Towards a zero-emission naphtha cracking industry in the Netherlands

A model-based exploration of policy options to accelerate electrification

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Executive summary

This research aims to support decision-making regarding the decarbonization of the naphtha cracking industry by analyzing the long-term development of electrification in the industry under deep uncertainty. The analyses suggest that profound changes in current policy instruments are required to achieve a significant degree of electrification in the naphtha cracking industry with sufficient certainty. It is advised to increase government funding for electrification, implement a fiscal shift away from gas towards electricity and to increase the effective carbon levy imposed on the industry. However, though the analyses show that government policy has a significant impact on the development of electrification, its success appears conditional on external factors, most importantly, developments in the energy and carbon markets. In fact, the electricity price and the ETS carbon price turn out to be more influential on emission reduction than most policy interventions. The availability of renewable electricity is the single most influential factor affecting CO_2 emissions and hence, is considered paramount in achieving emission reduction. Therefore, policy aimed at accelerating electrification should be accompanied by decisive government action regarding the development of renewable electricity sources.

In this management summary, first the context of the research will be sketched. Subsequently, the knowledge gap and main research question will be formulated and the research approach will be discussed, followed by a discussion of the results, the main conclusions and policy recommendations.

Introduction

In 2019, the Dutch government reached the Climate Agreement with more than a hundred organizations. The Climate Agreement outlines specific targets and measures for distinct societal sectors regarding emissions and energy use (Netherlands Climate Council, 2019). The industry sector, responsible for 31% of all CO_2 emissions in the Netherlands (CBS, 2019), is required to curb CO_2 emissions by at least 59% in 2030. To achieve this transition, the industry needs to implement efficiency improvements and move away from fossil fuel consumption, among other changes (Netherlands Climate Council, 2019).

The chemical industry accounts for 34% of all industrial emissions in the Netherlands (CBS, 2019) and is thus a major source of CO_2. Therefore, the decarbonization of the chemical industry can deliver a significant contribution to attaining the climate goals.
Electrification of the naphtha cracking industry is the main focus of this research. This industry produces various chemical compounds which in turn act as building blocks for many of the plastics we use on a daily basis (Wong & van Dril, 2020). This process is highly energy-intensive (Falcke et al., 2017) and consumes large amounts of natural gas. Through electrification, the energy supply of this process is switched from natural gas to electricity. Hence, electrification saves gas and can abate CO_2 emissions on the condition that electricity is sufficiently renewable (Wong & van Dril, 2020).

Knowledge gap and main research question

For energy-intensive industries such as the naphtha cracking industry, electrification is regarded as an important decarbonization strategy (Johansson et al., 2018; Chen et al., 2019; Wiertzema et al., 2020; Bataille, 2020). Its potential contribution to abating industrial emissions is significant (van Kranenburg et al., 2016) and due to the fast-decreasing costs of renewable electricity, it offers prospective economic advantages (den Ouden et al., 2018; Wiertzema et al., 2020).
However, the business case for electrification is complicated by various factors (den Ouden et al., 2018). For instance, uncertainties regarding the future energy market play a large role (den Ouden et al., 2018; Griffin et al., 2018; Wiertzema et al., 2020). To tackle these challenges, it is crucial that targeted, long-term policy is formulated (Chen et al., 2019). Based on these insights, the main research question is formulated as follows: *What robust policy options can the Dutch government employ to reduce CO_2 emissions in the naphtha cracking industry through electrification?*
In this regard, the following key performance indicators are defined: CO_2 emissions, production costs and policy costs (the total sum of subsidies granted to the industry subtracted by the total amount of taxes levied).

Research approach

The selected approach is based on the Robust Decision-Making (RDM) framework (Lempert et al., 2013). As RDM provides a framework for testing policy options under an ensemble of plausible futures (Walker et al., 2013a; Kwakkel, Haasnoot, & Walker, 2016; Lempert, 2019), it is suited for the formulated research objective.

The adapted RDM framework comprises three phases: (1) system description, (2) system dynamics (SD) modelling and (3) Exploratory Modelling & Analysis (EMA).
The system description phase involves gaining an initial understanding of the naphtha cracking industry and its multi-actor decision environment. In this phase, interviews are held among industry and government experts.
System dynamics (SD) is a modelling method widely used to study the nonlinear behavior of complex systems. SD aims to capture behavior by means of feedback loop structure (Vogstad, 2004). This principle is based on the notion that existing conditions trigger certain changes in the system, which in turn alter the conditions, thus leading to subsequent system changes (Forrester, 1993).
Exploratory Modelling & Analysis (EMA) is a methodology for analyzing the behavior of complex systems under deep uncertainty. In contrast to SD, it is not a modelling method but rather "a particular way of developing and using models to support decision-making under deep uncertainty" (Kwakkel et al., 2015). EMA is especially suited for the development of robust policy and hence, fits well within the RDM framework. Instead of trying to *predict* the future, EMA aims to *explore* the future by considering a large number of plausible future states of the world (Kwakkel et al., 2015).

System description & system dynamics model

In the naphtha cracking industry, naphtha, a hydrocarbon mixture produced from fossil fuels, is processed into high-value chemicals (HVCs) such as ethylene and propylene. Ethylene and propylene are the world's most-produced chemical compounds and are used as building blocks for several types of plastics (Wong & van Dril, 2020). In the production process, a mixture of naphtha and steam is first fed into a furnace, where it is heated to over 750°C. Under these conditions, the naphtha's hydrocarbon chains break apart into smaller molecules. The cracked gas that leaves the furnaces then enters a chain of consecutive steps of cooling, compression and distillation. This chain features several steam-driven compressor turbines. The high-pressure steam that drives these turbines is provided by boilers, which also produce steam for other parts of the process (Wong & van Dril, 2020).
The furnaces and boilers are fuelled by natural gas and hence, naphtha cracking consumes large amounts of gas and is a major source of CO_2. In this research, the focus is on the decarbonization of furnaces, compressor turbines and boilers through electrification. These installations feature long lifetimes of up to multiple decades which are repeatedly extended through retrofits. Retrofitting entails the upgrading of existing installations by installing new parts, thus extending their lifetimes (Wong & van Dril, 2020; Interviews, 2021).
Investment decisions regarding electrification of these installations, which feature investment costs of hundreds of millions of euros, is impacted by various uncertainties. For instance, the capacity of the electricity grid is a major concern. Moreover, challenges arise from factors specific to the naphtha cracking industry. One is the high degree of integration between systems onsite which implies that the electrification of certain parts of the process requires adjustments in other systems and cycles (Interviews, 2021).

Based on these insights on the industry, a system dynamics (SD) model is developed that describes the development of electrification in the naphtha cracking industry. Investment decisions within the industry are taken as the starting point for this model. Only investment decisions regarding retrofits are considered. Depending on the development of external factors such as energy prices and policy options such as energy taxes and subsidies, the model computes the aggregate cost of electrification versus the aggregate cost of retrofits based on conventional technologies for three types of installations: furnaces, compressors and boilers. The ratio between these costs then determines which portion of the industry's investments is channeled towards electrification. According to the distribution of investments the development of electric and conventional capacities is modelled over time, along with its effects on CO_2 emissions, production costs and policy costs.

