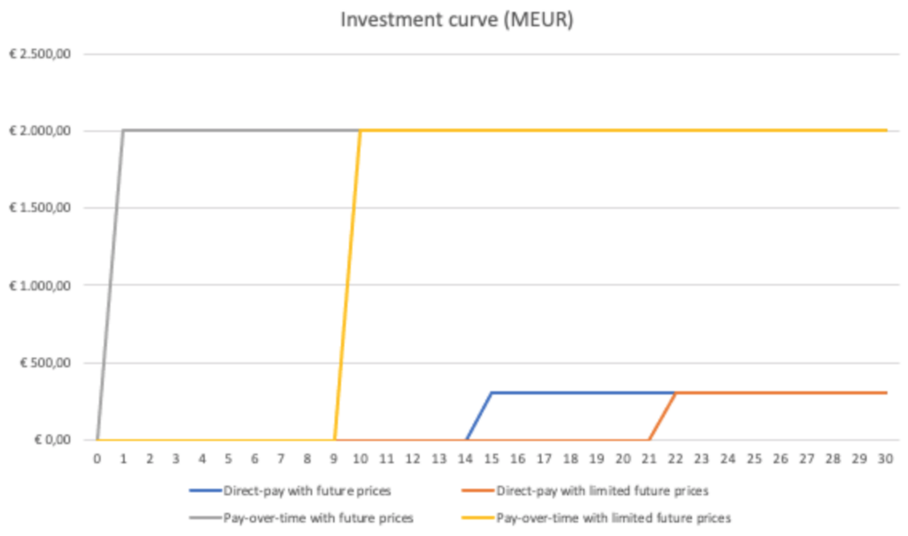

Figure 24: Investment curve of the pay-over-time structure and direct pay with and without future knowledge of prices

The figure shows that having full knowledge accelerates the time step in which the model will invest. Or, by arguing the other way, if the model has limited knowledge of future prices and capacity, it will invest in technologies at a later point. Meaning, that if the look ahead is very low or even 0, it can cause the model to even not invest in a technology. This is quite obvious, because having full knowledge allows the model to calculate the amount of cash flow the cluster will make, and based on that it can determine whether the investment will be profitable in the long-term or not. The knowledge removes the risk of losing money on an investment. Finally, having full knowledge also influences the CO_2 emissions, which can be seen in the figure below

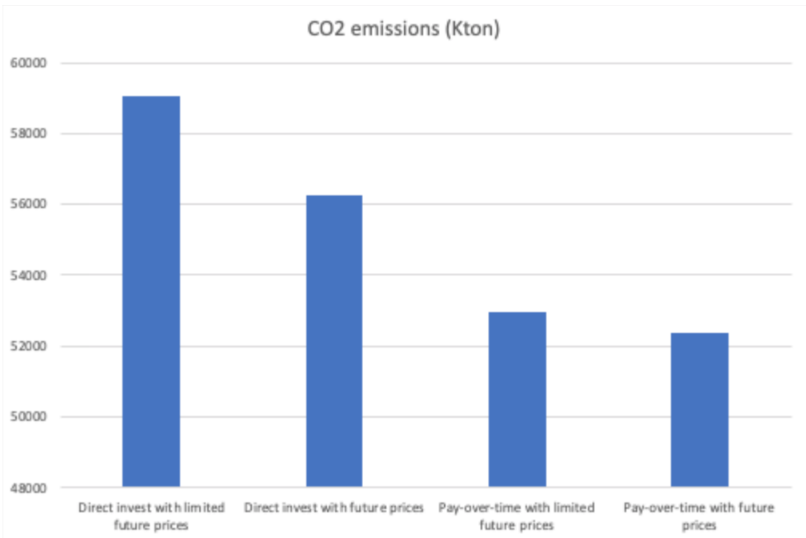

Figure 25: CO_2 emissions comparison of the pay-over-time structure and direct pay with and without future knowledge of prices

This shows that both the investment strategy, and the amount of knowledge influences the amount of CO_2 emissions. This is the consequence of the model being able to invest into a CO_2 emission reducing technology at an earlier time step, and that it is able to invest more. Having full knowledge of future prices is an unrealistic scenario, but the scenario does give insights on how clusters should or could behave if the risk is totally removed from the equation.

5.3.3 Effects of CO_2 cap versus CO_2 price

For the final experiment, the influence of a CO_2 cap versus a price put on CO_2 is analyzed. Currently, companies within the industrial sector have a CO_2 cap, but can exceed that cap by paying for emission certificates. Using the model provided in figure 18, two experiments have been performed with 2 simulations each. The first experiment has a CO_2 cap being implemented where each actor is allowed to emit 1400 Kton of CO2 in time step 0, and 0 Kton in time step 30. The second experiment has instead a CO_2 price implemented and no cap imposed on the emissions. Furthermore, every experiment is performed with full knowledge and limited knowledge, to further quantify the effects of the CO_2 cap versus CO_2 price, but also to look at the influence that knowledge has in this situation. By looking at the cash flow first, a large difference can be seen between the CO_2 cap and the CO_2 price in the figure below.

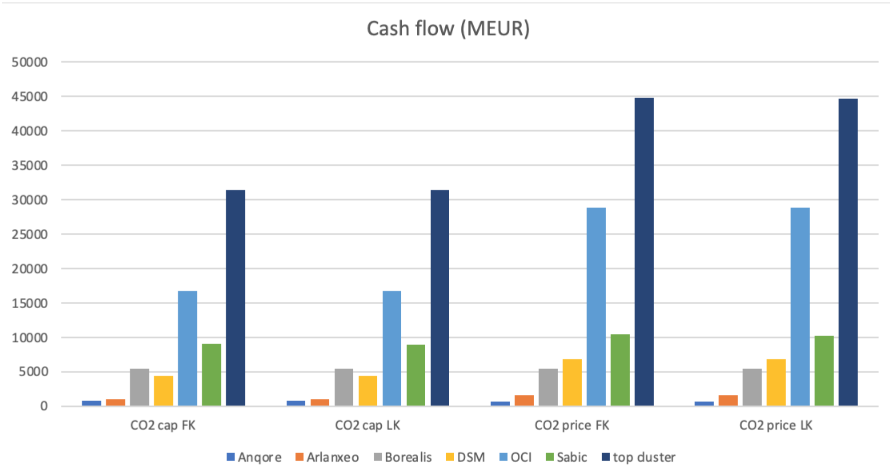

Figure 26: Cash flow comparison between the CO_2 cap and CO_2 price experiments

By capping the amount of CO_2 that can be emitted, the cluster needs to invest in CO_2 reducing technologies. The CCS alone is not enough to remove all CO_2 from the cluster, therefore, it has to reduce its production. However, reducing the production jeopardizes the cash flow of the cluster. This leads to new investments being made in CO_2 removing technologies such that production can be up-scaled again to remain profitable. This is also clearly visible in the investment curve below.

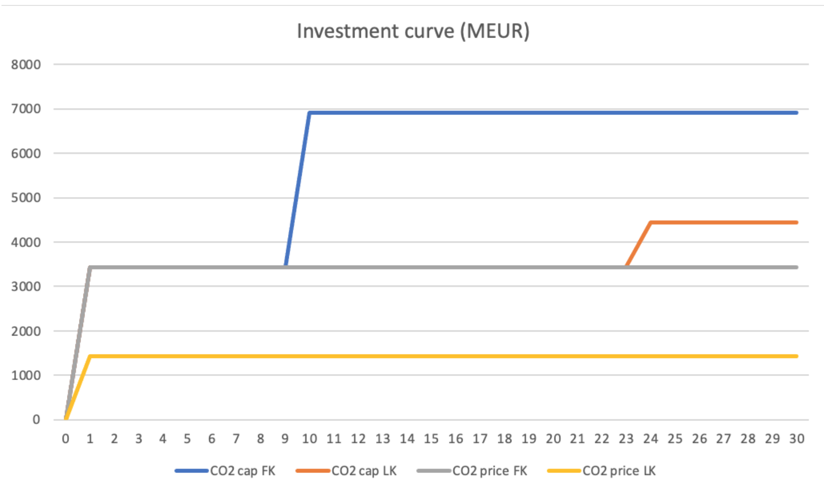

Figure 27: Investment curves for the CO_2 cap and CO_2 price experiments

The curve shows a clear difference in money invested in technologies between the CO_2 cap experiments and the CO_2 price experiments. the CO_2 cap does promote investment behaviour, but it comes at the cost of large amounts of cash. So, it becomes questionable what is a more efficient strategy to push the industrial sector towards CO_2 neutrality whilst also remaining profitable. The figure below shows the emission levels.

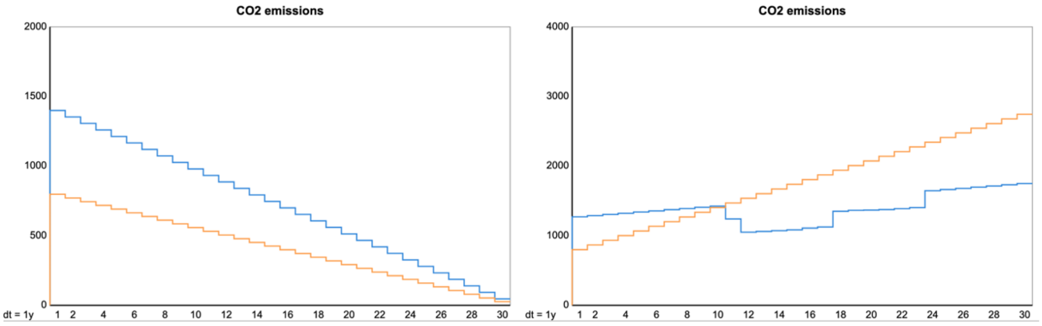

Figure 28: Emissions comparison between the CO_2 cap and CO_2 price experiments

The figure clearly shows that a CO_2 cap effectively reduces the cluster towards CO_2 neutrality. Whereas, the CO_2 price just forces the cluster to pay for the emissions and only reduce their emission levels when the price of CO_2 becomes too high. For the sake of this research, cash flow is still the most important measurement since staying profitable for industrial clusters is the most important thing. CO_2 emissions reduction is also an important aspect, but if making the investments causes the cluster to not be profitable anymore, the investments will not be made. So, this shows that putting a price on CO_2 allows the model to have a higher production level, which in turn generates a higher cash flow. More investments are realized under a CO_2 cap, however, this does compromise the cash flow with significant amounts. Therefore, it is decided to move onward with the CO_2 price. By looking at the difference between the models with limited knowledge and with full knowledge, a clear difference can be noted in the investment behaviour, which translates to a difference in cash flow. The difference in investment behaviour is because the model can determine the optimal investment trajectory when it has full knowledge, whereas, with limited knowledge, the model has to determine based on 4 years of information whether the investment is profitable. Finally, for the experiment with a CO_2 price implemented, the model with full knowledge has less emissions than the model with limited knowledge, due to the investment behaviour. The difference can be seen below.

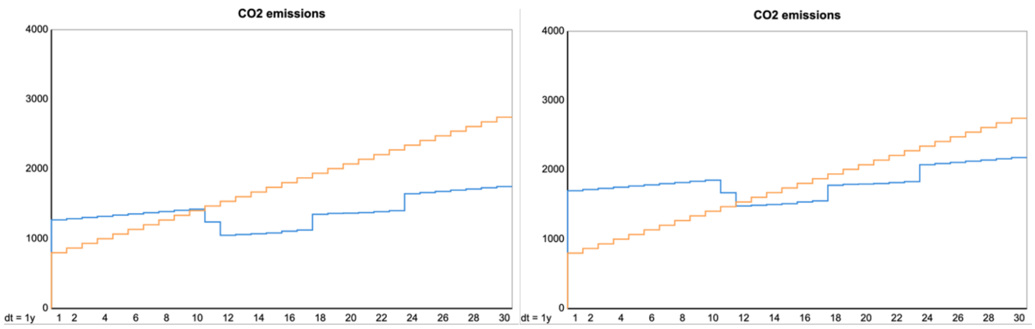

Figure 29: Emissions comparison between the full knowledge (left) and limited knowledge (right) CO_2 price experiments

5.4 Verification of the investment model

Having provided the different implementation steps for the model, it should be noted that there is always room for human error. Therefore, the verification of the model is needed to make sure that it is correctly implemented. Testing the model with a benchmark or a similar model is not possible since no other model with the same scope and inputs such as the model in this research has been developed. However, what can be done is to verify the model by isolating and investigating certain inputs and outputs of the components in the model. The verification is performed by first making sure all the steps that have been implemented are carefully checked and all the input parameters in every step of the calculations are cross referenced with the results. Then, the calculations will be performed and will be cross referenced with the values implemented in the model. Finally, the model will be tested for very high and very low input values, to check whether its performance and robustness is up to par with the expected behaviour of the implemented model.

5.4.1 Implementation steps check

Whilst looking at all the steps of the calculations performed, all the parameters in the model are carefully inspected. Especially looking at the mass balances of the processes and investments that are implemented into the model, extra attention has been devoted to making sure that the calculations are correct, that they are correctly implemented into the model and that all the inputs are consistent with each other. Processes such as Olefin 3/4 and AFA 2/3 have been carefully inspected to make sure that the balances of all the inputs and outputs are correct, with the correct values of those inputs and outputs. Furthermore, the investment costs, investment structure and mass balances have also been carefully inspected, making sure that the model can choose for those options, resulting in a potential higher cash flow. This also means that the model is able to compare the prices of different commodities and make a decision based on that comparison. All of the above is then tested through multiple checks that have been performed in the model. Finally, no large obstacles or implications have been discovered whilst checking the steps above.

5.4.2 Model checks

The model checks are then performed by making isolated calculations of simple steps with different parameters implemented in the model, which are then cross referenced with the outputs of the model. Below is an overview of the model checks that have been performed as a verification step.

Model check	Description	Performed	Results
Investment costs payed over time	The investment costs will be first charged when it is turned on for the first time. After this, the debt will be payed of over 20 years. Turning the option on or off should have no effect on the debt	Yes	Correct implementation of the investment cost structure.
Commodity price comparison	The prices of different commodities should be monitored by the model to optimize the cash flow for every time step	Yes	Correct implementation of variable prices for commodities.
Multiple investments	The model perceives different investment options to maximize the cash flow for ever time step using the investments.	Yes	Correct implementation of multiple investments which can be turned on.

Table 26: Data derived from (IEA, 2018; Consortium, 2019; IEA, 2019)

5.4.3 High and low input values

As with previous verification steps performed in this research, extremely high and low input values will be implemented again to test the robustness of the model. This will verify that the model works exactly like it should, even with the newly implemented investment structures. This step is similar to the ones performed in chapter 3.3 and 3.4, however, adding the actual values of the current situation, future prices and implementing multiple investments at the same time is where the verification steps differ. So, adjustments to commodity prices, as well as investment costs to very high or very low values will be performed, which are then compared to the results that are expected to be gained from the model. Table 20 and table 21 shows the price adjustments, the value to which they are adjusted, the expected outcome and whether the expected outcome matches the actual outcome.