Results of the Exploratory Modelling & Analysis

By applying Exploratory Modelling & Analysis (EMA) the system dynamics model is used for simulation. The simulation takes into account a range of plausible future scenarios given the large degree of uncertainty that characterizes the system. From the analyses of the simulation results, it follows that the development of electrification in the naphtha cracking industry hinges on the future state of the energy and carbon markets. Regarding cumulative CO_2 emissions, the availability of renewable electricity turns out to be the single most influential parameter.
Moreover, the development of electrification varies across the different installations considered. The highest electrification rate across the scenarios is attained in compressor turbines, which display an electrification rate of over 80% in almost all scenarios. It also appears that, regardless of the degree of electrification, the production costs of ethylene may be under pressure due to rising energy prices. Furthermore, simulation outcomes

with far-reaching electrification feature relatively higher government expenditures.

Besides analyses of the simulation results, a robust policy search is performed. Robust policies are defined as policies that are relatively insensitive to deep uncertainty and display a certain performance under an ensemble of plausible futures (Giuliani & Castelletti, 2016). As part of the robust policy search, the system dynamics model is subjected to an optimization algorithm which seeks to minimize cumulative CO_2 emissions while also minimizing cumulative production costs and policy costs. Based on the results of the optimization, a selection of robust policies is made.
From the robust policy search, it is found that policy has a significant impact on the development of electrification and CO_2 emissions. On the other hand, the robust policy search shows that even with rather radical policy adjustments, there remains considerable uncertainty about attaining a significant emission reduction. The resulting robust policies introduce profound changes to the current policy instruments and require adjustments in multiple aspects: a substantial SDE++ subsidy (the Dutch government's Stimulation Scheme for Sustainable Energy Production and Climate Transition), a fiscal shift favouring electricity over gas and an increase in the carbon levy, either by abolishing dispensation rights or by substantially raising the carbon levy increase rate post-2030.

Main conclusions

From a qualitative study of the system, the development of electrification appears highly sensitive to external factors. This sensitivity is confirmed by the analyses. Fundamental uncertainties, most importantly the availability of renewable electricity and the capacity of the electricity infrastructure, make the industry hesitant to invest in electrification. Therefore, these uncertainties should be analyzed and accounted for in the design of policies to reduce emissions in the naphtha cracking industry.
The suggested robust policies feature considerable adjustments in almost all current policy instruments in parallel. However, though policy does have a significant impact on the development of electrification, even far-reaching policies cannot guarantee that significant decarbonization is attained. Developments in the market, i.e. the electricity and ETS carbon prices, and the availability of renewable electricity turn out to be the main drivers, or inhibitors, of emission reduction. Policy-makers should be aware of the fact that emission reduction in the naphtha cracking industry is strongly dependent on the availability of renewable electricity.
Moreover, considerable electrification on the medium term does not guarantee far-reaching electrification on the long term as rising electricity prises may pose a limit to electrification.

Limitations of this research

The research presented in this thesis has several limitations, of which a few important ones are listed here. For instance, the choice of system dynamics (SD) as a modelling method poses a limitation as SD is a continuous modelling tool. In reality, however, investment decisions are taken at discrete moments in time and investment sums, capacity acquisitions, etc. are all discrete.
Second, it is questionable whether the development of electrification for the three installations considered can be analyzed separately from the other installations onsite as these processes are all highly interconnected.
Third, electrification is just one of the decarbonization pathways for the industry and should be considered in relation to other decarbonization alternatives, including hydrogen-fuelled cracking.
Regarding investment costs, only the costs for the installations in themselves are considered and adjustment costs for integrated systems onsite caused by electrification have not been taken into account.
Moreover, grid capacity and grid connection upgrades, which feature significant lead times (Scholten et al., 2021), have not been considered. These could lead to substantial delays in the deployment of electrification. Hence, this omission may result in rather optimistic simulation outcomes regarding the development of electrification.

Recommendations for policymakers

First, as the availability of renewable electricity is the most influential factor regarding emissions, policy change to accelerate electrification in the naphtha cracking industry should go hand in hand with more decisive action regarding the development of renewable electricity sources.
Second, a category for electric compressor turbines should be included in the SDE++. The electrification of compressor turbines appears a no-regret measure which also reduces the required boiler capacity.
Third, the introduction of a novel subsidy instrument should be considered as it could be questioned whether the subsidy amount foreseen by the suggested robust policies fit within the current SDE++ system. Hence, the results justify the possible introduction of a novel subsidy instrument.

Moreover, raising the effective carbon levy (*nationale CO_2-heffing*) should be considered, either by phasing out the dispensation rights granted to the industry or through a significant increase of the carbon levy post-2030. Furthermore, to stimulate electrification a more extensive fiscal shift from gas to electricity should be taken into consideration.

Finally, given the dynamism of the future energy market, policy should be designed in an adaptive fashion. Adaptive policy-making involves the construction of a sequence of policy options, which contains both policy options that are implemented upon enacting the policy and contingency plans that are activated based on certain indicators (Walker et al., 2001).

Recommendations for further research

Regarding further research, it is recommended to consider the integration of systems onsite and within industrial clusters. In this manner, the simulation model yields a more realistic estimation of the system costs caused by electrification. It is also recommended to diversify the electrification options for each installation and include additional decarbonization pathways, such as hydrogen cracking, Carbon Capture, Utilization and Storage (CCUS) and feedstock decarbonization. In this way, a more integral approach towards decarbonization is adopted, ensuring a more accurate reflection of the breadth of options that feature in investment decisions.

In light of the dynamism of the future energy market, it is also advised to improve the model such that it allows for the specification of adaptive policies. Furthermore, in future model-based studies of electrification, it is advised to make the modelling process more participatory; this will enhance both the quality of the model and the quality of the explored plausible futures.

Finally, it is suggested to include the product side of the industry in future models. In this research, only operational and capital expenses have been considered. However, it is expected that electrification will impact the composition of the production output, which, in turn, influences revenues (Interviews, 2021). Moreover, developments in the high-value chemical markets may have an impact on the development of electrification as well.

Contents

1 Introduction

In 2015, 190 parties including the European Union signed the Paris Agreement. By doing so these parties have committed to limiting global warming to 1.5°C above pre-industrial levels (Masson-Delmotte et al., 2018). In its pledge to this global agreement, the EU has committed to reducing its carbon emissions by 40% in 2030 compared to 1990 levels (European Commission, 2019). Following the Paris Agreement, the Netherlands adopted a Climate Law in 2019 which legislates a goal of 49% CO_2 reduction in 2030 and 95% in 2050 (Government of the Netherlands, 2020b). In the same year, the national government reached the Climate Agreement together with more than a hundred organizations.

The Climate Agreement outlines specific targets and measures for the five societal sectors that need to reduce carbon emissions: the built environment, electricity, mobility, agriculture & land use and industry sectors (Netherlands Climate Council, 2019). The industry is responsible for 31% of all CO_2 emissions in the Netherlands (CBS, 2019) and to reach the 2030 target, it is faced with the major challenge of 59% CO_2 reduction. This transition needs to be achieved through improved process efficiency, energy-saving, Carbon Capture, Utilization and Storage (CCUS), electrification, use of hydrogen and the implementation of circularity (Netherlands Climate Council, 2019).

Among the industry sectors in the Netherlands, the chemical industry is one of the main sources of CO_2, accounting for 34% of all industrial emissions (CBS, 2019). Like the oil industry and base metal industry, it is a highly energy-intensive industry. Together these three industries account for 65% of all industrial CO_2 emissions in the Netherlands (Kaashoek et al., 2018). Therefore, decarbonization of these industries can potentially deliver a large contribution to attaining the goals set in the Climate Agreement. However, their large heat demand and the high carbon intensity of their processes makes the decarbonization of these industries rather challenging (Davis et al., 2018).

This research specifically focuses on the electrification of the naphtha cracking industry. This industry converts naphtha, a hydrocarbon produced from fossil fuels, into chemical compounds such as ethylene and propylene, which are in turn building blocks for many of the plastics we use on a daily basis (Wong & van Dril, 2020). To convert the naphtha feedstock into these chemical compounds it needs to be cracked, which means the naphtha is broken down into smaller molecules by heating it to over 750°C. This process is the most energy-intensive process in the chemical industry (Falcke et al., 2017) as it requires burning large amounts of natural gas to reach the desired temperature. Natural gas is also consumed for the production of steam, which is required in the post-processing of the cracked molecules. Through electrification, the energy supply of these processes is converted from natural gas to electricity. Hence, electrification saves gas and can abate CO_2 emissions on the condition that electricity is sufficiently renewable (Wong & van Dril, 2020).

Electrification is regarded as an important decarbonization strategy for the naphtha cracking industry but is currently hindered by several barriers. These include uncertainties surrounding future market prices, the capacity of the electricity infrastructure and the availability of renewable electricity. Moreover, several technologies are currently not commercially viable and the prospective capital expenditures for electrification technologies are high. In addition, the large degree of integration of technical systems onsite imply that electrification requires adjustments in other parts of naphtha cracking plants (Interviews, 2021). Government policy could play a pivotal role in giving electrification momentum, for example by providing fiscal incentives that increase the economic feasibility of enabling technologies (van Kranenburg et al., 2016; den Ouden et al., 2018).

The objective of this research is to explore what national-level policy options can accelerate electrification in the Dutch naphtha cracking industry while being robust against uncertainty. In this regard, an exploratory modelling approach grounded in the Robust-Decision Making (RDM) framework (Lempert et al., 2013) will be applied. With this approach, the impact of various policy interventions on the naphtha cracking industry will be tested under a range of plausible futures.

This thesis starts with the identification of the (academic) knowledge gap and the formulation of the main research question (Chapter 2). In Chapter 3 the research approach is outlined and the subquestions are formulated. Moreover, the corresponding research methods will be laid out. Then follows Chapter 4 with a description of the naphtha cracking industry system. Chapter 5 gives a description of the system dynamics model used to study electrification in the naphtha cracking industry. In Chapter 6 the simulation model will be subjected to Exploratory Modelling & Analysis (EMA) which will elicit the most influential parameters on the system and the common features of policy-relevant outcomes of interest. Moreover, a robust policy search will be conducted, which is concluded with the suggestion of several robust policies. Finally, in Chapter 7 an answer will be given to the main research question, followed by a discussion of the limitations of this research and recommendations for policymakers and for further research.

2 Knowledge gap and main research question

The goal of this chapter is to identify the (academic) knowledge gap and formulate the main research question. To do so, both academic literature and reports about electrification in the chemical industry were reviewed. Based on the background information obtained (Section 2.1) the knowledge gap and main research question are formulated in Sections 2.2 and 2.4, respectively.

2.1 Background

This section contains background information about electrification in the chemical industry based on a review of the literature. First, energy and trends in the chemical industry are discussed in Section 2.1.1. Second, the potential of electrification is outlined in Section 2.1.2, followed by a description of strategies, application areas and technology options for electrification (Section 2.1.3), the challenges involved (Section 2.1.4) and the uncertainties that impact electrification (Section 2.1.5). Finally, possible policy interventions are discussed in Section 2.1.6.

2.1.1 Energy use and trends in the chemical industry

With a final energy consumption of 301.5 PJ the chemical industry accounts for 52% of the final energy consumption in the Dutch industry (574.9 PJ) (CBS, 2017). In the chemical industry, heat demand is substantial, accounting for approximately 85% (240 PJ) of the final energy consumption (Rooijers, 2015). In addition, the chemical industry consumes 440.2 PJ in feedstock (CBS, 2017). This illustrates the great challenge of decarbonizing the chemical industry since renewable alternatives need to found not only for the electricity supply but also for the supply of heat and, predominantly fossil, feedstocks.
The chemical industry has already made great advancements throughout Europe: while production increased by 59% since 1990, energy intensity was reduced by 50% (van Kranenburg et al., 2016). Up until 2030 it is expected that, under current policy, the carbon emissions of the Dutch industry as a whole will remain constant, while final energy consumption will also remain constant. This indicates that energy efficiency measures are effective (PBL, 2020). However, more radical change is needed in order to comply with the Dutch Climate Agreement and the goals formulated in the international Paris Agreement. In the Climate Agreement (Netherlands Climate Council, 2019) the Dutch industry pledged to a goal of 59% CO_2 reduction in 2030 with respect to the 1990 level and (near) climate neutrality in 2050. To attain these goals, the following developments are necessary (den Ouden et al., 2018):

- Increasing industrial symbiosis: the exchange of (heat) waste and by-products originating from a certain industry or industrial process that may serve as a raw materials for another (European Commission, n.d.)
- Increasing energy efficiency.
- Reducing fossil feedstock consumption. This can be achieved through electrification (e.g. adopting electrolysis to produce hydrogen), recycling and using bio-based feedstock.
- Deploying low-carbon technologies.

The first three developments are seen as the most pivotal in achieving a substantial reduction in carbon emissions. With regard to low-carbon technologies four different transitions are envisaged for the (chemical) industry: (1) geothermal energy, using the earth's internal heat as a heat source, (2) bioenergy from biomass and green gas, (3) Carbon Capture, Utilization and Storage (CCUS) and (4) electrification (den Ouden et al., 2018).
It should be noted that combinations between these transitions are possible and perhaps necessary to achieve deep decarbonization. As has become apparent above electrification emerges in two developments: the reduction of fossil feedstock consumption and the deployment of low-carbon technologies (den Ouden et al., 2018).