Variable changed	Low value results	High value results	Verification
Natural gas	Large profits achieved by using natural gas instead of alternatives. Pre-CCS and Post-CCS investments can still be made	Model invests in alternatives because of higher profitability.	Matching results
Electricity	Electric investments become interesting because of low electricity costs, resulting in low amount of fossil-fuel used and CO_2 emitted	The high electricity demand of electric investments are unattractive because of the commodity price. H_2 powered investments can still be made if the H_2 is imported.	Matching results
Naphtha	Large profits are realized because margins increase drastically. All investments remain their attractiveness due to no change in other commodities	Because Olefin 3/4 is always forced to produce, extremely large losses are incurred. If the process could be turned off, it would be turned off	Matching results
Hydrogen	Importing H_2 becomes very attractive, due to low costs and reduced CO_2 emissions. Investments in processes that use H_2 will be made	The high H_2 prices cause investments in an electrolyzer to be made, making processes that use H_2 still viable	Matching results
CO_2 emissions	Because emitting CO_2 has low cost associated, little investments are made in processes that reduce the emissions. Storage is also unattractive because of the lower emission costs.	Sustainable investments are made as well as investments in CCS due to high costs associated with the CO_2 emissions.	Matching results
CO_2 storage	Storage becomes attractive, and because the CO_2 costs are increasing, the model will opt for either pre-CCS or post-CCS.	Storage is very unattractive due to being more expensive than emitting CO_2. Other investments remain their attractiveness and can still be opted for.	Matching results
NH_3	Having a low value on NH_3 causes OCI to make large losses, and companies that use NH_3 as a feedstock will incur large profits.	The high value of NH_3 provides OCI with large profits, companies using NH_3 as a feedstock make large losses.	Matching results

Table 27: Commodity verification results

Investment costs changed	Low value results	High value results	Verification
Post-combustion carbon capture	Favourable to make investment, reduces CO_2 emissions and associated costs	Unfavourable to make investment, cost associated with emitting CO_2 is cheaper alternative.	Matching results
Pre-combustion carbon capture	Favourable to make investment, reduces CO_2 emissions and associated costs	Unfavourable to make investment, cost associated with emitting CO_2 is cheaper alternative.	Matching results
Electrification of Olefin 3/4	A low investment cost makes the technology interesting. The increased electricity demand combined with electricity price can cause losses when invested, however, it will most likely choose to invest.	The high costs make the investment unfavourable, combined with the increased demand and electricity price will cause large losses, so model will not invest	Matching results
Methanol to olefin	Low investment costs make producing Ethylene and Propylene using Methanol interesting. It does depend on the costs of the feedstock whether the model will opt for the investment. However, with the costs very low, the model will invest in it	The combination of very high investment costs with the commodity prices in place cause the model not to invest in the Methanol to olefin, but rather keep producing as it was doing already	Matching results
Hydrogen fueled steam cracking furnace	The technology is dependent on the price of H_2, even with low investment costs, the commodity price is leading in the decision making on the technology. Model will not invest	With higher investment costs, and the dependency on the price of H_2, the model will not invest with current prices.	Matching results
Green hydrogen for ammonia production	Low costs make the investment interesting, but the overall profits are dependent on the price of electricity and H_2. Because of those prices, the model will not invest in the technology.	The high costs make the investment uninteresting, combined with the prices for electricity and H_2 results in no investment being made by the model	Matching results

Table 28: Investment verification results

5.5 Validation

Validating the model for the exogenous factor refers to assessing the degree to which the model with its implemented data and connections is able to accurately model the dynamics of a real world cluster (Cook & Skinner, 2005). A large part of the data that would be required to compare the output of the model with real life results is classified, such as real-time price of finished products and location-related profits. However, through the use of collaborative reports and an expert, the inputs of the model can be validated to which extend they are accurate. Normally, the more complex a model is, the larger the possibility for errors. When implementing multiple data points into a model for a single input, the risk for faults and inaccuracies increase. For the model in this research, the inputs that are subject to these kinds of risk are the prices related to feedstock, finished products and investments. These inputs are validated by making use of reports that have been established through collaboration of multiple companies situated in the selected industrial cluster. Because the reports and literature have been published in collaboration with multiple actors situated on Chemelot, they are considered to be accurate. These have then been cross-referenced with other data sources that provide insights on prices in the past and literature that provide predictions on future prices. More specifically, the value of CO_2 and H_2 for example are obtained and benchmarked against other predictions and projections from multiple sources, providing extra insights on how to set the value for these in the model. Furthermore, some inputs require manipulation to adhere with the model, this also increases the risk of the output being inaccurate. Examples of this are prices of certain feedstocks that are highly volatile such as electricity and naphtha and literature falls short in its projections. Through linear extrapolation from historical data found, the calculations are validated. Finally, with the use of an expert, the developed model has been validated by investigating the interconnections of the actors, degree of reaction to certain exogenous factors and demands for different actors. From this validation round with the expert, suggestions on extrapolating the prices of finished products and implementing of additional electricity demands for all actors have been included, completing the validation round.

Having validated the inputs for the model does not guarantee that the outputs will also be validated, however, the risks of inaccuracies and outliers in the output are lowered significantly. Meaning that through validating the input, it can be concluded that the model is successfully validated. Results from verification experiments have proved the robustness of the proposed methodology. Such experiments shown that the amount of knowledge and investment strategy have a fundamental role in the analysis of investment opportunities for the energy transition, and allow a simultaneous optimization of both individual actors' cash flows and of the total cluster wealth. The input complexity has been assessed, the reliability of the data points have been checked and the results of the model are in line with expectations, it is determined that the inputs of the model are validated. Ultimately, we have provided a solid method that allows to represent exogenous factors and investment opportunities in a way that is functionally correct, simulating rational behaviour of actors. The following chapter will provide the results from the simulations of the model, and they will be further discussed.

6 Results of modelling and discussion

This chapter will discuss the results of the model experiments performed in Linny-R following the proposed model in chapter 5. This will lead to answering the final sub-question: *What is the effect of exogenous factors on the investment behaviour for the transition of industrial clusters towards a CO_2 neutral future in 2050?*.

6.1 Exogenous factors results

This chapter answers the last sub-question: "*What is the effect of exogenous factors on the investment behaviour for the transition of industrial clusters towards a CO_2 neutral future in 2050?*" by looking at the results

The results derived from the experiments using the model provided in figure 18, makes a comparison between the simulation with full knowledge of future prices versus limited knowledge of future prices. This allows for quantification of the effects that the different exogenous factors have on the investment decisions, but also to see whether the effect of the exogenous factors increase if the knowledge of future prices is removed from the simulation. If no large difference can be detected, conclusions can still be made on the results because it will show that the knowledge of future prices does not make a large difference. Furthermore, by comparing the different simulations, with knowledge of future prices and with limited knowledge of future prices, further insights on the effect of exogenous factors as well as whether an increase of effect occurs. If no large difference are detected here, conclusions can be made on the structure of the model and assess how optimal the model is. The complications encountered during the construction of the model are discussed in chapter 6.2.4.
By changing the values of the data points provided in table 22 and 23, the simulations are performed and the solver provides the returns in two different forms:

- Cash flow per actor per time step
- Investment costs per actor time step
- Production levels per time step
- CO_2 emissions per time step

By using these forms of visualizing the results, insights can be derived on which investments are activated, which actor is largely influenced by changing exogenous factors and who is barely influenced, how it changes the production levels and what it does to the CO_2 emissions.

6.1.1 High and low CO_2 price

Here, the results for a high and low CO_2 price (price of CO_2 given in table 22, multiplied or divided by 0.01) are presented. The simulations were also performed with the model having full knowledge and with the model having limited knowledge (denoted as FK and LK in the graphs). The figure below shows the individual and collective cash flow per simulation.

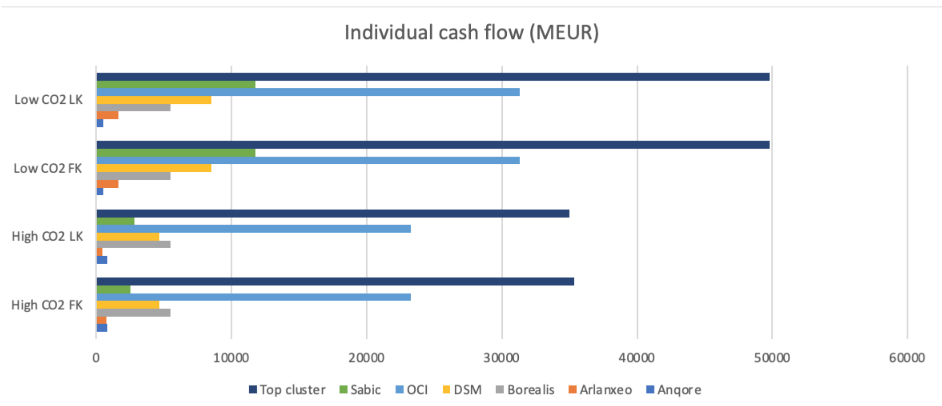

Figure 30: Cash flow results of high and low CO_2 prices with full knowledge and limited knowledge

In terms of overall cash flow, no big surprises occurred. When the price of CO_2 is low, the cluster can produce at a lower cost rate, thus, making more money. For the low CO_2 scenarios, no difference exists between the cash flow of the full knowledge and the limited knowledge. The costs costs associated with producing are now only the costs of raw materials and feedstock, which seem to be lower than the profits from selling the products at any point in time. Meaning that if CO_2 is removed from the equation, future price knowledge does not matter in this simulation.

Looking at the high CO_2 simulations, interesting things arise. First of all, the overall cash flow is lower, with the reductions being experienced by OCI and Sabic. They are at the front of the Chemelot value chain, and are largely responsible for the CO_2 emissions. Furthermore, a small difference in the overall cash flow can be seen for the simulation with full knowledge and the simulation with limited knowledge. It seems that since the CO_2 price is very high, having full knowledge allows for a more optimal production level, or earlier investments to be made to increase the overall cash flow. To analyze this more deeply, the investment curve is presented in the figure below.

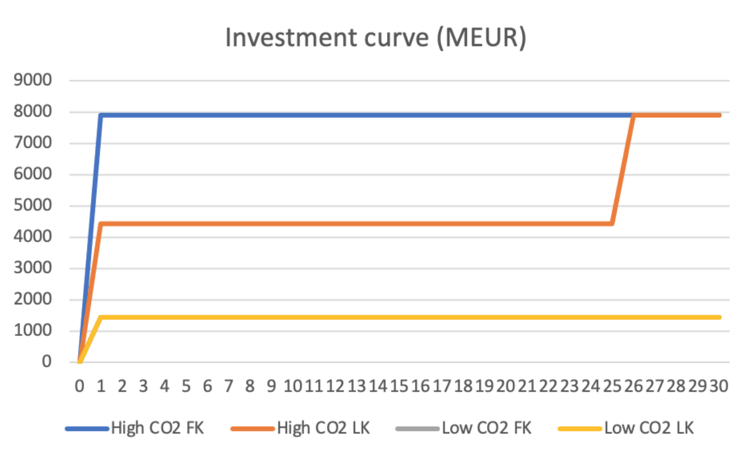

Figure 31: Investment curves for high and low CO_2 prices with full knowledge and limited knowledge

What can be seen in the investment curve, is that for the low CO_2 simulations, investing in technologies that reduce CO_2 are not profitable. The investment costs far exceed the CO_2 costs, since they are so low in this simulation. Looking at the high CO_2 investment curves, it can be seen that with full knowledge, more investments are made at the first time step. The simulation with limited knowledge does invest the same total amount of money after 30 years, but not all at once. Those 24 time steps that the simulation with full knowledge has invested and the simulation with limited knowledge has not invested, can explain the difference in cash flow. The difference in cash flow is €304.000.000 between the high CO_2 full knowledge and limited knowledge. This does mean that for this model, Chemelot could save up to €10.000.000 per year if they had full knowledge of the prices. It also shows the difference in investment behaviour and how companies within clusters could benefit from more accurate price predictions. By looking at the production levels, it can be determined whether the early investment increases the production levels or not.
No difference occurs between the low CO_2 price simulations, which makes sense because they can operate at a very high capacity since the costs of CO_2 are so low. For the simulations with a high CO_2 price, a small difference occurs in the production levels between the simulation with full knowledge, and the simulation with limited knowledge. This supports the statement that the earlier investment allows for more products to be produced, and thus more cash flow being generated. However, to verify the statement, a comparison between the overall CO_2 emissions must be made.
No unexpected occurrences can be seen in the figure. When the CO_2 price is very high, it is necessary to invest in technologies that remove CO_2 from the value chain. Whereas, when the price is very low, removing CO_2 from the value chain will only cause large losses. This also supports the statements that the difference in cash flow is caused by the earlier investment, allowing for a higher production level and thus more products being sold. In conclusion, when CO_2 is very low, knowledge has no influence on the cash flow, investment behaviour, production levels or emission rates. Whereas, when the CO_2 price is very high, more knowledge allows for better results to be gained.

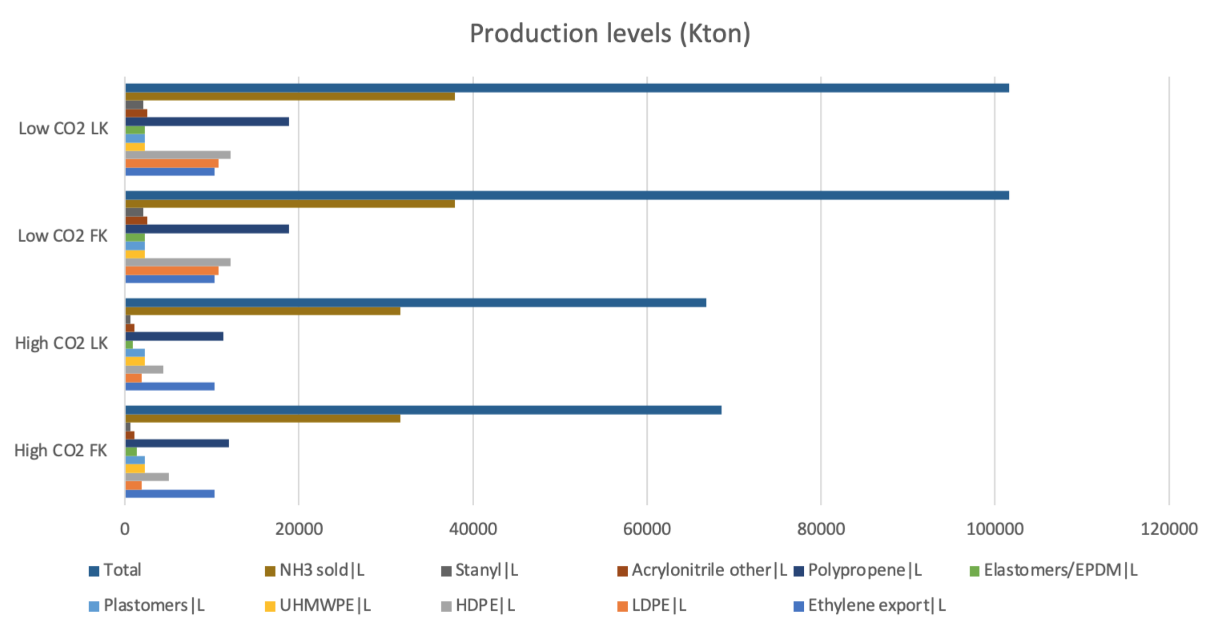

Figure 32: Production levels for high and low CO_2 prices with full knowledge and limited knowledge

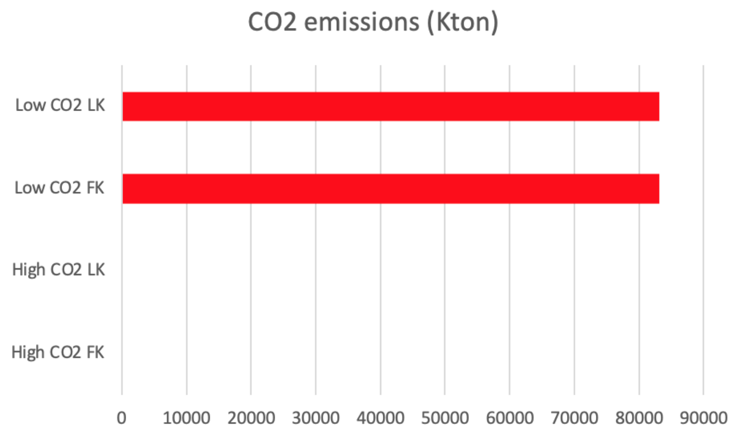

Figure 33: CO_2 emissions for high and low CO_2 prices with full knowledge and limited knowledge

6.1.2 High and low naphtha prices

Here, the results for a high and low naphtha price (multiplication or division by 0.01) are presented. The simulations have been performed with the model having full knowledge and with the model having limited knowledge. The figure below shows the individual and collective cash flow per simulation.
Starting with the high naphtha price simulations, no difference exists. Producing in the naphtha chain becomes too expensive, resulting in the entire chain being shut off. The NH_3 chain does keep on producing, but only to sell the NH_3 it makes, it is not used to make any other products. In the low naphtha price scenario, Sabic can operate with very profitable margins because of low raw material costs. Producing as much as possible results in large profits being realized. Looking at the graph, a very small difference exists between the cash flows, €26.000.000 in favor of the simulation with full knowledge. This difference can be the result of a small change in production levels, or emission levels. To investigate this more deeply, the investment curve will be analyzed first.
For the high naphtha price simulations, no investments are made since the entire chain is shut off. For the low naphtha price simulations, a difference in investment behaviour occurs. The simulation with full knowledge performs all its investments in the first time step, whereas, the simulation with limited knowledge does invest in the first time step, but only after time step 9 are they at the same level. This difference can explain the difference in cash flow, since more CO_2 is reduced in earlier time steps and, therefore, costs being cut. However,

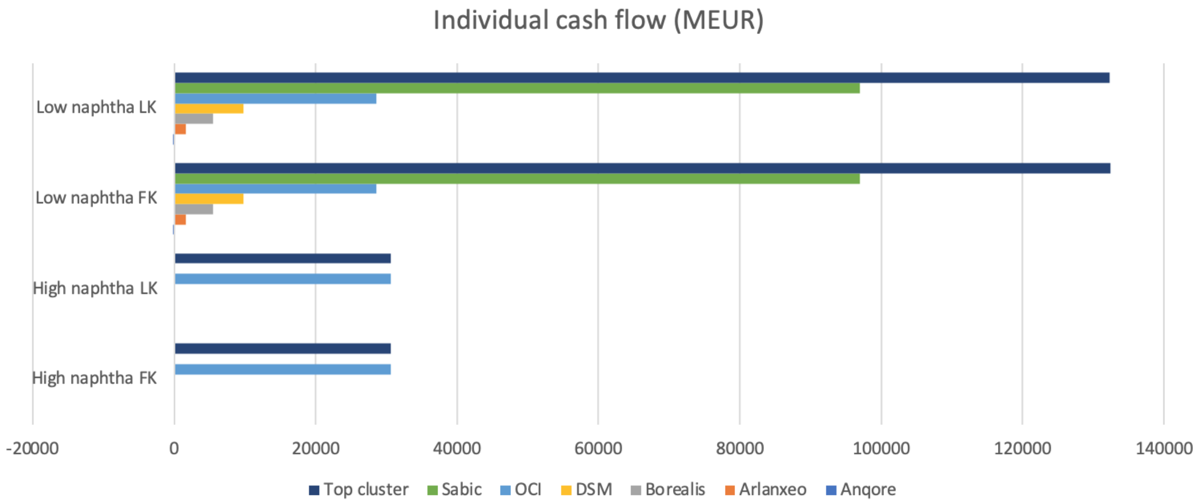

Figure 34: Cash flow for high and low naphtha prices with full knowledge and limited knowledge

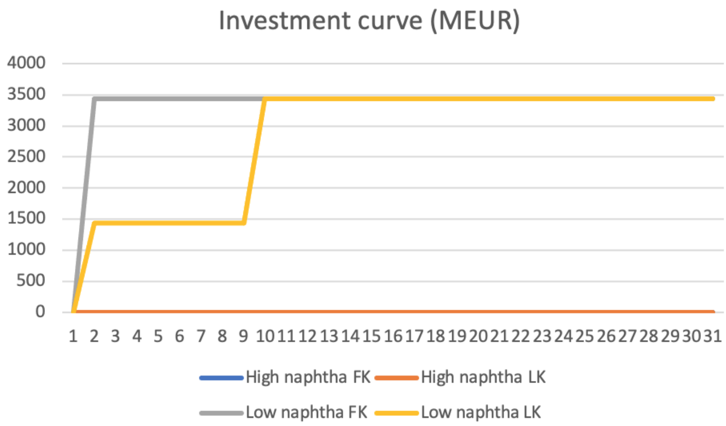

Figure 35: Investment curve for high and low naphtha prices with full knowledge and limited knowledge

it could also lead to more efficient production levels, which lead to more cash flow. Therefore, the production levels are presented below to analyze it more deeply.
The high naphtha simulations have the exact same production levels, its just the NH_3 that is being produced and sold immediately. For the low naphtha simulations, a very small difference exists, the simulation with limited knowledge produces 24 Kton more in total. This can be caused by the difference in investment behaviour, and making it seem that producing more will result in more cash flow. However, the difference in cash flow could also be related to a difference in emissions. Therefore, the CO_2 emissions are presented below to analyze it more deeply.
Here, it shows a significant difference between the low naphtha FK and low naphtha LK, which can be related to the difference in investment behaviour. Meaning, that the difference in cash flow can be related to the difference in CO_2 emissions. For the high naphtha price simulations, no difference occurs in emissions, which corresponds to the equal production levels and equal cash flow.
This shows that having full knowledge of future prices in a scenario where producing with naphtha is profitable, stimulates investment behaviour, allows for more efficient production levels and reduces the CO_2 emissions.

6.1.3 High and low electricity prices

Here, the results of the simulations with a high and low electricity price will be presented. The simulations have been performed with the model having full knowledge, and with the model having limited knowledge. The figure below shows the individual and collective cash flow per simulation.
First of all, no differences occur between the simulations with full knowledge and limited knowledge for both electricity prices. Furthermore, the low electricity price allows for very large amounts of cash flow to be

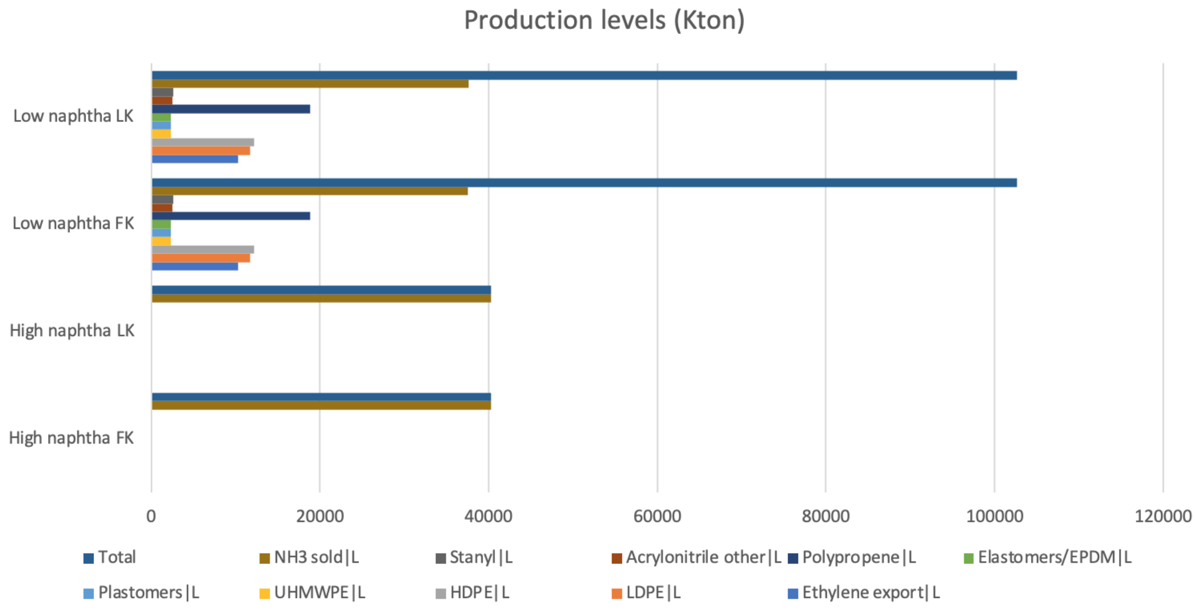

Figure 36: Production levels for high and low naphtha prices with full knowledge and limited knowledge

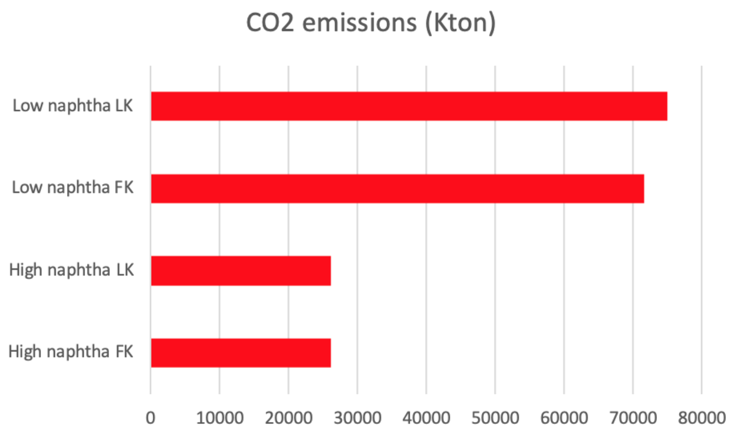

Figure 37: CO_2 emissions for high and low naphtha prices with full knowledge and limited knowledge

generated. This is partly because of low costs, but also because investments that require large amounts of electricity become interesting in this scenario. With the high electricity costs, it can be seen that OCI mainly dictates the cash flow of the cluster, and Sabic produces a negative cash flow. This can be the result of the cluster producing a product that requires both the naphtha chain and the NH_3 chain, making a large profit for Borealis and OCI, but makes a loss for Sabic. To analyze this more deeply, first the investment curve will be presented to see whether any differences occur.

Again, no differences occur in the investment behaviour, which was expected. If a large difference would have occurred here, it would have been shown in figure 35 most likely. The investment curve shows that when the price of electricity is very high, it is not worth to invest in technologies that have a higher electricity demand, because that would drive op the costs even higher. Furthermore, if electricity is already one of the biggest cost item in the cluster, cutting down on production levels can be better in terms of cash flow and emission levels than to try and remove them by investing in CCS for example.

In the scenario with a low electricity price, investments that move away from fossil-fuel as feedstock and use electricity become very interesting. The lower variable costs result in larger profit margins and thus a higher cash flow. Looking at the production levels can confirm the statement regarding similar investment behaviour.

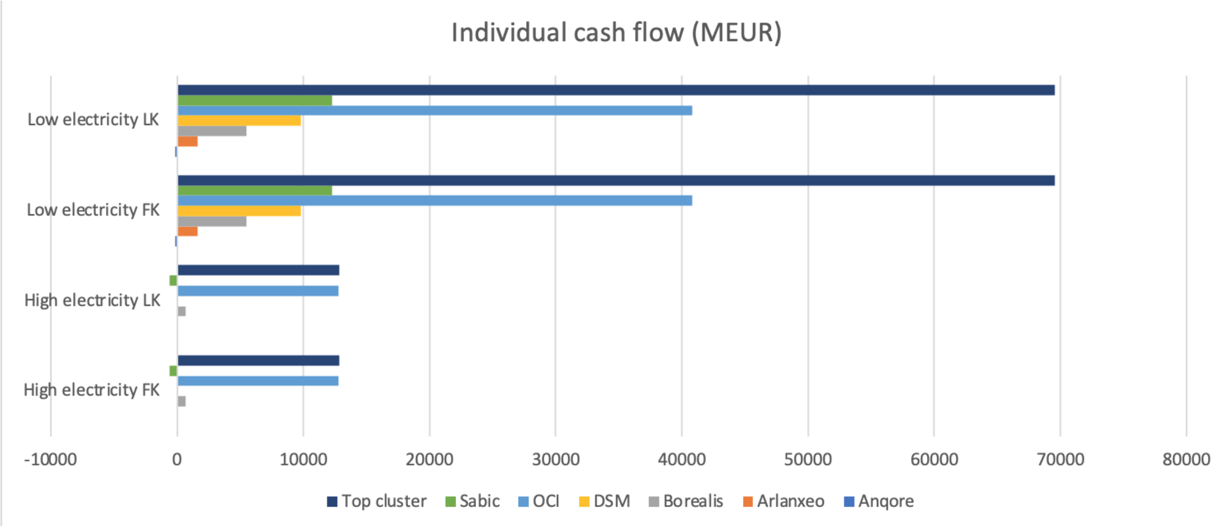

Figure 38: Cash flow for high and low electricity prices with full knowledge and limited knowledge

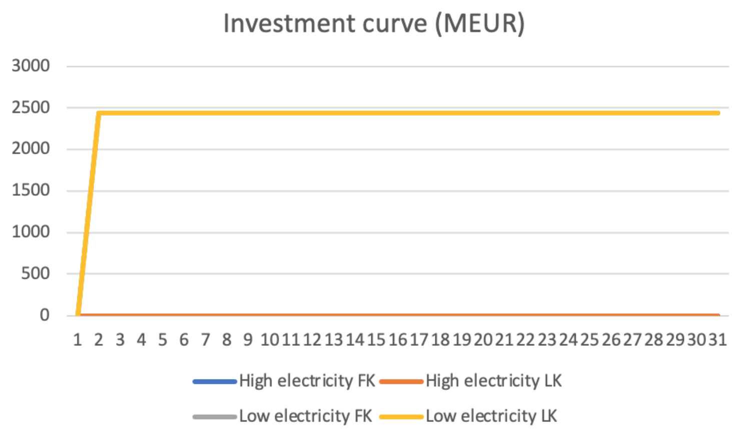

Figure 39: Investment curve for high and low electricity prices with full knowledge and limited knowledge

The production levels show no difference between the simulations with full knowledge and limited knowledge. Furthermore, it shows that in the high electricity price scenario, that nearly all production is NH_3 that is being sold directly, and a very small amount of plastomers and polypropene. Meaning, that the statement regarding the loss of Sabic can be confirmed, they make a loss because the model has calculated that producing plastomers will increase the overall cash flow of Chemelot, which is produced using ethylene. Because Sabic has to provide this ethylene, it must "get rid" of its remaining propene, which is further processed into polypropene to generate the largest cash flow given the circumstances. This should also mean that the emission rates are the same regardless of the knowledge that the model has.
As expected, no differences in the emission rates exist. This confirms the statement that having more knowledge in a scenario with varying electricity prices does not increase or decrease the cash flow, influence investment behaviour, increase or decrease production levels or emission rates. However, it has shown that the electricity price largely influences the cash flow, investment behaviour, production levels and emission rates. Electricity is essential in the energy transition and if the price increases drastically, it slows down the energy transition of Chemelot substantially.

6.1.4 High and low natural gas prices

Here, the results of the simulations with a high and low natural gas price will be presented. The simulations have been performed with the model having full knowledge, and with the model having limited knowledge. The figure below shows the individual and collective cash flow per simulation.
The figure shows that the natural gas price heavily dictates the overall cash flow of the cluster. The feedstock is for both the naphtha and NH_3 chain important to produce. The low natural gas price also removes the need

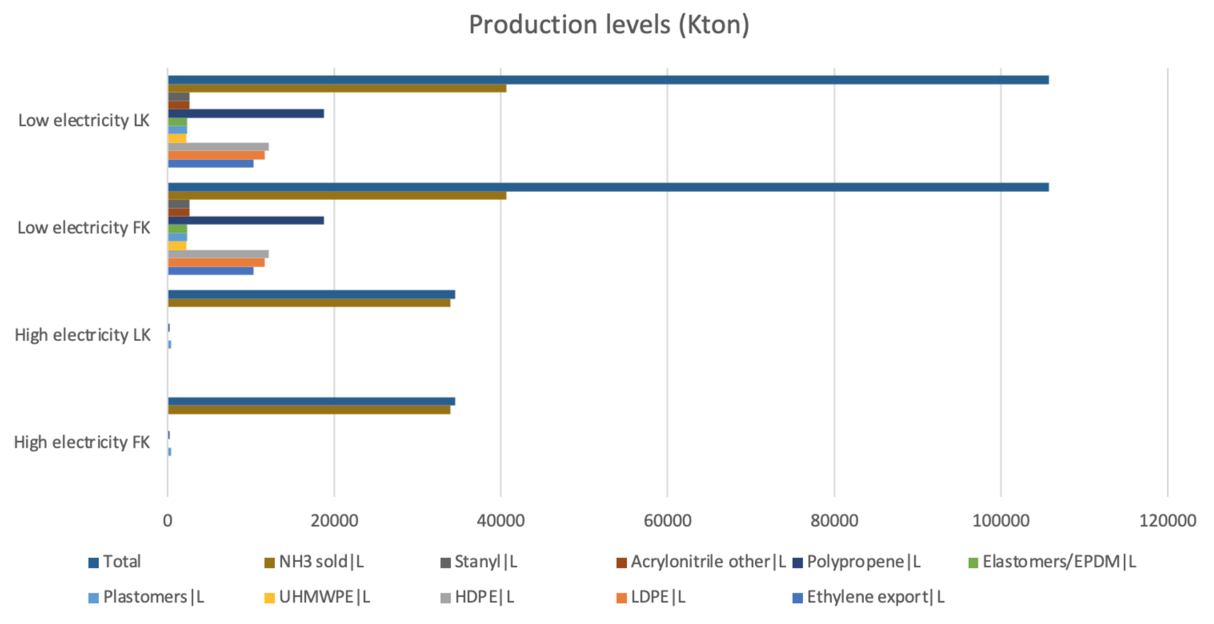

Figure 40: Production levels for high and low electricity prices with full knowledge and limited knowledge

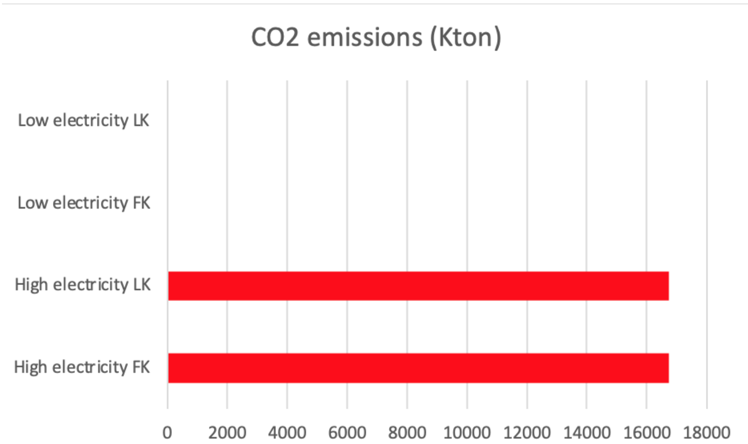

Figure 41: CO_2 emissions for high and low electricity prices with full knowledge and limited knowledge

to invest in technologies that move away from natural gas, since they will use other feedstock which is more expensive than the natural gas. Looking at the high natural gas price simulations, both chains are still active, but the cash flow of Sabic and OCI have been reduced drastically. Furthermore, other actors such as DSM and Borealis generate large amounts of cash. Finally, no difference exists in the cash flow between the high natural gas simulations, whereas, with the low natural gas price simulations, a cash flow difference of €170.000.000 exists. To explain the difference, the investment curve will be investigated first.
Both of the high natural gas price simulations follow the same investment path, in the first time step, investments are performed to reduce the dependency on natural gas to lower the costs of feedstock and increase cash flow. The amount of knowledge does not matter in these simulations, the price of natural gas is so high that investing is always profitable. Looking at the simulations for the low natural gas price, a difference in investment behaviour occurs. The full knowledge simulation immediately makes all its investments to be able to operate at full capacity whilst reducing its CO_2 emissions. Looking at the simulation with limited knowledge, the total amount of money invested is the same, but the rate at which the investments are made is slower. The difference in cash flow can be explained by the differing investment behaviour, however, to analyze it more deeply, the production levels will be investigated.
The production levels show no difference for all simulations performed. This means that knowledge does not make the production levels more efficient in this scenario. It also allows for the revision of the previous statement regarding the cash flow, and changing it to the difference in cash flow most likely being generated through a