2.1.2 Potential of electrification

Electrification is regarded as a key strategy in achieving deep decarbonization of the chemical and other energy-intensive industries (Johansson et al., 2018; Chen et al., 2019; Wiertzema et al., 2020; Bataille, 2020). Even if Carbon Capture, Utilization and Storage (CCUS) becomes widely applied and energy efficiency-enhancing measures are implemented, substantial electrification will still be required to achieve deep carbonization (Johansson et al., 2018; Bataille, 2020). First, electrification can contribute to substantial reduction in the emission of CO_2 and other greenhouse gases. Even without relying on renewable electricity, full deployment of electrification will lead to substantial CO_2 savings due to the higher energy efficiency of electric technologies (van Kranenburg et al., 2016).

Regarding economic incentives, the increasing share of renewable electricity - from 18% (2019) to 75% (2030) (PBL, 2020) - is an important driver for electrification (den Ouden et al., 2018; Wiertzema et al., 2020). In part due to the substantial subsidization and the consequent scale-up of renewable energy, major cost reductions have been achieved over the last decade: 71% for wind energy and 90% for solar PV between 2009 and 2020. As a result, newly built renewable energy capacity is competitive with existing conventional generation capacity, such as coal, nuclear and gas-combined cycle (Lazard, 2019). Due to further cost reductions, the market price for renewable electricity in the Netherlands is expected to be much lower in 2030 than the wholesale electricity price of 51 euro per MWh: 34, 39 and 41 euro per MWh for onshore wind, offshore wind and solar PV, respectively (PBL, 2020). However, according to den Ouden et al. (2018) the increasing supply of renewable energy will be insufficient "to meet the industrial heat demand for which electrification is technically possible towards 2030." Moreover, it is expected that the increasing supply of renewable energy will not be reflected in the market price of electricity in the near future yet. On the contrary, the market price of electricity is projected to increase up until 2030 (PBL, 2020).

Wind and solar energy do not only drive electrification through low-cost electricity but also through the opportunity for the chemical industry to act as a buffer for the electricity system. With more wind and solar energy generation, the electricity supply will increasingly be subject to weather-dependent fluctuations on an hourly, daily as well as a seasonal basis (den Ouden et al., 2018; van Kranenburg et al., 2016). At the same time, electricity demand also shows fluctuations, because for example households consume more energy at the beginning of the evening when people come back from work and require heat in the winter. Therefore, for energy suppliers and grid operators it is paramount that more flexibility is created within the electricity system in order to smoothen peaks and valleys in both the supply and demand of electricity (den Ouden et al., 2018; van Kranenburg et al., 2016). With more flexibility, energy suppliers and grid operators will be better able to align demand and supply. With more electric installations the chemical industry can contribute to creating the desired flexibility. During peaks in the electricity supply plant operators can switch from conventional energy sources to electricity. This offers an opportunity for the chemical industry as well, because during peak supply electricity prices will be low. As a result, operational margins will increase. As such, the chemical industry will become on actor on the wholesale electricity market (den Ouden et al., 2018; van Kranenburg et al., 2016).

Lastly, because electrification leads to reductions in air pollution and water use, it has societal benefits as well (Bataille, 2020).

2.1.3 Electrification strategies, application areas and technology options

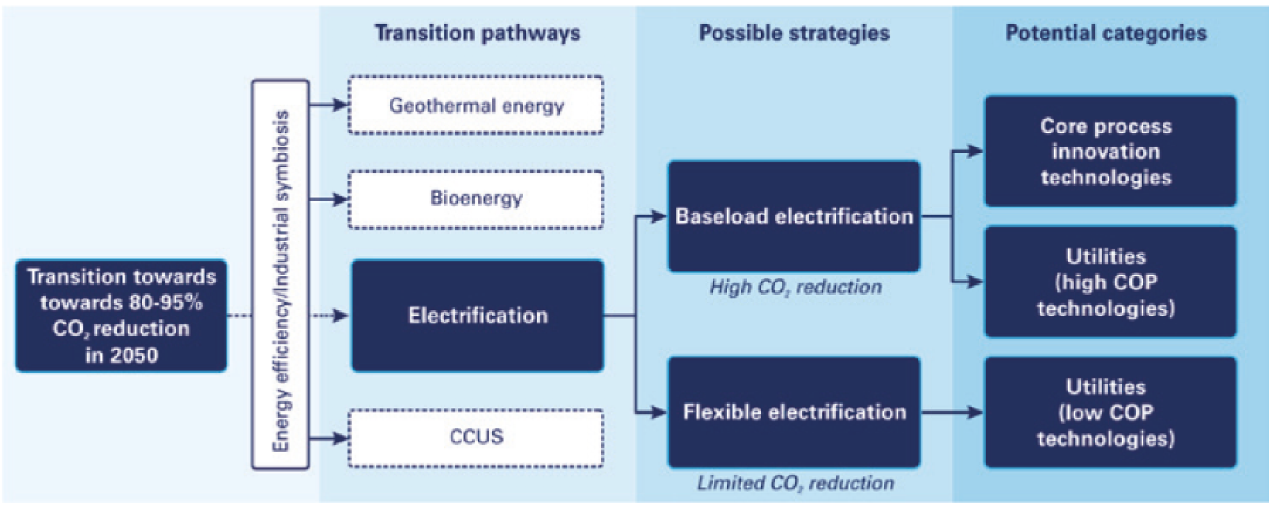

Figure 1: Overview of electrification strategies and their application areas inside the chemical industry. Source: den Ouden et al. (2018).

Electrification can be deployed in a variety of ways. Different strategies, application areas and technologies exist, which are visualized in Figure 1.

With regard to strategies, industrial decision-makers can opt for either *baseload electrification* or *flexible electrification* (den Ouden et al., 2018). Through baseload electrification industrial processes are redesigned such that they operate on electricity in a baseload fashion. The CO_2 reduction potential of this strategy is high but it is less attuned to the expected larger fluctuations in the future electricity supply. (den Ouden et al., 2018). Flexible electrification, on the other hand, means that installations operate on (renewable) electricity on a part-time basis. In this case, installations use renewable electricity when there is sufficient supply and thus, electricity prices are low. In this way, chemical plants are able to respond to fluctuations in the supply of renewable energy and exploit drops in the electricity price (van Kranenburg et al., 2016; den Ouden et al., 2018).

When it comes to application areas, electrification can either be applied in core processes (direct electrification) or in utilities, facilitating systems that are not core to the process (indirect electrification). However, flexible electrification cannot be applied to core processes as these processes require a stable, baseload supply of energy (den Ouden et al., 2018; Wiertzema et al., 2020).
Different technology options for electrification exist. Some involve the direct use of electricity in certain industrial processes to produce heat (Power-to-Heat), mechanical power or pressure. However, the chemical industry uses fossil fuels not only as a source of energy but also as feedstock. In this case, electricity is used to produce hydrogen which can be used as low-carbon feedstock (Power-to-Hydrogen) or to produce chemicals through electrochemical synthesis (Power-to-Chemicals) (Chen et al., 2019; Wiertzema et al., 2020; Bataille, 2020).
In Appendix A electrification strategies, application areas and technologies are discussed in more detail.

2.1.4 Challenges for electrification

Despite the potential of electrification and its presumed indispensability in the chemical industry's pathway to carbon neutrality, challenges remain. First of all, despite the major cost reductions achieved in renewable energy, the electricity price is expected to increase in the short term (PBL, 2020). As a result, switching from fossil fuels to electricity poses an unattractive business case for the chemical industry (den Ouden et al., 2018) and may increase production costs in an industry already characterized by strong competition and small profit margins (Griffin et al., 2018; Bataille et al., 2018). Another economic barrier is posed by the high investment costs of some key electrification technologies (den Ouden et al., 2018).
Secondly, the intermittency and variability of renewable energy sources pose a significant challenge for the stability and capacity of the electricity grid (Chen et al., 2019; Wiertzema et al., 2020). Hence, improved planning and coordination are required to balance the demand and supply of electricity (Chen et al., 2019) and large investments are needed in the grid distribution capacity (Wiertzema et al., 2020). This may cause high additional grid connection costs, which, in the current grid tariff system, are for the chemical industry to bear. Moreover, new flexibility mechanisms will be required in the long term (den Ouden et al., 2018). On the other hand, electrification may also offer grid operators an opportunity to create more flexibility in the electricity system (van Kranenburg et al., 2016; den Ouden et al., 2018).

Another challenge lies in the chemical industry's substantial heat demand, which accounts for approximately 85% (Rooijers, 2015) of its final energy consumption. Current commercially viable Power-to-Heat technologies are only applicable to low temperatures ($<200°C$) (van Kranenburg et al., 2016; Wiertzema et al., 2020) while 65% of the final energy use for heat is for temperatures above 200°C (van Kranenburg et al., 2016). Hence, further technological development is required for electrification to become an option for high-temperature heat (Chen et al., 2019; Wiertzema et al., 2020).

That said, not only the final energy consumption is of concern. Indeed, the chemical industry consumes fossil fuels also for non-energetic purpose, namely as feedstock for the production of chemicals. With 440.2 PJ per year, this consumption is even larger than its final energy consumption, which accounts for 301.5 PJ per year (CBS, 2017). For these purposes, innovative technologies like Power-to-Hydrogen, Power-to-Gas and Power-to-Chemicals are key. However, many of the technologies in these categories are not commercially viable yet and are currently expected only to play a role in the long term (van Kranenburg et al., 2016; den Ouden et al., 2018).

Finally, electrification has consequences beyond the chemical industry as well. This is due to the interconnectivity within the physically concentrated production clusters that characterize the Dutch industry. This interconnectivity concerns both energy and material flows. Hence, altering the energy supply configuration has effects for the entire chain (den Ouden et al., 2018). Among other things, this concerns the increased demand for CO_2 feedstock that electrification involves (Wiertzema et al., 2020).

2.1.5 Uncertainties impacting electrification

Uncertainties also pose a barrier to a decisive adoption of electrification. These include uncertainties concerning the future energy market (den Ouden et al., 2018; Griffin et al., 2018; Wiertzema et al., 2020). In their study Wiertzema et al. (2020) find that specific electrification strategies perform well in certain energy market scenarios, but are not robust in others. They note that the potential for emission reduction and costs is strongly scenario-dependent. These uncertainties are reflected in the development of the electricity price, as well as the market prices of fossil fuels and the carbon price in the EU Emissions Trading System (ETS) which tend to show a rather large bandwidth (PBL, 2020).

Technological development is also uncertain. While current electrification options with high technology readiness levels will reduce energy consumption and carbon emissions in the short term, it is uncertain whether more innovative technologies will reach a commercial breakthrough in the longer term (Griffin et al., 2018). However, without these innovative technologies, such as Power-to-Chemicals, it will be difficult to achieve substantial decarbonization (Chen et al., 2019; Bataille, 2020). This complicates investment decisions (Wiertzema et al., 2020).

2.1.6 Possible policy interventions

There is a need for targeted, long-term policy to accelerate electrification (Chen et al., 2019). Johansson et al. (2018) and Bataille et al. (2018) add that such policy should be adaptive in light of emerging technologies and a dynamic energy market.
Adaptive policy-making encompasses the construction of a sequence of policy options. This sequence specifies policy options that are implemented upon enacting the policy, as well as corrective actions. The implementation of these corrective actions depends on so-called *signposts*, indicators that signal whether the policy should be adjusted or reconsidered entirely in light of developments in the decision-making environment. In this way, adaptive policies account for uncertainties and allow for responding to changing conditions (Walker et al., 2001).
According to Bataille (2020) current government programs to support decarbonization in energy-intensive industries are insufficient to carry emerging technologies over the market threshold and bring about transformative change. Instead, the author argues for making “transition plans” involving a wide range of relevant actors. Moreover, Johansson et al. (2018) and Bataille (2020) agree that carbon pricing alone is not sufficient to encourage the development of new technologies. In part, this is due to the fact that carbon pricing has a limit; after all, a carbon price that is too high would incur carbon leakage. To improve the business case for electrification, den Ouden et al. (2018) suggest adapting grid tariff structures for high capacity connections and reassessing grid connection. Moreover, financial and fiscal incentives are needed, e.g. in the form of funding for pilot projects or guarantee schemes and revolving funds. Another possible solution is to alter energy taxes which currently make natural gas a relatively attractive energy source compared to (renewable) electricity (den Ouden et al., 2018).
Johansson et al. (2018) further highlight the importance of policy packages with mutually reinforcing elements. In such packages, incentives that reward positive action, e.g. R&D funding and risk sharing arrangements, are combined with negative incentives, such as carbon pricing and emission regulations.

2.2 Knowledge gap

The current literature on electrification provides useful insights in the technological options, the potential of electrification and the challenges involved. Though some literature (e.g. Johansson et al. (2018), den Ouden et al. (2018) and Bataille (2020)) do recommend policy interventions to accelerate electrification, no research yet has specifically concentrated on quantitatively evaluating the impact of policy interventions in the chemical industry. Such evaluations have been performed at a macro-level by e.g. Isley et al. (2015) and Li & Strachan (2019) and for other sectors, such as the electricity sector (see e.g. Moallemi, de Haan, et al. (2017). Indeed, Johansson et al. (2018) articulate the need for new approaches to evaluate the effects of policy interventions on the long-term while also taking into account interactions between such interventions.

With regard to long-term planning of energy transitions, Moallemi & Malekpour (2018) argue that the combination of a deeply uncertain future and the involvement of many different actors make energy transitions a so-called wicked problem. Conventional modelling approaches are unable to adequately deal with wicked problems due to their deterministic nature. Therefore, wicked problems call for the application of exploratory modelling, which takes into account many plausible futures (Moallemi & Malekpour, 2018).
The context of electrification in the chemical industry fits this observation since uncertainty with regard to

the future energy market is currently a main barrier to electrification (Griffin et al., 2018; Wiertzema et al., 2020). On the issue of climate policy in a broad sense, several scholars suggest the development of an alternative approach to long-term climate policy-making. Such an approach should explicitly address uncertainty (Workman et al., 2020; Thiele, 2020). Furthermore, Li & Strachan (2019) emphasize that not only technological and environmental relationships should be reflected in the model but also complex societal and political processes should be incorporated.