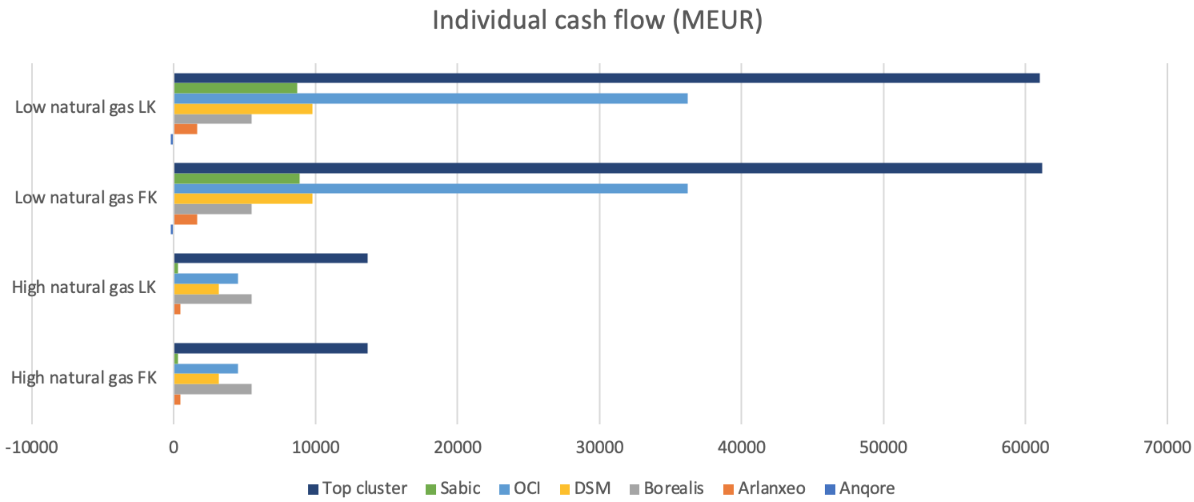

Figure 42: Cash flow for high and low natural gas with full knowledge and limited knowledge

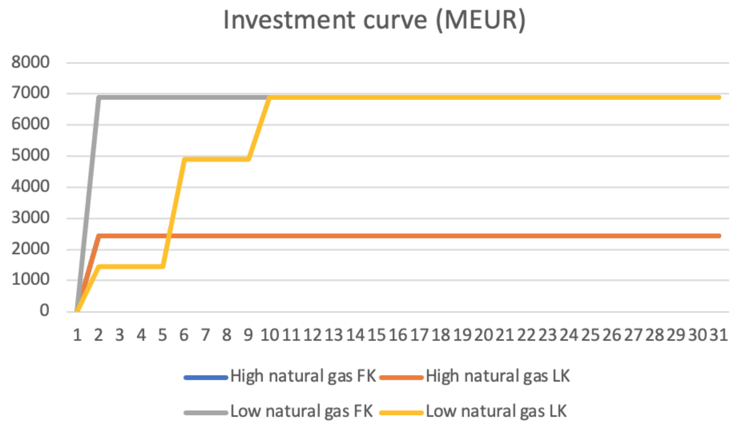

Figure 43: Investment curve for high and natural gas prices with full knowledge and limited knowledge

difference in emission levels because of the investment behaviour. Below are the CO_2 emissions presented.
As expected, a difference exists between the simulations for low natural gas price. This difference is because of the speed at which the model will full knowledge is able to invest, and results in CO_2 being able to removed from the model in earlier time steps. For the simulations of high natural gas price, both are 0. With such a high natural gas price, it is more profitable to move away from natural gas as a feedstock and invest in electrification or other sustainable investments. In conclusion, if the natural gas price is very high, the model will move away from it as a feedstock and move towards more sustainable investments. Here, having knowledge does not influence any of the analyzed parameters. When the natural gas price is very low, a difference occurs in the cash flow, investment behaviour and emission levels. Here, having full knowledge improves the overall cash flow and thus, benefits Chemelot.

6.1.5 Comparison of all exogenous factors simulations performed

The results of the exogenous factors have shown the influence they have on the cash flow, investment behaviour, production levels and CO_2 emissions of the actors within Chemelot. By comparing all the results, it can be determined which factors have a larger influence on certain parameters, and also allows for establishing realistic scenarios. First, the cash flow of all simulations will be compared.
In terms of largest influence on the cash flow, we see that naphtha has a large impact. Natural gas and electricity also have a large influence on the overall cash flow of Chemelot. The price of CO_2 does influence the cash flow, but it does not have an impact as large as the other factors. What is also worth noting, is that of all the simulations performed, Sabic is susceptible for changes in commodity prices, whereas, OCI is more robust in that regard. Anqore, Arlanxeo, Borealis and DSM are largely dependent on the outcome of Sabic and OCI,

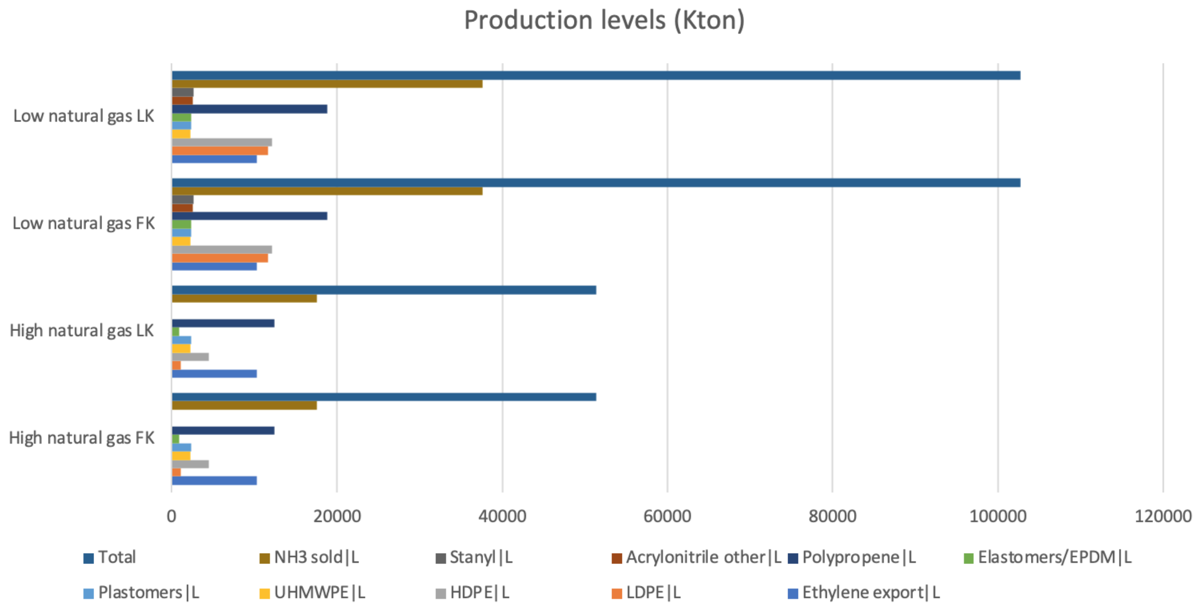

Figure 44: Production levels for high and natural gas prices with full knowledge and limited knowledge

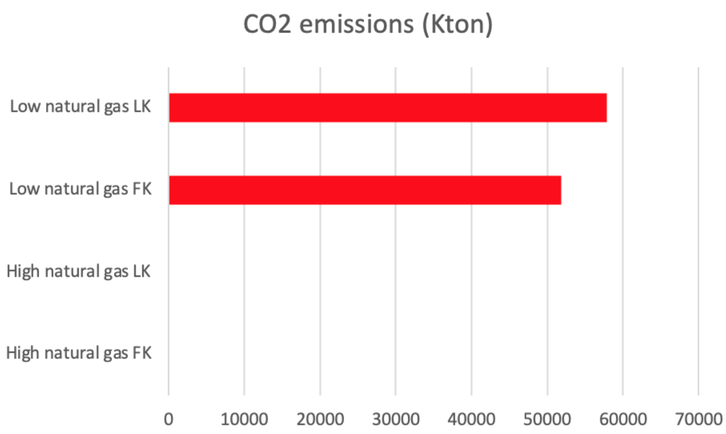

Figure 45: CO_2 emissions for high and natural gas prices with full knowledge and limited knowledge

making their cash flow also dependent on the production levels of Sabic and OCI. If we look at the differences between the high and low price simulations, the differences become more evident.

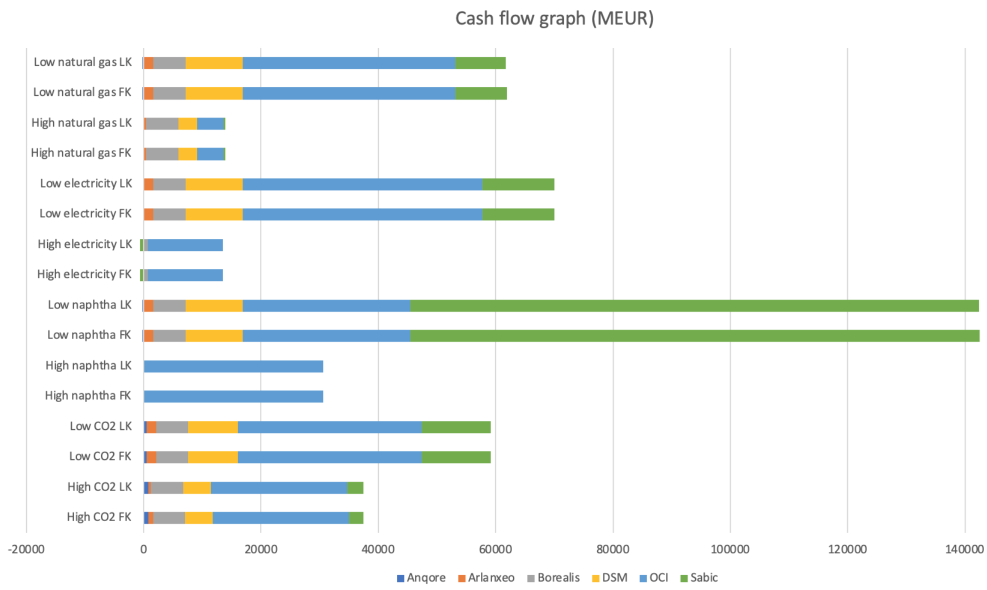

Figure 46: Cash flow comparison for all simulations

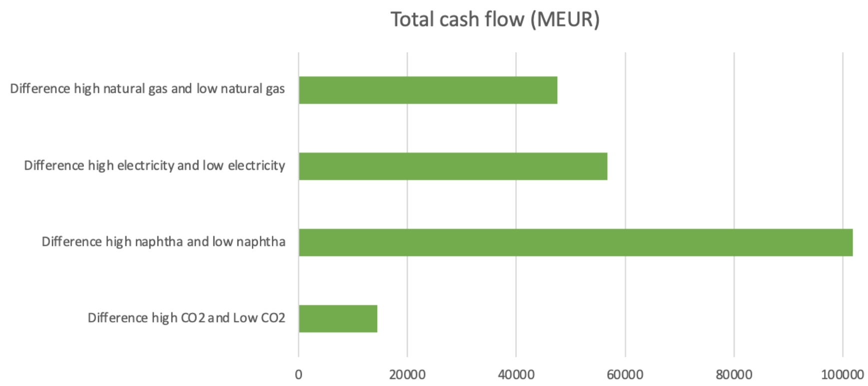

Figure 47: Difference in cash flow for all simulations

As previously mentioned, the CO_2 price does influence the cash flow of Chemelot, but not as large as a drastic increase in the other commodities. This shows that Chemelot should be able to overcome the challenges faced with increasing CO_2 prices towards 2050, but it also shows that Chemelot is more vulnerable to feedstock and raw material price increases. These changes also influence the overall production levels, which are presented below.
For the product levels, its noticeable that whenever the price of a commodity increases drastically, the production levels are reduced. Furthermore, OCI is more robust than Sabic when it comes to these price changes. This could be the result of higher profit margins for OCI, since their feedstock consists mainly of natural gas and electricity. Whereas, Sabic also has to use naphtha to produce its hydrocarbons. Only when the price of the finished products is lowered with a large amount, will Chemelot completely shut off. In all other cases, Chemelot is still able to make a profit. To inspect the differences between the high and low price, the figure below is presented.
The figure shows that the difference in production levels is the lowest for the high and low CO_2 price. This is in line with the statement made earlier regarding the resilience of Chemelot when it comes to increasing CO_2 prices. Furthermore, the difference between the high and low natural gas price is also less than the others, this is because in this scenario, Sabic was still able to produce products by making use of electrification, thus making it independent of natural gas. This also shows that Chemelot is resilient when it comes to increasing natural gas prices, however, less resilient than increasing CO_2 prices. Finally, the emissions will also be compared.
Here it shows, that when a lot of product can be produced with very profitable margins, the emission rates will almost always be high as well. The only exception is when the electricity price is very low, this makes investments in electrification and other technologies that have high electricity demands very attractive. In this

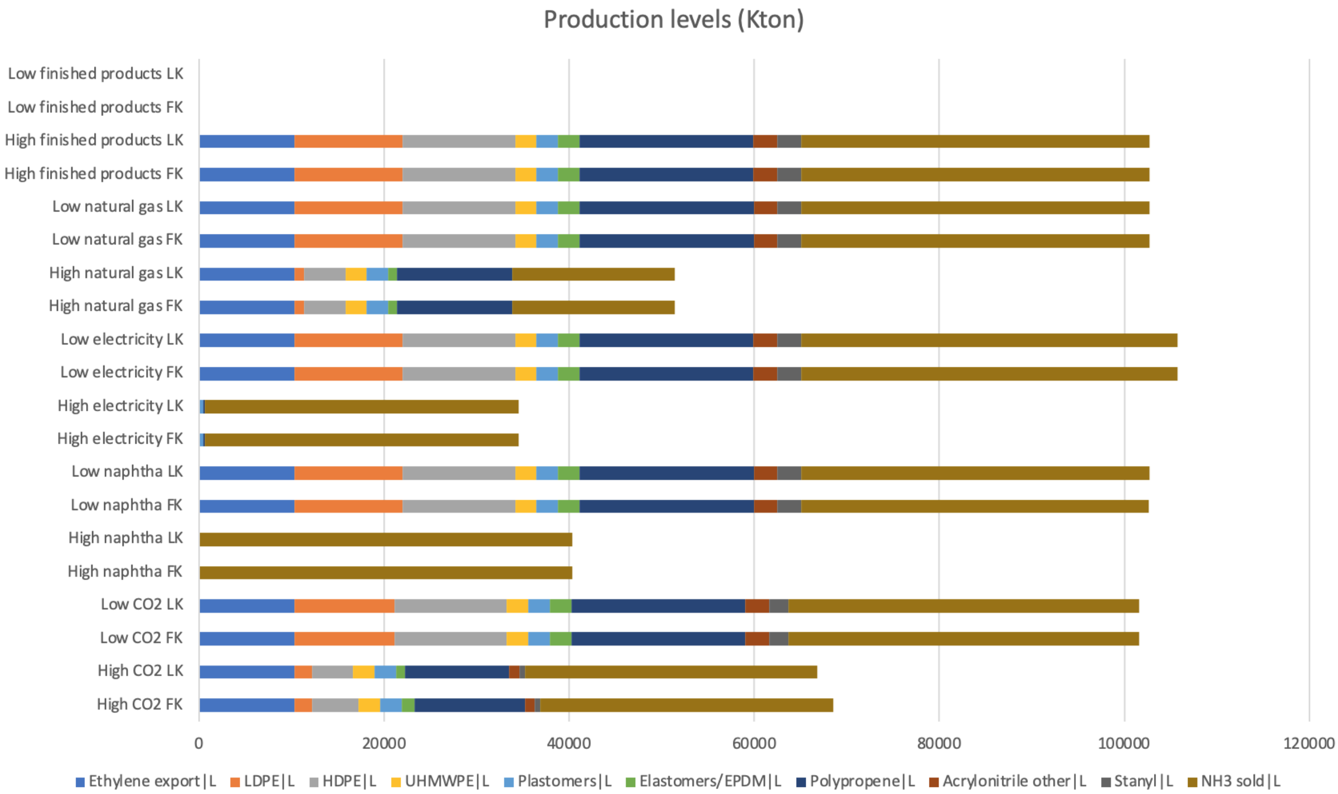

Figure 48: Production levels for all simulations

scenario, all the CO_2 is removed from Chemelot since producing through these high electricity demand technologies becomes very profitable. It also seems that the low finished product simulations are very sustainable, however, no actor in Chemelot produces in this scenario, so no CO_2 is emitted. By comparing the differences, a better insight is created for the emission levels.
The CO_2 difference is the highest for when the price of CO_2 increases and when the price of finished goods decreases. Furthermore, it seems like electricity price has a low influence on the CO_2 emissions, however, when the price is high, the production levels are largely reduced, which also reduces the emission levels already. This also shows that the simulation with the least CO_2 emissions definitely does not mean that it also has the highest cash flow.

6.2 Scenario analysis

With the results of the exogenous factors showing the influence they have on the cash flow, investment behaviour, production levels and CO_2 emissions of the actors within Chemelot, the realistic scenarios that have been established in chapter 5.2.3 can now determine optimal investment trajectories for Chemelot. The results of the scenario analysis will not only give insights in what optimal investment trajectories exist, but also how the knowledge of future prices influences Chemelot when the commodities do not take extreme values, but are realistic. Below are the cash flows for all the simulations provided.