In conclusion, a need is identified to evaluate the impact of policy interventions on electrification in the Dutch chemical industry, while incorporating uncertainty. This need calls for the development of an exploratory socio-technical modelling approach that establishes a link between technology and policy in the context of electrification in the chemical industry. Furthermore, in light of the Dutch Climate Agreement, the impact of policy interventions should be evaluated against the set climate goals.

2.3 Scope: electrification of the naphtha cracking industry

Including all possible electrification technologies and all chemical industry processes with potential for electrification would be infeasible due to the time constraint and purpose of this research. Therefore, this research will focus specifically on the electrification of the naphtha cracking industry.

Firstly, this industry was selected because it is highly energy-intensive (Haribal et al., 2018); according to Ren et al. (2006) it is the most energy-intensive process in the chemical industry, consuming 8% of the sector's primary energy demand (as of 2006). In the Netherlands, six steam crackers are operated at three locations (Wong & van Dril, 2020). As such, naphtha steam cracking provides an important potential for reducing large amounts of CO_2 emissions in one fell swoop. Secondly, the scope was limited to electrification. It should be emphasized that other decarbonization options exist this industry, which can be combined with electrification.
However, electrification options exist for both the very large-scale equipment (furnaces) which may play a role in the longer term, as well as for supporting equipment, such as compressors, currently driven by steam, which may play a role in the shorter term. Limiting this research to electrification does not mean that the industry's options are limited to electrification. However, it helps to limit the scope, while considering a sufficient number of options with a spread in both time and size in order to illustrate the potential of this research approach.
Though the electrification of the naphtha cracking industry offers a large CO_2 abatement potential it also features very large investments (in the order of hundreds of millions of euros) and long-term planning due to turnaround times of 6-7 years (Interviews, 2021). Therefore, decision-making with regard to electrification of these processes is highly sensitive to uncertainties.

2.4 Main research question

The knowledge gap formulated above leads to the following research objective: to explore potential policy options aimed at accelerating electrification in the naphtha cracking industry while being robust against uncertainty. Consequently, the following main research question can be deduced: *What robust policy options can the Dutch government employ to reduce CO_2 emissions in the naphtha cracking industry through electrification?*

Curbing CO_2 emissions in the naphtha cracking industry may induce higher production costs for the industry as well as higher government expenditures for the required policy options. Hence, in this research, we are interested in policy options that reduce CO_2 emissions, while keeping production costs and policy costs limited. Hence, the selected key performance indicators in the context of the research objective are:

1. CO_2 emissions of the naphtha cracking industry
2. Production costs of the naphtha cracking industry
3. Policy costs: costs of the combined policy options aimed at reducing CO_2 emissions

3 Research approach, subquestions and methodology

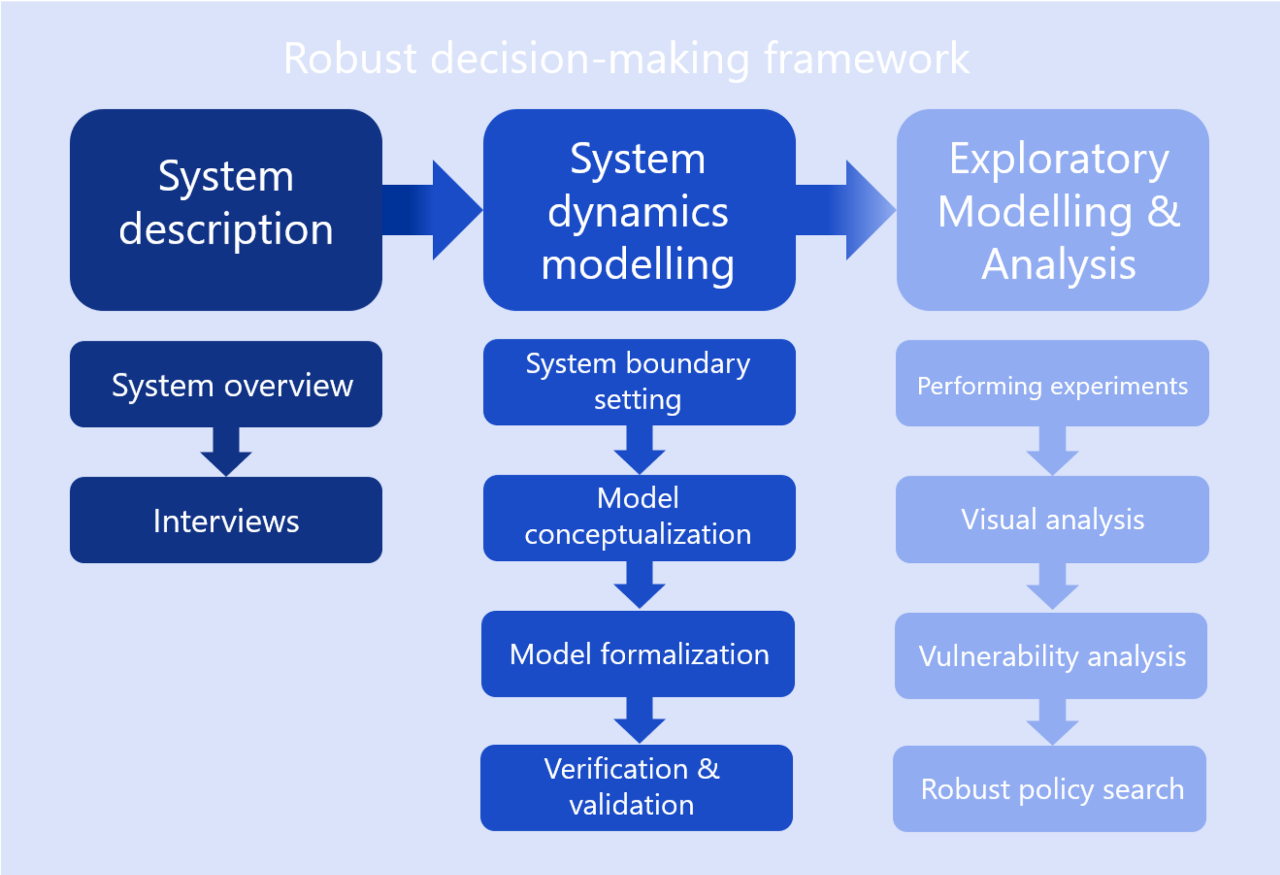

Figure 2: Research roadmap: overview of the consecutive phases of this research.

In order to answer the main research question formulated in Section 2.4 an approach grounded in the Robust Decision-Making (RDM) framework will be used. The RDM approach used consists of different phases, an overview of which is provided in Figure 2.

In this chapter the choice for an RDM approach will be outlined and motivated (Section 3.1). Afterwards, the research subquestions will be formulated. Methods and data will be outlined in Section 3.2 per research phase.

3.1 Research approach and subquestions

Given the research objective, the exploration of policy options, a modelling approach is apt. The future is highly uncertain, yet policymakers are required to act to meet the goals set in the Climate Agreement. As is it impossible to experiment with policy intervention in the real-world, simulation models offer an alternative for virtual experimentation. Hence, simulation models can aid evidence-based decision-making with regard to a deeply uncertain future (Gilbert et al., 2018; Ssser et al., 2021).
Next question is what type of modelling approach should be applied.

In general, climate change mitigation concerns a deeply uncertain future, from a natural systems, a technological and a political perspective (Thiele, 2020). This is also true for policy targeted at the naphtha cracking industry as was explained in Chapter 2. Specifically with regard to electrification in the naphtha cracking industry, energy market uncertainties also play a role. Moreover, the system is characterized by a multi-actor decision-making environment. Hence, it is characterized as a wicked problem (Incropera, 2016) which conventional (predictive) modelling approaches are unable to deal with (Moallemi & Malekpour, 2018). Therefore, studying policy interventions to accelerate electrification in the naphtha cracking industry calls for the application of an *exploratory modelling* approach to develop policy that is robust against uncertainty.

In contrast to *predictive modelling*, which aims at optimizing performance in a limited set of future scenarios, exploratory modelling recognizes that there is a large number of plausible future circumstances and focuses on testing the system's behavior under a wide range of scenarios through simulation (Moallemi & Malekpour, 2018). Exploratory modelling is useful for studying the behavior of complex socio-technical systems since they are surrounded by uncertainty and insufficient knowledge. Hence, the modeller needs to make a rather large number of assumptions and consequently, the resulting model cannot be viewed as predictive of the system's behavior. Instead, the model should be viewed as a way to conduct experiments, testing various plausible assumptions and exploring their consequences (Bankes, 1993).

The Robust Decision-Making (RDM) framework, originally developed at the RAND Corporation (Lempert et al., 2013), can form the basis for an exploratory modelling approach. RDM is a widely used approach to tackle complex decision-making problems featuring deep uncertainty. It revolves around the question: "How can we make good decisions without making predictions?" (Pardee Rand Graduate School, 2021; Lempert et al., 2013). Using a selection of model-based methods and tools, RDM provides a framework for testing policy options in a large number of plausible future scenarios. These tests reveal possible vulnerabilities in the selected policy options, which can then be adapted to be better prepared for certain scenarios. (Walker et al., 2013a; Kwakkel, Haasnoot, & Walker, 2016; Lempert, 2019). In this manner, robust policies can be developed, *robust* meaning that the number of plausible futures in which the policy options perform sufficiently well is maximized, although the policy may not achieve satisfactory performance in every single plausible future (Walker et al., 2013a).

The usual steps that RDM features have been adapted to fit the scope and purpose of this research (Walker et al., 2013a; Kwakkel, Haasnoot, & Walker, 2016; Lempert, 2019), resulting in the following steps:

1. **System description**. This first phase involves outlining an initial understanding of the socio-technical system of electrification in the naphtha cracking industry. This is done by establishing the actors' objectives and their potential actions, including policy interventions. Part of this step is also to determine the uncertainties that may impact the outcome of these actions and the key relationships within the system (qualitatively).
   (a) **System overview**. First a broad overview of the system under consideration is constructed through studying both academic and "grey" literature.
   (b) **Interviews**. Through interviews with representatives from the industry and the government (specifically, the Ministry of Economic Affairs & Climate) a better understanding of the system is gained, including actor objectives, uncertainties, potential policy interventions and relationships existing within the system.
2. **System dynamics modelling**. RDM does not specify a standard modelling method; multiple modelling methods are possible. For this research, system dynamics (SD) modelling will be used, which forms the basis for the following modelling steps (Sterman, 2000; Vogstad, 2004; Vensim Documentation, n.d.-b). The SD paradigm and the justification for using SD in this research will be explained in Section 3.2.2.
   (a) **System boundary setting**. Based on the system description and the system boundary the system boundary is set. This phase revolves around the question: which elements of the system are crucial for studying the system's behavior and which could be omitted? In this manner, it is determined which variables are endogenously modelled (being internal system variables) and which are exogenously modelled (being external factors). System aspects that are considered outside of the scope of this research will be omitted.
   (b) **Model conceptualization**. This phase involves formulating a dynamic hypothesis about the system. A dynamic hypothesis is a theory that describes the system's structure. Moreover, the list of external factors and policy options included in the model is finalized.
   (c) **Model formalization**. In this step, the conceptual model is translated to a set of mathematical relationships. With these relationships, the model can be used for simulation: numerical integration of the equations.
   (d) **Verification & validation**. This step involves testing of the model to examine whether it produces the expected behavior and to validate that the model presents an adequate representation of reality.
3. **Exploratory Modelling & Analysis**. Once the SD model has been established, it is subjected to Exploratory Modelling & Analysis (EMA). EMA is a methodology to analyze complex systems characterized by deep uncertainty (Bankes, 1993); it is further explained in Section 3.2.4.

(a) **Performing experiments**. In this phase, plausible future scenarios will be defined. Moreover, numerical bandwidths for the identified policy interventions are established. The SD model is then used for simulation under an ensemble of plausible futures, while testing different policy interventions. This yields a database of simulation results.

(b) **Visual analysis**. The database of simulation results generated in the previous step is subjected to visual analysis to study the behavior of the system under the different plausible futures and policy interventions.

(c) **Vulnerability analysis**. This step aims at characterizing so-called *regions of interest* in the simulation results: results which feature either very good performance or very poor performance. Under which conditions will the system succeed in achieving or fail to achieve the established objectives of reducing emissions while keeping production costs and policy costs limited? In this way the input parameters (policy options or external factors) with the highest influence on the system will be elicited. (Kwakkel, 2017a)

(d) **Robust policy search**. In this step the SD model is subjected to an optimization algorithm that identifies *robust* policies: policies that maximize system performance across a range of plausible futures (Walker et al., 2013a).

Based on the research phases formulated above the following research subquestions can be formulated:

1. How can the socio-technical system of electrification in the naphtha cracking industry be described and modelled? (Phase 1 and 2)

2. How does the system behave under an ensemble of plausible futures and policy interventions? (Phase 3a and 3b)

3. How do the input parameters map onto the system's key performance indicators? (Phase 3c)

4. Which policies qualify as robust given the system's performance across an ensemble of plausible futures and policy interventions? (Phase 3d)

3.2 Overview of the used methods

In the following, the methods used in this research will be outlined and the data specifications elaborated. First, an overview will be provided of the research methods: semi-structured interviews, system dynamics (SD) and Exploratory Modelling & Analysis (EMA). Then, for each subquestions the methods and data specifications will be detailed in Section 3.3.