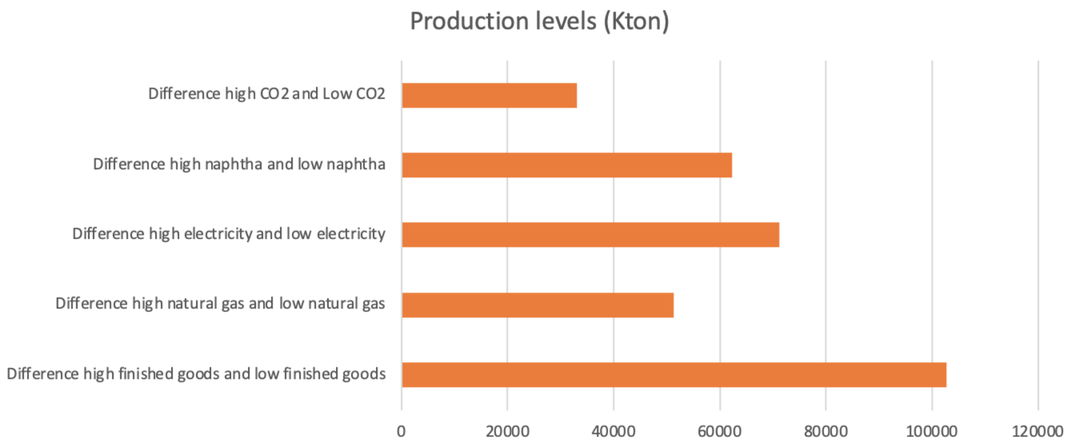

Figure 49: Production level differences between high and low simulations

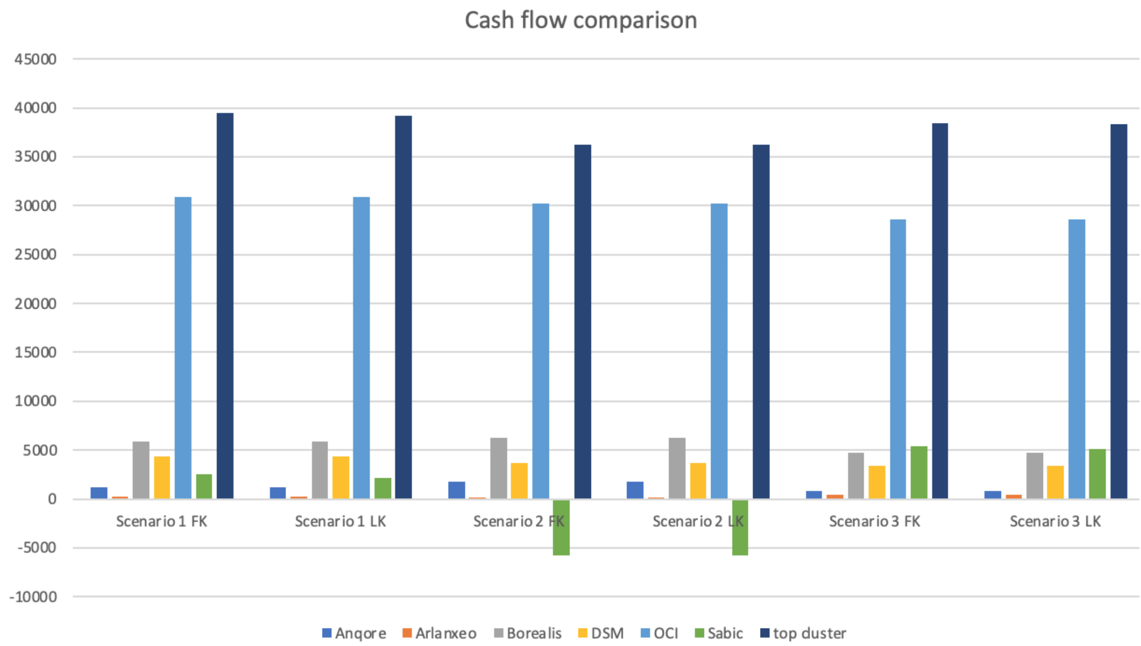

Figure 52: Cash flow comparison for all scenarios

Small differences in cash flow occur for Sabic in scenario 1 and 3. The differences can be due to a difference in investment behaviour. By taking into account what has been learned from the previous section, it would seem that having full knowledge allows for investments to be made that would not seem profitable with limited knowledge. To further analyze the cash difference, the investment curves will be presented.

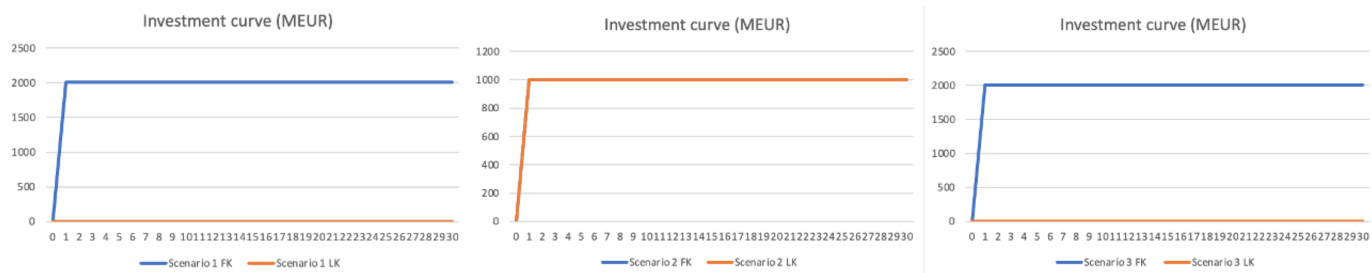

Figure 53: Investment curve comparison for all scenarios

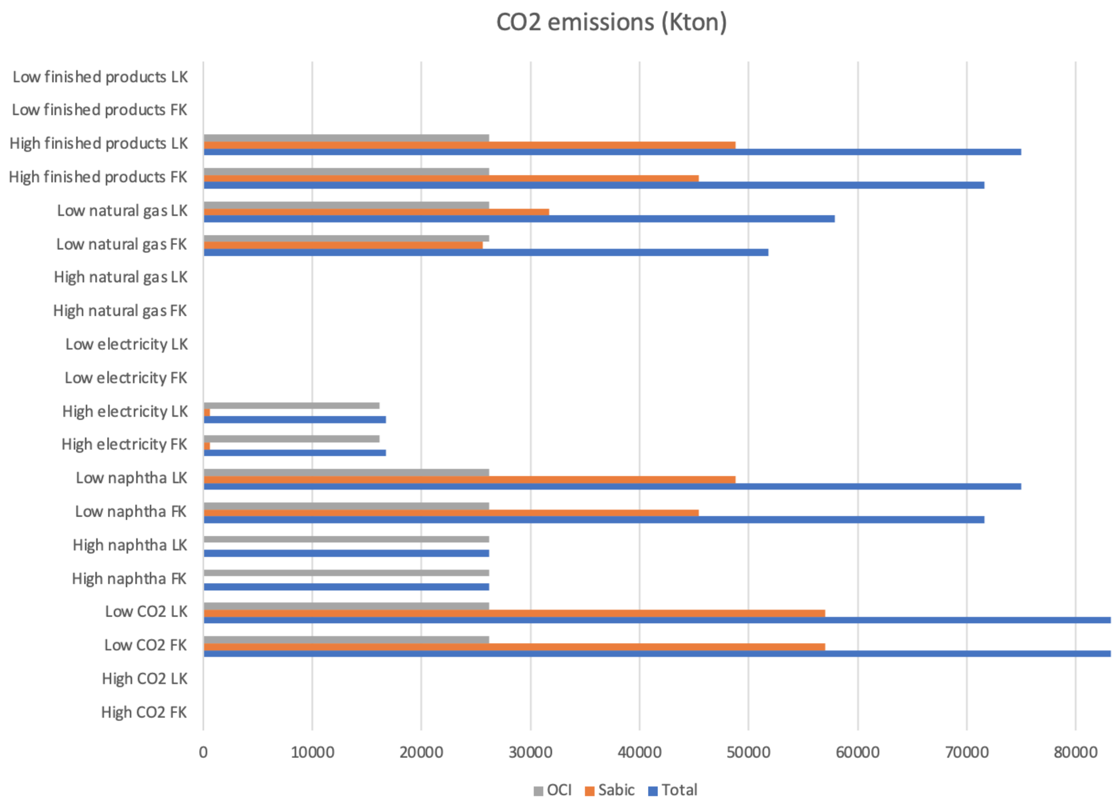

Figure 50: CO_2 emissions for all simulations

The curve for scenario 1 and 3 shows that having full knowledge of the prices allows for making investments because the risk is removed from the equation. This investment allows for a reduction in CO_2 emissions and can result in an increase in cash flow if enough CO_2 is removed. To support this statement, the emission rates are provided below.

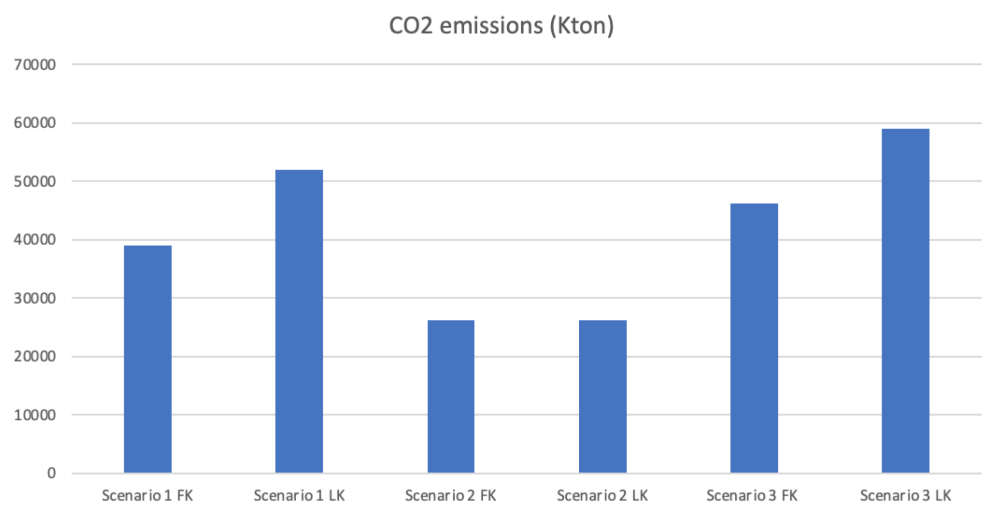

Figure 54: CO_2 emission comparison for all scenarios

A difference in scenario 1 and 3 is clearly visible, which explains the cash flow difference. This would also mean that the production levels for all scenarios are the same with full knowledge and limited knowledge. To verify this statement, the production levels are provided in the figure below.

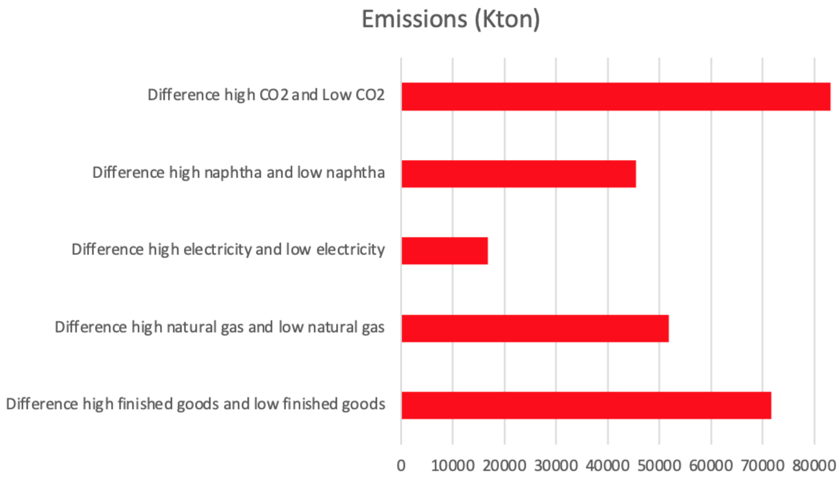

Figure 51: CO_2 emission differences for all simulations

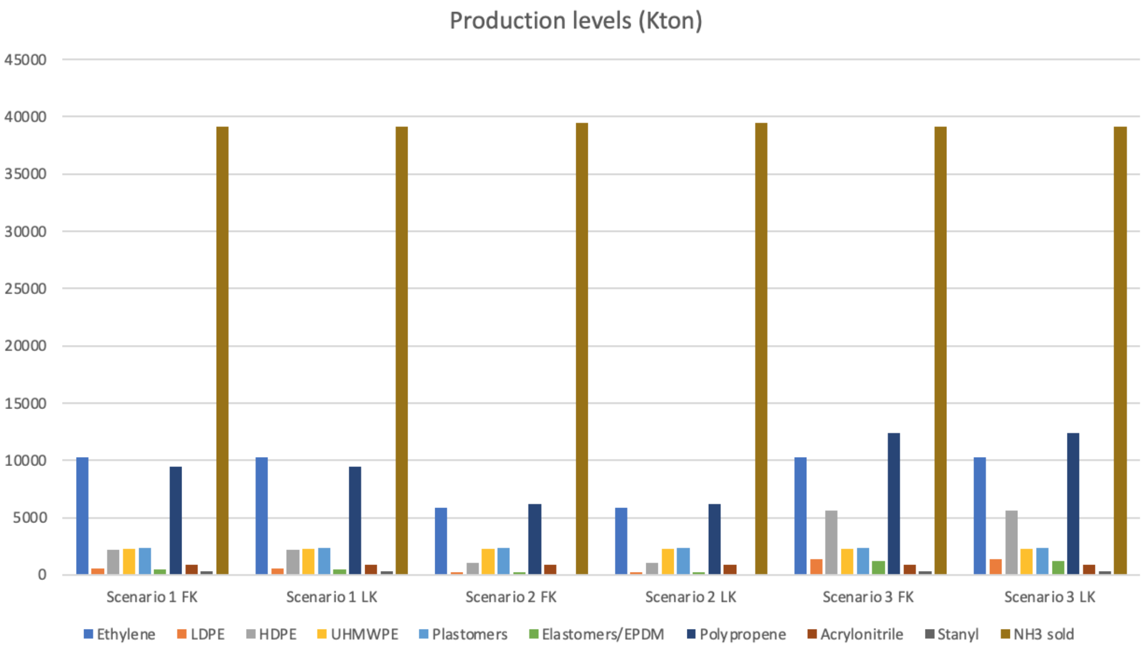

Figure 55: Production level comparison for all scenarios

The figure confirms the statement made earlier. The cash flow difference is caused by having full knowledge of future prices, which allows for making investments that reduce CO_2 and thus saves costs. This shows that with the model, optimal investment paths can be determined for the demarcated part of Chemelot and compare it with with sub-optimal investment trajectories. The results will further be discussed in the following subsections.

6.3 Results analysis

A more in-depth analysis will be performed on the different exogenous factors that have been included into the model. Next, a more in-depth interpretation of the quantified results with full knowledge and with limited knowledge. Finally, any remarks regarding the investment options will be presented.

6.3.1 Discussion of effect of exogenous factors on the investment behaviour

The emission reduction policies were implemented in the model by applying a price to the CO_2 that is emitted. Any emission comes at a price, and the higher the price, the faster an actor would want to become more sustainable to save costs. The price of emissions heavily influences the investment behaviour because the model will calculate a tipping point where it is more interesting to invest in a technology that reduces the CO_2 emissions, than to just offset it. Figure 27 shows the cash flow for high and low CO_2 prices, and shows how much CO_2 influences Chemelot. By combining it with figure 28, which shows the investment curve, it shows clearly that a higher emission price stimulates investments in emission reducing technologies. The emission reduction policies could also be integrated in the model by using a cap on the amount that could be emitted, forcing the model to invest in certain technologies to make sure the CO_2 would be captured. However, offsetting CO_2 is also a viable option right now, and removing that possibility from the model would create less realistic investment trajectories. Furthermore, from a cash flow perspective, this would give the best insights on what would happen with which actor according to the increase of the emission price. But, reflecting on the model, it can be stated that including this modelling choice in the model and alternating it with the current implementation could lead to other or new insights on how the actors would react to a cap on the CO_2 emissions. This is currently not included in the model, also because the model is only a demarcation of Chemelot. Some actors on Chemelot rely on the emissions of other actors, which they would include to produce certain products, as is the case with the Methanol to Olefin process. Extending the emission reduction policies to also include NOx emissions or any other type of emission will increase the complexity of the model, but will also provide new insights on how incorporating more of the emission reduction policies will influence the investment behaviour of actors.

The increase of naphtha has shown important the raw material is for Chemelot. When the price becomes incredibly high, a very large part of Chemelot shuts down. A large amount of actors on Chemelot are dependent or part of the naphtha chain, and if it is not operating, incredibly large losses are incurred. If the price is very high, no investments are profitable to keep on operating. This also shows how certain investments are not mature enough yet to be interesting for certain actors. Interestingly, when the naphtha price is low, investments are performed. Due to the high operation level because of the low price, investments that reduce CO_2 emissions become interesting as they remove the correlated costs. It is not expected that the naphtha price will become lower in the near future, meaning that as long as no new innovations are discovered or the methanol to olefin technology matures, it will become difficult for Chemelot to stay profitable. However, the naphtha chain in the experiment performed in chapter 6.1.2. was increased by 100 times, which is very unrealistic. By comparing it with the experiments performed in chapter 6.2, the naphtha chain remains profitable with an increase in the naphtha price among other increases. It still remains a subject of interest, because in the second scenario of chapter 6.2, Sabic does make a very large loss, and the price increases and decreases implemented in that scenario are realistic. So, efforts need to be put into making the naphtha chain as profitable as possible with increasing naphtha prices, or try to move away from naphtha as a raw material to produce hydrocarbons.

When it comes to the electricity prices, a low value promotes investment behaviour, whereas high electricity prices slows it down. A lot of the decarbonizing investments in Chemelot are focused on electrification. Moving away from fossil-fuels to provide the energy and heat required for certain processes, and using electricity to provide both. If the electricity is renewable, large amounts of CO_2 are removed from the process. However, the electricity demand increases drastically during electrification, and when the electricity prices increase, these investments become less and less profitable. Electrification does remove the need for investments such as CCS to be made, which does make it very interesting if CO_2 storage becomes more expensive in the future. Furthermore, it is not expected that the electricity price will decrease drastically in the near future, especially if the electricity price trends of 2021 and 2022 will continue to persist. Even large breakthroughs in electricity production or storage will not make the electricity price near zero, therefore, electrification is still very tricky in terms of profitability. Looking at the cash flows, it can be seen that the naphtha chain is more susceptible to large fluctuations of the electricity price, whereas, the NH_3 is more resilient. A very small amount of plastomers is produced since it increases the overall cash flow of Chemelot, but it does also result in a loss for Sabic because they have to provide the ethylene for Borealis, which is produced at a loss.

For natural gas prices, a low price generates enormous amounts of cash flow and really promotes investment behaviour. Interestingly enough, even when the price is very high, investments still occur. This is because the increase in natural gas price makes investments that use a different source as fuel more profitable. So, electrification and producing NH_3 through H_2 instead of natural gas also becomes interesting here. Removing natural gas from the equation becomes very profitable. When the price is low, the production levels go up to very high levels, which also causes large amounts of CO_2 emissions. To compensate for those emissions, a lot of money is spent on investments, but still, a large amount of CO_2 is emitted. This shows that as long as it is profitable to produce whilst emitting CO_2, it will still happen and be compensated for by paying for it. With such low natural gas prices, its more profitable to just produce as much as possible and collect the costs of emitting CO_2. When the natural gas price is very high, every actor that produces still makes a profit. This shows that

Chemelot is quite resilient to the influences of natural gas prices and has the options to cope with increases in the future. As the world starts moving away from coal, natural gas will be in more demand, and since there is a limited stock of natural gas in the world, it is expected that the price of natural gas will increase in the near future. Therefore, the resilience to increasing natural gas prices in these simulations seems promising for Chemelot.

Finally, simulations varying the finished goods price have also been performed. No unexpected results were derived. When the price of the finished goods is very high, production is maximized to maximize cash flow. When the price of the finished goods is very low, no production will take place since producing does not become profitable. Furthermore, whenever production levels are increased or maximized, investments take place to compensate the extra CO_2 emitted. Making the comparison between the cash flow, production levels, investment curve and CO_2 emissions between a high price for finished goods and a low price, since for the low price, both chains were shut off. This also shows that the model behaves accordingly to extreme values and, therefore, functions well.

6.3.2 Full knowledge and limited knowledge results

As shown in the figures throughout chapter 5 and 6, the experiments have been performed twice per scenario, one with full knowledge of future prices, and one with limited knowledge of future prices. The limited knowledge was defined as the model being able to look ahead 4 years into the future. By performing every scenario simulation twice, one with full and one with limited knowledge, insights can be gained on how it affects the investment behaviour.

The simulations throughout chapter 6.1 have shown the effects that having full knowledge can have on the system. First, in all experiments, the simulations with full knowledge would always perform equally, or better in terms of cash flow than the simulation with limited knowledge. This is expected, the model can optimize every aspect since it knows the risks that can come in the future. Secondly, the full knowledge simulations always had an equal or higher amount of money invested in new technologies and always performed at an equal time step or earlier than the simulation with limited knowledge, meaning that no future setbacks were experienced. Since having full knowledge removes any risk that comes with making an investment. If the costs and gains are known to the model, its a simple calculation whether it will be profitable for the model to invest, which can be seen for the simulations with full knowledge, as it always invests in the first time step. When comparing the production levels, the simulations with full knowledge produced as much, or less than the simulations with limited knowledge. Linny-R optimizes the cash flow of the model, which does not mean that producing as much as possible generates the largest amount of cash flow. In certain cases, producing a bit less might be more profitable since the prices can increase rapidly. This is especially evident in the simulations for the low naphtha price. Here, the simulation with limited knowledge actually produces 25 Kton more, which results in €26.000.000 less cash flow. So, having full knowledge allows for the optimization of production levels and flow, making it more cost efficient. Finally, having full knowledge always results in an equal or lower amount of CO_2 emitted. The reduced risk in investments that comes with having full knowledge, and therefore, the faster investment behaviour allows the simulations with full knowledge to reduce more emissions. This is also the main cause for the increase in cash flow when there exists a difference between the model with full knowledge and with limited knowledge. However, the optimization of production levels can also lower the emissions, so the investment behaviour is not the sole reason for a difference in emission levels.

So, the simulations with full knowledge always perform on an equal level, or better compared to the simulations with limited knowledge. However, it must be noted that the simulations with limited knowledge still perform at a very good level. This shows how well the conceptual model in this research has performed throughout all the scenarios. For the cash flow, only small differences exist, same goes for production levels and emission rates. The only large difference is the speed at which investments are made when there is limited knowledge. In cases where it is extremely evident that the investment will be cheap from the first time step, the limited knowledge simulations will also invest in time step 1. However, if natural gas or naphtha prices are 100 times cheaper, or when CO_2 prices increase by 100 times, the investments come relatively late. It takes at least 10 time steps for the model to notice that a profit can be made by investing in a certain technology, whilst over the course of 30 time steps, it is profitable. This shows how much influence having knowledge can have, and what difference it makes in investment behaviour. It should also be noted that small differences that occur in the results of the simulations might seem small, but the cash flows are presented in MEUR, so a small difference is still a very large amount of money. For now, a look ahead of 4 has been taken to represent the limited knowledge model, as it seems realistic for industrial clusters to try to predict and incorporate those prices for their short-term and long-term goals. Especially since the (sustainable) goals change every so often, it would not be smart for Chemelot to take prices beyond that into account since the environment but also the goals are dynamic. The look ahead of 4 comes quite close to the optimal investment trajectories, proving it to be an effective and realistic modeling choice for this research.

6.3.3 Investment options remarks

The results produced by the model show a medium amount of variability in the investment trajectories for the industrial cluster, for both with full knowledge and with limited knowledge. Out of the 6 investment options, 4 are chosen consistently. These are the post-CCS, Electrification of Olefin 3/4, Ammonia synthesis through H_2 and pre-CCS. Because of this, the attractiveness of the remaining investment options are assessed as well as the amount of available investments for different actors. First of all, the majority of the investment options presented are technologically very immature. They have not been implemented on a large scale, even need to be implemented or can only decarbonize a very small part. This results in the costs being very high to opt for such an innovation, whilst having a very low impact on the overall system. A scale has already been applied to the investments to make them seem more attractive to the model, but the CAPEX and OPEX combined with the capacity still causes them to be unattractive for the model. Another explanation for the low variability of the investment trajectories is the amount of available investments. The model is a simplified representation of the petrochemical part of Chemelot, where the focus is mainly on the actors in the system that have the highest levels of CO_2 emissions. These actors produce high amounts of CO_2 because they run on natural gas and use feedstock that also causes emissions. Other emissions such as NOx, emissions resulted from producing products using intermediary products and actors that emit CO_2 because they use electricity to power their systems have been left out. This resulted in the available investments for the model to engage with were reduced to different innovations that mainly focus on moving away from natural gas as an energy source or innovations that capture CO_2 emissions. Having a more detailed model of Chemelot would allow for increasing the amount of decarbonizing investments the model could opt for.

Other observations on the available investments show that investments that do not require extremely large amounts of electricity are always firstly favoured in the model. The electricity price as presented in chapter 5 shows that it could increase with 30-50% in the near future. Electrification of processes or investing in innovations that move away from natural gas as an energy source causes the electricity demand to increase by huge amounts. This increases the price of operating such an investment by multiple times because of the electricity demand. Investments such as CCS, using imported H_2 as an energy source or even using H_2 as a feedstock could be favoured in reality because they do not depend on electricity as its main source. Furthermore, integrating H_2 in Chemelot seems could be an attractive option to further decarbonize the cluster, but the technologies seem to be too immature right now. The model does not engage in these innovations in the scenarios presented, to which the conclusion is made that they are not attractive enough right now. Furthermore, the imported H_2 has to be green H_2 to cause the largest impact. Blue H_2 has not been integrated in this model, but it is also considered less favourable for an industrial cluster because the costs of producing blue H_2 are considerably higher if the associated CO_2 costs are integrated in the price. So, the model has shown that introducing H_2 in Chemelot still faces barriers. However, as mentioned before, the simulations performed in this research are all without including a subsidy of some sort. Where other studies might have different conclusions on introducing electrolysers in industrial clusters, or how the price of blue H_2 might be lower than natural gas because of subsidies (Consortium, 2019), the results in this differ in that sense. The validity of the results are dependent on the accuracy of the system that is modelled, but it does show that the model is capable of looking at which investment options seem more attractive because they are not dependent on a certain commodity which increases drastically in price. This shows different opportunities for introducing certain innovations on industrial clusters which will reduce emissions and in turn might result in synergies down stream.

The results show that electrification and CCS are currently the most attractive in reducing the CO_2 emissions of Chemelot and to increase cash flow. Even with the increasing electricity prices, electrification is still profitable in most scenarios. However, CCS alone is not enough to cover the emissions if the production levels are high. This means that multiple investments should be made to make sure that Chemelot is working towards a CO_2 neutral future. The lack of H_2 engagement in this research allows for new questions to be researched regarding how it should be integrated, whether electrolysis to produce H_2 on site is attractive in the (near) future with subsidies and how it influences actors that are dependent on CO_2 emissions of actors upstream.
So with CCS and electrification being the most attractive investment options, and a combination of those being enough to fully decarbonize Chemelot in terms of CO_2 emissions, it does raise the question whether similar results will be achieved if the model is extended and increased in complexity, including other emissions such as

NOx.

6.4 Discussion

6.4.1 Discussion of the applied methodology

Since exogenous factors and sustainable investments had not been implemented in Linny-R in the way as proposed in this research, it posed quite the challenge, to come up with a methodology that would implement exogenous factors and investments and to see what the influence was of the one on the other. However, the research has shown that institutional components can be added to an optimization model and to also see their influence under different circumstances. The methodology also allows for defining an investment trajectory that is optimal given the scenario it takes place in, showing how actors may act. The implementation has shown that the investments that are made are dependent on the different exogenous factors in place, prices of feedstock and how far the model can look ahead. Resulting in the proposed methodology allowing for the analyses of how actors behave in a cluster, which is a rudimentary part of analyses within dynamic environments and environments where individual actors aim to optimize its own cash flow given the dynamic rules they play by. The methodology has provided different insights in the investment behaviour of different actors for optimal investment trajectories. It has been shown that industrial clusters would need to shift towards sustainable investments that rely on electricity and remove CO_2 from their processes.

It also shows that investments that are being made are not only dependent on fluctuating commodity prices, but also how technologically mature an innovation is, availability of the (renewable) energy alternative and how much knowledge they have of future prices. The simulations with full and limited knowledge of future prices showed that the speed of investment behaviour is largely dependent on this. The model allows for analysing the behaviour of actors within the system and can be of importance for analysing environments where multiple actors want to move towards more sustainable production, where the model could add value to the coordination of making those multi-actor decisions. A model was created using the methodology presented in this research, which showed what influences different exogenous factors have on the investment behaviour of actors. The conclusions derived from this model have been presented earlier, however, the results also provide useful insights on the methodology. The methodology has now been tested on an environment where a petrochemical cluster wants to decarbonize, however, with small adjustments, the methodology should be applicable to a larger amount of different systems. Adding more specific processes and including more investment options should allow the methodology to be applied to different systems in similar environments. Finally, the experiments have also shown that the methodology of this research has been executed properly.

6.4.2 Discussion of investments and exogenous factors implemented

The representation of investments and exogenous factors is considered to be sufficient. Mainly because the methodology that was implemented accompanied by experiments allows it to be adjusted and redone for future researches in similar scenarios and environments. It has been shown that the investment representations can be applied in multiple situations where a single investment option is available for the model, as well as multiple options. It also showed that paying upfront and paying over time both work well. Furthermore, the different exogenous factors applied are factors common in multiple environments and scenarios, meaning that implementing this in a different multi-actor situation would not cost large amounts of effort. The proposed investment representation also allows for easy adjustments such that different kinds of investments can be represented with the desired degree of complexity. If more complexity would have been added to the proposed representation, more challenges could have been faced but also more accurate results could be derived. For example, by not representing the Olefin 3/4 as a single process in Linny-R, but as multiple sub-process building blocks with each intermediary step, and adding associated investments related to those sub-processes, insights could be derived on smaller sustainable investments. Doing this would also allow for more sustainable innovations to be added to the model more downstream. However, this would add significantly more constraints to the binary variables for the solver and could increase the chance for error as well as the computational time.

Subsidies have not been included in this research for multiple reasons. The existing subsidies in the Netherlands are very complex in terms of funds available per actor. It also differs per subsidy and depends on the ETS 100 year border. Adding the subsidies in the model gives a significantly more realistic picture of what investments are more attractive and when/how actors and clusters should invest to remain profitable during the energy transition. The subsidies have not been included because of the time frame given for this research. For the subsidies alone, substantial time and efforts should be committed to getting at least a ballpark of the funds that could be provided through the multiple subsidies. Therefore, future research committed to the implementation of subsidies could generate new and interesting insights on the investment behaviour of industrial clusters. Finally, the payment structure of the investment was not based on literature regarding how such large investment payments take place. This limitation can be further addressed in future research by performing research on how those large investments take place to make a more accurate representation within the proposed methodology. Another limitation is the amount of available sustainable investment options for all actors. In the current model, the investment options are limited to the two largest actors in Chemelot, whom both stand at the beginning of the value chain. Therefore, the investment curve that is derived from the results is limited in creating an optimal investment trajectory for the entire industrial cluster, whereas right now it is more focused on the two largest players in the cluster. As mentioned before, adding more complexity to the model and by integrating additional investment options for actors more down stream could overcome this limitation, which will produce more extensive investment trajectories for all actors.

This research mainly focused on the choices to be made regarding sustainable investments under different exogenous factors in different situations. Similar analyses in different clusters can be performed if sustainable investments are included in the model related to that cluster. So the proposed representation and implementation should allow for similar insights to be gained in different research purposes with a focus on the energy transition.

6.4.3 Discussion of the model

As mentioned before, by modelling Chemelot in Linny-R, certain simplifications of the real-life situation had to be made to decrease the complexity. The simplifications started by not incorporating the entire Chemelot cluster, but rather the entire naphtha stream and a part of the NH_3 stream. This scoping decision was made because of the given time frame and because the increased complexity would not directly lead to more ground-breaking findings. However, the level of complexity and the given time still allowed for the necessary analyses to be performed in order to answer the research questions set out in this research. With respect to the model, simplifications and assumptions had to be made to with respect to sustainable investments and future prices of products. The assumptions presented in this research have been based on grey literature, expert information and logical reasoning, however they still present a shortcoming in the research. Adding more complexity in the model is easily implemented since Linny-R does allow for nested modelling to add more detailed processes or other components. The model currently functions by solving the MILP for a high number of variables. If the complexity of the model increases, so does the computational time. Therefore, given the time frame, a certain level of simplicity is required to maintain a manageable computational time, whilst staying at a specific level enough to come up with deep analyses. The model could also become more complex by choosing for smaller time steps. Currently, a time step of 1 year was decided on, because it was easier to look at production levels and data on prices on a yearly basis instead of a monthly, weekly or even daily basis. Given more time, more level of depth can be added to the model by taking a smaller time step.

The data used to set the price for feedstock, emissions and final products are based on projections made for reports and papers, they do not include large fluctuations that are currently experienced because of the war in Ukraine. However, it is expected that when the commodity prices experience unusually large increases because of a crisis situation, it will only slow down the transition speed of an industrial cluster and will make actors behave more individualistic, and in terms of game theory move away from the cooperative game and go 'back' to the non-cooperative game. This will give rise to interesting questions such as: Who will be the first to move away from the cooperative game? How do these large fluctuations influence the cash flow in the industrial clusters? Will investments actually be put on hold in times of large uncertainty? By adding more critical data, more accurate results can be derived from the model. As mentioned, the current data entered is based on (grey) literature and reports. When using real-time data for raw materials, feedstock, intermediary products and final products, the results can provide more accurate insights and by adding more complexity to the model, it can be used as a foundation to look at what investments might be the most attractive under certain situations. The model is limited in this aspect because real-time data is extremely critical and classified, making it not able to use this data for any research purposes.

An interesting approach for further research would be to take a look at contracts between different actors and whether investment contracts would result in different investment trajectories. This could gain new insights in the dynamics between actors on a more contractual level and with minor adjustments can be applied to multiple researches in the future. Furthermore, the model has been developed in such a way that the demand in the market is restricted, and that the large processes such as Olefin 3/4 always need to produce on full capacity. In real-life, the market demand is dynamic of course and will increase in the future most likely. The production capacity has now been restricted and investing in new capacity was only possible if it replaced the existing capacity. In reality, the capacity can be extended through investments such as the Methanol to Olefin production, or producing NH_3 using green H_2. This was not implemented in the model because future demand of the market is very hard to predict, but another implication met was that by setting the demand of the market as the lower bound and setting the upper bound to infinity, caused the model to fail. This was another error found in the model that was not able to be solved. This together with the limitations mentioned above caused the results to be limited in its value.

6.4.4 Discussion of encountered implications

During the development of the model, an implication regarding the green hydrogen to ammonia investment and the electrification of Olefin 3/4 investment was encountered. The investments were first designed to replace the current AFA 2/3 or Olefin 3/4 in terms of capacity, because electrification often involves the existing structure to be adjusted. The way this was implemented was according to the methodology provided in figure 10, however, this restricted the model from using a look ahead larger than 1 to be used. This lead to a decision having to be made regarding the importance of keeping the structure as it is, where the electrification functions as capacity replacement, or removing this from the model to allow for a larger look ahead to be used. The latter was chosen since it is possible for a normal processing unit and an electrified processing unit to operate parallel. Furthermore, the insights that were derived by using a look ahead of 4 were of far greater value than using only a look ahead of 1. Ideally, no choice would have had to be made regarding this issue, but for the sake of the research and the quality of the results, it was decided to go for the larger look ahead.

6.4.5 Discussion of the research limitations

The limitations of the research have been addressed on a few earlier occasions, mainly regarding how the model was created and the setup of the experiments that have ran. Because this has been highlighted before, this chapter will mainly focus on the limitations regarding the methodology applied in this research and the design of the research. MILP has been used to model the dynamics and optimize the cash flow of different actors on Chemelot. Achieving relevant results without getting lost in the details required simplification of the real-life dynamics happening in Chemelot. By reducing the complexity of the cluster, a model could be created using single processes and allowing for multiple analyses to be performed on the achieved results. To simplify the cluster, certain decisions regarding what encompasses the applied scope had been made to reduce the complexity of the model whilst it was still able to answer the main research question. Simplifications were made in the investments and how they are represented and when the investment was made, it could be operated immediately. In real life, constructing a new ammonia plant for example could take op to a decade before it can operate at full capacity. Furthermore, all the production processes are represented as a single process. This simplification was required to reduce the complexity of the model and is a limitation of this study. Future research could be committed to including more details of the processes and not representing them as a single process, as well as including a delay in the model that forces the model to look even further ahead with its investments. In addition to this, only a part of Chemelot was represented as the cluster, which was another limitation of this research. The model did not include the entire NH_3 stream, which could lead to different investment decisions if they would have been included. They were excluded due to the given time, available data on the actual dynamics and increase in complexity. By extending the scope of the research and including the extended boundaries into the model, this limitation can be addressed. Finally, the model mainly focused on providing insights in how private companies should invest in different options. However, given more time, there would also be the possibility to add more governmental support programs, options between public and private companies and more. This rather large limitation could be addressed by including financial incentives for sustainable options or subsidies. By addressing this, an interesting knowledge gap could be filled with rather exciting opportunities in further research to be committed.

7 Conclusion

The conclusion of this thesis will be presented by first addressing the main contributions of the research by first highlighting the sub-questions and then the main research question. After the questions have been addressed, opportunities that have followed from the discussion will be further elaborated on.

7.1 Contributions and research questions

A methodology has been created in this thesis to determine the effects of various exogenous factors on the investment behaviour of actors within industrial clusters and to provide a proof of concept for applying the developed model on Chemelot. This serves as the main contribution of this research. Literature, reports and data from experts allowed for an overview of multi-actor investments, their contractual structure which determines how the investment is organized and how they behave according to Game theory. This allowed for answering sub-question 1. It was determined that large investment projects involving infrastructure development were most of the time performed by one or several actors combined with a state-owned company. Smaller investments such as investing in an electrolyzer or the electrification of a process are usually performed by a single actor. Quite often, the larger investments will be performed under a joint venture or consortium agreement, where smaller investments that could produce a certain (by)product will function under a bilateral contract. However, the use of contractual agreements would go beyond the scope of this research, therefore, they were excluded from this point on in the research.

By extending the literature and reports, exogenous factors were identified that influence industrial clusters in multiple ways. It showed that different governmental decisions such as emission reduction policies, but also not realizing the required infrastructure, limits industrial clusters in the sustainable investments it can make. This shows that the rate at which an industrial cluster becomes more sustainable is not only dependent on internal variables, but also on exogenous factors, answering sub-question 2. From all the identified factors, a selection was made to further investigate because of their impact and the given time frame. With the theoretical lens established at that point, it was important to come up with a methodology to build the model that would be used in this research. By making use of Linny-R, a model was presented which included constraints regarding capacity, investment possibilities and the products that an industrial cluster makes. Furthermore, an adjusted investment structure was presented that allowed for actors to make an investment over time, instead to having to pay for it up front. answering sub-question 3. With this knowledge, it was necessary to start looking at different investment strategies and what the effect was of a different strategy. But, it also had to be tested in a structured way, therefore, the developed methodology was verified by creating a simple model and testing it under different circumstances. This showed that the model was able to invest under different circumstances and that different scenarios could be implemented.

By extending the model that was made, the effect of different investment strategies were able to be examined, and showed that the opportunity to invest over time would always encourage the investment behaviour. This answered sub-question 4. From there, it was necessary to test the proposed modelling methodology in a realistic environment to determine its robustness and whether it would be applicable to other similar systems. By performing a case study on Chemelot, the proposed modeling methodology was tested. Investment options had to be identified for Chemelot, however, writing down every possible renewable investment option would be outside of the scope of this research.Therefore, 6 investment options to decarbonize the naphtha chain and the NH_3 chain were identified and used for this research. Furthermore, data on Chemelot was collected and interviews were conducted to gain more insight in the actors on Chemelot, but also on the interactions and its sustainable plans. This showed that Chemelot was a good fit as a case study to test the proposed modeling methodology, answering sub-question 5. After the model of Chemelot was developed, single exogenous factors were applied to the model to investigate the influence it has on the investment behaviour. This has shown that having full knowledge of future prices very much encourages investment behaviour, and that the model of Chemelot was quite resilient to price increases of various commodities. This all together has answered sub-question 6. Finally, the model that was designed was validated by making use of an expert from Chemelot to determine whether the model was an accurate representation of Chemelot and its dynamics, and whether the preliminary results made sense in terms of cash flow.

The methodology that was used throughout this research adds value to any research attempting to model the interactions, exogenous factors and investments for any industrial cluster following an MILP approach. The implementation of the investment structure allows for actors to invest in a sustainable option whilst not jeopardizing its future of existence. Decarbonizing investments in industrial clusters costs enormous amounts of money, and this structure allowed for actors to invest in such options. It served as a representation of the lack of available funds factor, because in reality, a lot of decarbonizing investments are enabled through subsidies and loans. Other exogenous factors were implemented by putting caps on commodities or by increasing the price over time. With this methodology, insights were derived in the investment behaviour of an industrial cluster, which adds value to any other method that evaluates investments, especially because this methodology allows for a systems perspective. The model that followed from the methodology identified investment trajectories under different scenarios, taking into account all the dynamics present in the industrial cluster. The different exogenous factors implemented in the model changed the investment behaviour of the industrial cluster by having it to speed up its transition to adhere with the regulations and still remain profitable. The insights derived here can serve as an important guideline for actors within industrial clusters using it as a guide for coordinating decisions in multi-actor environments. But, also for policy-makers to see what the influence is of new regulations and policies on industrial clusters and how they will react. The research has also shown how to identify exogenous factors in a systematic manner for industrial clusters and how they could transition towards a CO_2 neutral future. It has been shown that the industrial cluster is very responsive to changing commodity prices, demand in the market and that the investment behaviour is very reliant on how much knowledge it has of future prices. The model also showed which investments appeared the most attractive, given the scenario that the model was in.

The results have shown that the industrial cluster moves towards CO_2 emission reducing investments that have large electricity demands and towards carbon capture investments. On a policy level, infrastructure is very important since it the sustainability of an industrial cluster is not only dependent on how it transitions internally, but also how fast the country it is situated in transitions. Regulators and policy makers should use the findings to engage with actors within industrial clusters to realize a CO_2 neutral future. The societal relevance of this research is provided by showing that implementing exogenous factors and sustainable investment options using the presented representation allows for analysing how an industrial cluster behaves, because it serves as an accurate representation of how actors within the cluster behave. Incentives in the form of cash flow are taken into account as well as the restrictions set by the exogenous factors to identify optimal investment trajectories under different scenarios, providing relevant insights on how multiple actors behave following through a systems perspective.

7.2 Future research

Following from the discussion above, multiple suggestions for future research have already been touched upon. They will be discussed more extensively here.

The limitations described earlier should be first addressed in future research to improve the quality of the results obtained in this research. By focusing on a better representation for investments to be paid over time in combination with capacity replacement instead of parallel expansion creates new insights on the investment behaviour. It is not expected that the results will be very far from each other, but it is worth noting that it might provide interesting new insights. Furthermore, the research could be extended by incorporating more detailed processes to prove the scalability of the model, and performing the research with a different industrial cluster could provide more insights on how exogenous factors might impose different behaviours, and how much geographical factors such as being located near a harbor vs not is a limiting factor in the transition of an industrial cluster towards CO_2 neutrality. Additionally, using extended data sets that include more accurate prices or have insights on future market demand of the finished products will further increase the level of the results. Finally, the research could also use a smaller time step to gain more in-depth results or even implement startup and shut down costs to make the results even more accurate.

Other future research could be committed by using the presented research and include contractual structures between actors in an industrial clusters for investments. The model that could be constructed including these contractual structures can give more insights on how actors behave if costs are shared, but also perhaps if profits are split under said contract. By including bilateral and multilateral contracts such as joint ventures and consortium agreements, can perhaps allow for more investments to be made due to cost sharing and also more insights on the individual versus collective actor behaviour. Furthermore, future research using this research but including detailed information and representation of subsidies for sustainable investment options could examine whether the investment behaviour would change. Currently, large investments are being performed using subsidies to make sure they result in a positive cash flow. In this research, the subsidies have been included by allowing for paying over time, but using the subsidies that governments provide to accurately lower the price of the investments or including an extra revenue stream in the model may result in different insights regarding the optimal investment trajectories. The future research could also include any other policy or regulation that has not been included in this research to further investigate the possible impact those regulations can have on the investment behaviour of actors within industrial clusters. The policy agreements have been limited to reducing the CO_2 emissions, but can be extended by including any other form of emissions and by also looking at the different emission scopes. Finally, by focusing on the interactions and the interconnections actors have within the system and with which contractual structure they work, future research could be committed to analysing what influences different actor weights have on the cash flow allocation, investment behaviour and speed of transition. Insights derived from this can contribute to the overall research on the energy transition for industrial clusters.

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A Implemented model representations

This chapter will elaborate on the investment representation presented below to further elaborate on the structure.

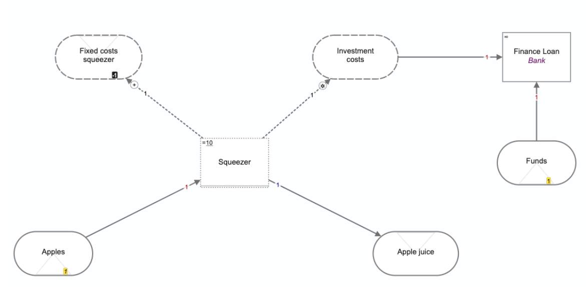

Figure 56: Annualized payment structure

Changing the investment structure from having to pay all costs upfront to allowing actors to pay over time required the incorporation of different processes and data products to facilitate this. The importance in this case was that once the investment was turned on, the payments were performed for each year, up to 20 years. However, if the investment was turned on in time step 3 and turned off 2 time step later, the payments still had to be performed. In reality, payments don't stop when you stop using the machine you have invested in. Therefore, this was a necessary addition to the structure. If the model decides to invest in a technology, a flow moves from the investment to the CAPEX data product. The flow level that goes to the CAPEX is dependent on the CAPEX of the investment, and on the risk value given to that investment. As described in chapter 3.3.1, the risk value is dependent on either a combination of the block length and look ahead, or a value can be given to it. Once the flow has gone from the investment to the CAPEX, a loan is being engaged with the bank by it going into the Finance Loan process. This process is connected to the CAPEX data product and pays for the CAPEX flow, which is implemented by adding a product called Funds. This means that the CAPEX is engaged by the actor that wants to make the investment, and paid initially for by the bank, which is then payed back in 20 equal payments. To prevent the model from "cheating" and making investments in time step 29, and not paying for it, a boundary was implemented in the structure that prevents this from happening.
Actor weights influence the the dynamics in an industrial cluster because it can prevent actors within the model to adjust their production level, or allow others to make larger profits than others. With the verification performed in chapter 4, actor weights were adjusted to see their impact and test the robustness of the model. Below is the configuration of the model. This configuration shows the model where the first actor produces a

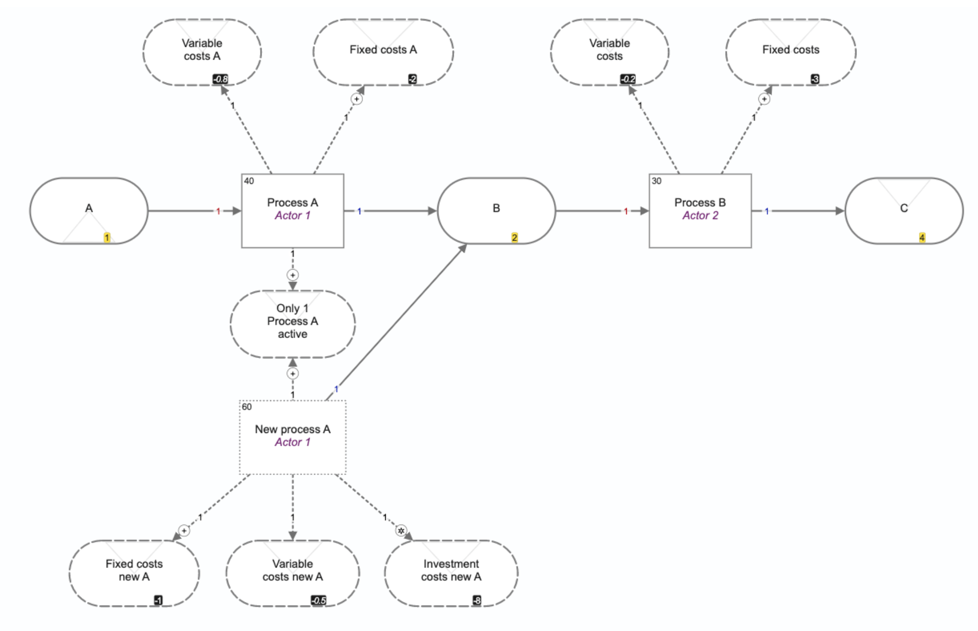

Figure 57: Model used for actor weight verification

half product which is then in turn used by the second actor to produce the final product. If all the actors would carry an equal weight, actor 1 and 2 would make a profit. If the actor weights are adjusted such that actor 2 has a higher weight than actor 1, making her more important, the same production will happen and also if the roles are reversed and actor 1 has a higher weight. Now, by changing the intermediary price of product B in the figure to 4 and changing the product C price to 2 creates an interesting structure. Now, if the model will run, actor 1 will make a profit and actor 2 will make a loss according to the figure 9. However, the cluster will incur a profit. Now, by changing the actor weights, changing the actor 2 weight to 1 will force the model to optimize the profit levels of actor 2. However, the moment that actor 2 will start producing, it will make a loss. Therefore, the model will not run. If the actor weight of actor 1 is changed to 1, the model will optimize the cash flow for actor 1 and it will produce at a maximum level, resulting in large profits for actor 1 and large losses for actor 2. This is in line with expectations regarding changing actor weight within the industrial cluster, but it also shows that interesting interactions can occur within clusters. If for example, profits can be split because of the dependencies actor 1 and 2 have, the overall profits could be maximized.

B Linny-R model of Chemelot

Below is a detailed description of the Linny-R model used for the experiments. The model can be split in two parts, the naphtha chain and the NH_3 chain. The naphtha chain consists of 4 main actors: Sabic, DSM, Borealis and Arlanxeo. The naphtha chain starts by taking naphtha, and process that into ethylene and propylene through cracking. The cracking is performed in the Olefin 3/4 cracker, owned by Sabic. To power the cracker, electricity is required and energy in the form of steam is required. The electricity is imported directly, the natural gas is imported and then combusted to heat up the steam, which in turn powers the Olefin 3/4. Part of the methane that is released in this process is recaptured by Sabic and reused. During this process, large amounts of CO_2 are emitted which are either captured or emitted in the air. After the naphtha has been processed into ethylene and propylene, the ethylene is then either sold as ethylene, or further processed into other products. Those products are: Low-density polyethylene, High-density polyethylene, Ultra-high-molecular-weight-polyethylene, plastomers, Ethylene Propylene Diene Monomer or polypropene. Sabic is responsible for producing the ethylene, LDPE, HDPE, and polypropene. DSM produces the UHMWPE, Borealis produces the plastomers and Arlanxeo produces the EPDM. Within the naphtha chain, various investment options exist. Two of those are carbon capture and storage investments. The more detailed description is presented in chapter 4, but the investment option focuses on either using a low carbon fuel to reduce the CO_2 emissions, or capturing the CO_2 after combustion. Other investment options focus on removing the natural gas from the naphtha chain to reduce the emissions, either through electrification or by using H_2 as a fuel. The last investment option focuses on moving away from naphtha as a raw material and using CO_2 combined with electricity and H_2 to produce ethylene and propylene.

The NH_3 chain starts by using natural gas, air, water and electricity to produce NH_3. This production process generates a lot of CO_2, which can be split in high purity and low purity CO_2. The high purity CO_2 is sold to another actor in Chemelot, which is not represented in this research. The low purity CO_2 can't be sold and is emitted into the atmosphere. After having produced the NH_3, it is either exported as NH_3, or combined with the propylene from the naphtha chain to produce acrylonitrile. From there, the acrylonitrile is either sold directly, or it is sold to DSM such that they can further process it into Stanyl. This makes the NH_3 more complex since it involves the naphtha chain and 3 other actors. The actors present are OCI, Anqore, DSM and Sabic. For the NH_3 chain, one investment option is available, which is a technology that allows for moving away from natural gas as a raw material and to produce NH_3 by making use of H_2. The investment involves an electrolyzer that is build internally and will produce the required H_2. This makes the investment very interesting, but the electricity demand increase makes it expensive if the electricity price is not attractive at the moment. Finally, all investment payments are represented in the "Investments" cluster. Here, the structure as presented in 3.3.2 are added such that the payments are made over time. This results in whenever an investment is made, the payment will not be paid all in once, but divided over 20 years such that more investments can be made since having so much cash is very rare for companies in industrial clusters.

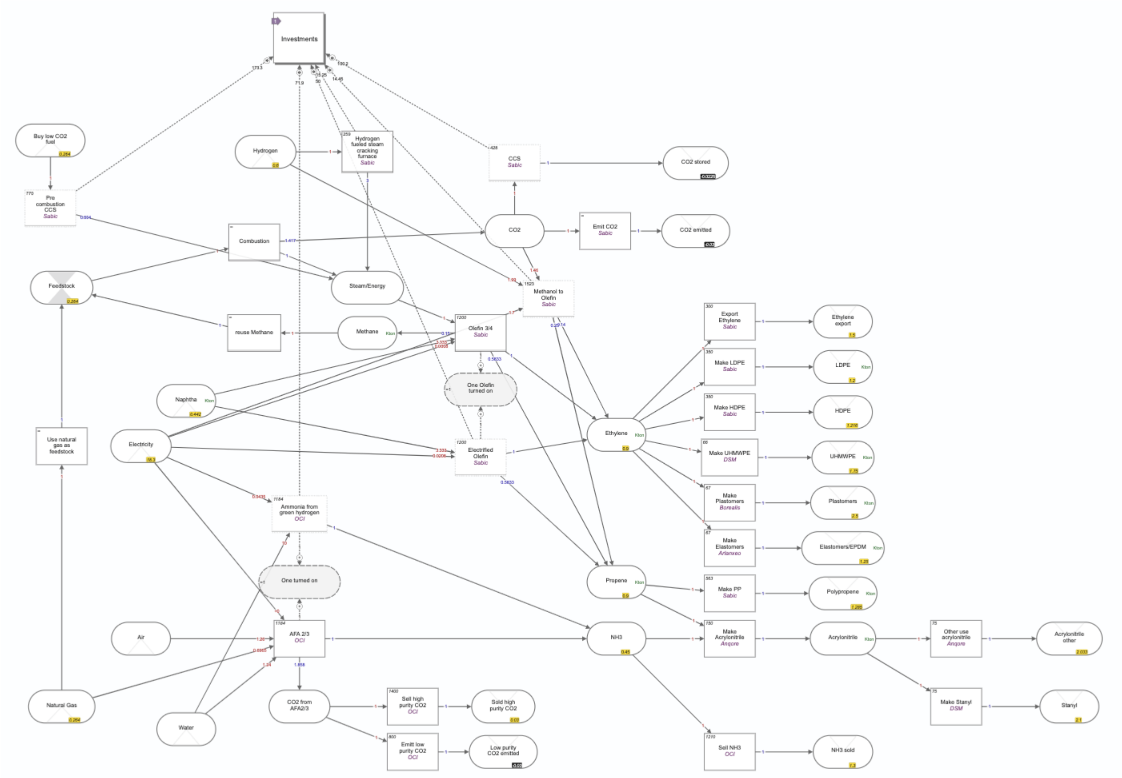

Figure 58: Linny-R model of Chemelot

C Verification results

As mentioned in the research, the model that has been implemented required verification and validation to test the robustness. Here, the verification results will be elaborated on. The first experiment was performed using a simple configuration where a single investment opportunity arose for the industrial cluster, a CCS system that would reduce CO_2 emitted. Depending on the price of CO_2 and the size of the investment costs, the investment would either be profitable because the amount of money saved on emission costs, or loss-making due to high investment costs. In this simulation, the profitability of the investment was adjusted by allowing it to make large amounts of money by saving on CO_2 emissions or by causing enormous losses to be made if the investment would be made.

Expected results - investment representation Below are the expectations for how the actor will behave in this setting:

High profitability results - The model always focuses on optimizing cash flow within the simulation. In this case, if the investment would increase the total amount of cash flow throughout the system, the model will opt for the investment.

High loss-making results - If the investment causes large losses to be incurred, the model will not opt for the investment. Instead, the model will maximize its profits by not changing anything within the system.

The expected outcomes might come over as results that seem very obvious, however, it should be kept in mind that the model will optimize the total cash flow and does not really take into account the effect of that decision on individual actors. Therefore, the expected results should be verified.

Verification results - investment representation
The results of the verification experiment of the investment representation are in line with the expected outcome:

High profitability results - The investment appears to be convenient for Sabic to invest in for every time step in the simulation. Therefore, it will opt for this investment in the first time step, since it will already provide

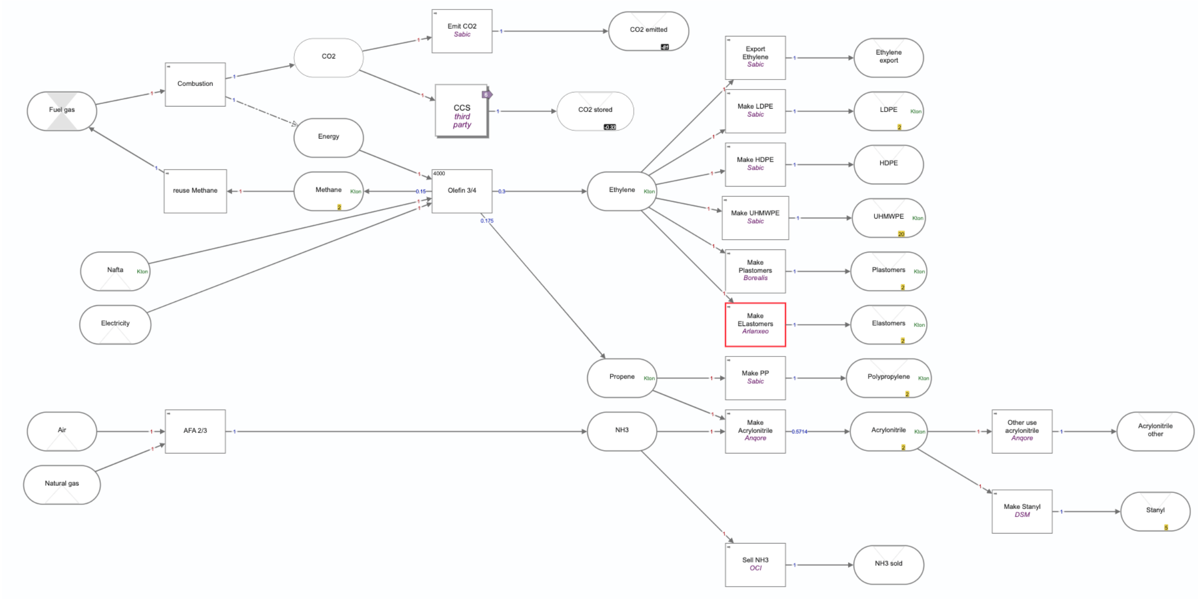

Figure 59: Model used for investment representation verification

an increase in cash flow compared to not investing.

High loss-making results - The investment appears to be inconvenient for Sabic to invest in, for any time step in the simulation. The costs associated with investing in the CCS are too high for the revenue generated by this option. The cash flow would decrease and, therefore, the model does not invest in the CCS.

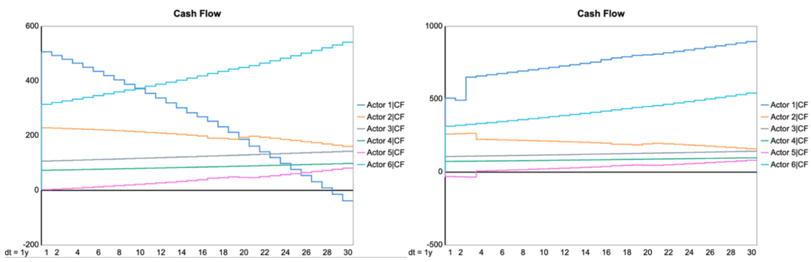

Figure 60: Cash flows of the verification experiment

On the left graph in the figure above, the cash flow of the verification experiment is provided where the investment would make large losses. No investment is being made, and the profits of Sabic (teal line) go down as the price of commodities increases. On the right graph is the cash flow of the verification experiment where the investment would result in extreme profits. Here it can be seen that with this investment, the profits will keep on increasing. This verifies the investment structure and shows the robustness of the model.

To extend the verification process, the model is adjusted, by incorporating a payment over time structure such that the exogenous factor "Lack of available funds" can be implemented in the model. The model still only contains a single investment, which is the CCS investment reducing the amount of CO_2 emitted. Because the setting does not change, only the investment structure, similar results are expected.

Expected results - pay over time representation
Below are the expectations for how the actor will behave in this setting:

Profitable investment - The model always focuses on optimizing cash flow within the simulation. In this case, if the investment would increase the total amount of cash flow throughout the system, the model will opt for the investment. Since the payments for the investment are now spread out over time, the model will invest in a very early time step.

Loss making investment - If the investment causes large losses to be incurred, the model will not opt for the investment. Instead, the model will maximize its profits by not changing anything within the system. The pay over time structure could still interest the model since the payments are low, however, the costs associated with the investment are set at such a level that the model still should not opt for the investment.

The expected outcomes might come over as results that seem very obvious, however, it should be kept in mind that the model will optimize the total cash flow and does not really take into account the effect of that decision on individual actors. Furthermore, the new investment structure might change certain steps or routes within the model, therefore, the expected results should be verified.

Verification results - pay over time representation
The results of the verification experiment of the investment representation are in line with the expected outcome:

Profitable investment - The investment appears to be convenient for Sabic to invest in for every time step in the simulation. Because the costs are spread out over time, the model invests in it at the very first time step, since it will already provide an increase in cash flow compared to not investing. The new investment structure does not provide new results compared with the old investment structure

Loss making investment - If the investment causes large losses to be incurred, the model will not opt for the investment. Even with the possibility to spread out the costs over time, the costs associated with the investment are still too high for the model to opt. Instead, the model will maximize its profits by not changing anything within the system.

The same cash flow results are derived from this verification experiment as the results in the figure above.

Verification of the model
The model used throughout this research needs to be verified, before using it for the case study. To verify it, extreme conditions will be imposed to test the model for multiple actors to gain insights on the robustness of the model. The results will have to be in line with the expectations provided in table 13 in chapter 4.4. For this verification step, the same model without any investment will be used. The model is a basic representation of Chemelot and will be used to verify the exogenous factors described in chapter 3.2.1. The verification experiments were done through implementing extreme values on variables within the model. Variables such as final product price and availability of products are variables with large influences on the profitability of the cluster. For the experiments, one extreme value manipulation was implemented and the rest was left unchanged. The cash flow statements of the experiments are presented below.

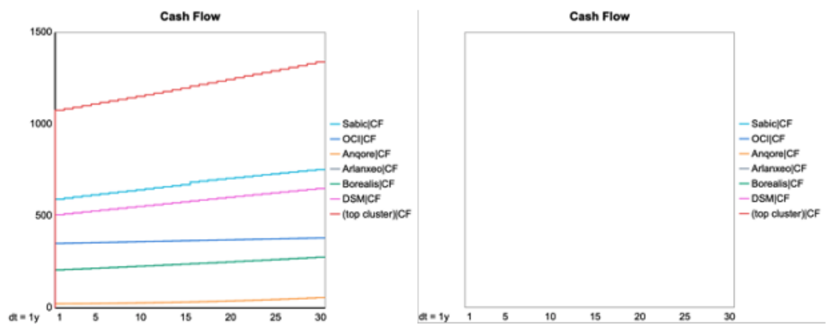

Figure 61: Cash flows for extreme low CO_2 price (left) and extreme high CO_2 price (right)

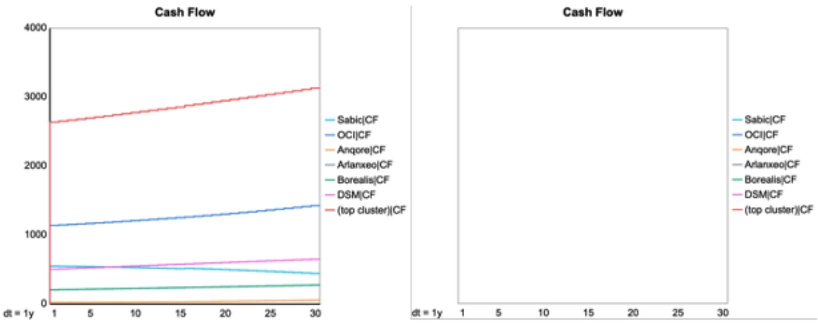

Figure 62: Cash flows for extreme low natural gas price (left) and extreme high natural gas price (right)

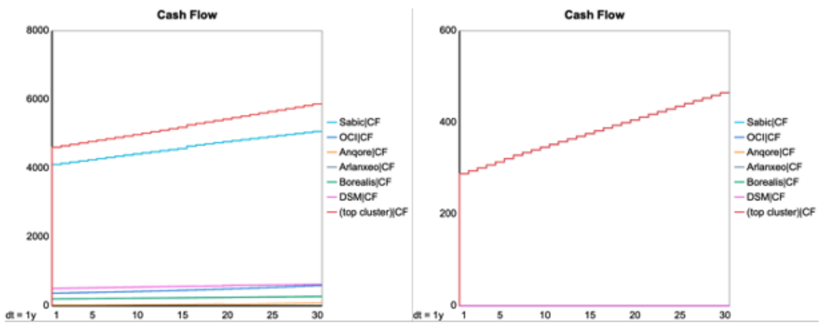

Figure 63: Cash flows for extreme low naphtha price (left) and extreme high naphtha price (right)

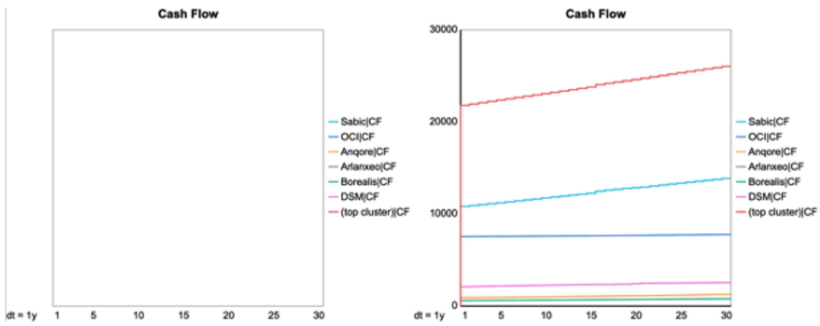

Figure 64: Cash flows for extreme low finished product price (left) and extreme high finished product price (right)

The model behaves according to the expected results presented in the table. What can be observed is that in certain cases such as an extreme low CO_2 price, natural gas price or naphtha price, the model will operate at full level to maximize the profits. This is also the case for when the price of the final product is extremely large. The model wants to optimize cash and in these cases, it will run at max capacity to optimize the cash flow. In the cases of extremely high CO_2 price, natural gas price and low price for final products, the model will not produce anything. The costs far exceed the possible profits and this makes it more profitable to not produce anything instead of producing. In the case of a high naphtha price, the naphtha chain will be shut down, however, the NH_3 chain will still operate since it does not use naphtha in its chain and since the price of NH_3 is set at a normal level, it is more profitable for the entire system to produce in that chain than not to.