3.2.1 Semi-structured interviews

In order to gain insight in the relationships in the socio-technical system of electrification in the naphtha cracking industry, the potential policy options industrial and governmental decision-makers are considering and the uncertainties that impact their decisions, consultation and deliberation with stakeholders is essential. This will be done through semi-structured interviews (Fylan, 2005). As opposed to structured interviews that feature a predetermined set of questions that are the same for each interviewee, semi-structured interviews are more of a conversation aimed at eliciting stakeholders' viewpoints, objectives and criteria. Questions and discussion topics will be prepared in advance, but the interview is flexible and can deviate from the prepared format (Fylan, 2005; Kelly, 2010). The semi-structured interviews will not lead to ready-to-use quantitative input for the SD model and EMA process. Rather, they provide a qualitative basis for establishing relationships in the system and elicit uncertainties that impact their decisions. Moreover, the interviews will yield narratives upon which policy options will be based.
Based on the actors identified in Section 4.1.5 the following actors will be interviewed:

- Naphtha cracking industry: four representatives from different chemical companies and other relevant companies, such as service companies. From these interviews it should become clear by what factors investment decisions are influenced. Also actors' objectives and criteria will be identified. Moreover, it should be elicited what uncertainties complicate decision-making in the naphtha cracking industry.

- Government: a representative the Ministry of Economic Affairs and Climate. Through this interview, policy options will be identified and detailed.

3.2.2 The system dynamics paradigm

System dynamics (SD) is a method to model the nonlinear behavior of complex systems using a feedback loop structure (Vogstad, 2004). SD builds on the notion that existing conditions trigger changes in the system, altering the conditions and thus influencing later changes. This is what the founder of the SD field, Jay W. Forrester, called a *feedback structure* (Forrester, 1993). SD can be applied to virtually every complex system, be it natural, societal, organizational, technical, economic or a combination of these. How the SD paradigm applies to a decision-making context can be explained based on Figure 3. It is the system characteristics displayed in Figure 3 (c), nonlinearity and multiple feedbacks, that SD strives to capture.

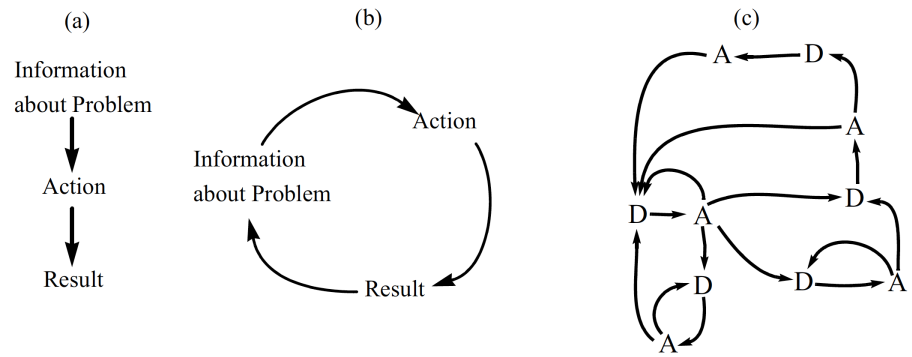

Figure 3: Different views of decision-making. (a) shows a linear approach to decision-making which functions as the framework for many discussions in society. (b) shows a nonlinear approach in which decision-making is recognized as a continuous process: each action changes the system's state, which in turn leads to future actions. In (c) we see a multiple loop information feedback structure with multiple different actor perceptions (D) lead to actions (A) which in turn influence future actions taken by other actors. This structure represents more closely how decisions are made in reality. Source: Vogstad (2004)

The four main characteristics of SD models are: (1) a bounded system with its basic structure composed of feedback loops, (2) so-called *stock variables* representing accumulation processes within the feedback loops, (3) *flow variables* representing changes (increases or decreases) in the stock variables, (4) actions determined by the discrepancy between the system's observed state and its desired state (Forrester, 1968, 1969; Papachristos, 2019). SD has an endogenous perspective to complex systems: it assumes that causal relations within a complex system create feedback loops that determine the system's behavior. Without these internal causal relations, the system's behavior would be determined by exogenous factors only (Richardson, 2011). Hence, "structure drives behavior" is a principle central to SD (Forrester, 1961).
Through its ability to capture feedback loops, accumulations, time delays and nonlinear behavior SD is geared to dealing with dynamic complexity in systems (Sterman, 2000; Lane, 2010) and simulating the system's behavior over time (Lane, 2000). Thus, SD models contribute to enhancing our understanding about complex systems (Sterman, 1994, 2000).
SD allows for an interdisciplinary research approach as it is able to capture not only technical factors, but also societal, economic and behavioral ones (Sterman, 2000). As such, SD can be used for the quantitative evaluation of policy interventions. Therefore, it is a tool for evidence-based decision-making (Holtz et al., 2015).

SD modelling usually consists of five steps: (1) problem definition, (2) model conceptualization, (3) model formalization, (4) verification & validation and (5) policy evaluation. In this research, the system description phases acts as the first step. During the fifth step the impact of policy interventions on the system's behavior are evaluated, which is done through Exploratory Modelling & Analysis (EMA). Hence, the EMA phases replaces the fifth step of SD in this research. All in all, integrating SD in the RDM framework leads to the research phases outlined in Section 3.1.

3.2.3 Justification for using SD in this research

SD is deemed an appropriate method to study electrification in the naphtha cracking industry and to evaluate the impact of policy interventions on this process. Several reasons can be given to justify this choice.

First, as explained in Section 4.1.4, the naphtha cracking industry sector can be viewed as a complex socio-technical system with interacting interdependent technical and social components and a multi-actor environment. From these characteristics, information feedbacks emerge (Chappin, 2011). For example, an increasing number of electric installations reduces the marginal costs for the additional grid connection required for electrification. This lowers the costs for further electrification as expected by the industry, fostering further investments in electrification. Furthermore, SD accommodates the study of transitions at the macro level as well as lower levels. Hence, SD is suited for studying transitions at the sector level (Geels, 2002; Geels & Schot, 2007; Geels et al., 2017; Papachristos, 2019), such as electrification in the naphtha cracking industry.

Second, electrification is essentially a transition: the evolution of a socio-technical system over decades. From a systems perspective, a transition can be regarded as a change from one system state to another system state (Chappin, 2011). SD is widely regarded as a modelling tool suited to study such changes since it draws upon the causal feedbacks between interconnected factors (Köhler et al., 2018). Moreover, electrification requires investments in production installations that have a very long technical lifespan: 30-50 years (Chappin, 2011). SD is well suited to model investment cycles that involve time delays, nonlinearities and feedbacks (Vogstad, 2004; Chappin, 2011). For these reasons, authors such as Vogstad (2004) and Moallemi & Malekpour (2018) have applied SD modelling to the transition of the electricity sector.

A third reason is the role of actor behavior in the electrification of the naphtha cracking industry. The development of electrification is determined by investment trade-offs: is it worthwhile to invest in new electric capacity while depreciating current assets or will current assets be kept in operation, delaying investments in electrification? Hence, actor behavior is at the core of these investment decisions. Through information feedbacks SD can incorporate actor decisions (Vogstad, 2004).
For this reason, it could be argued that agent-based modelling (ABM) would be even more suitable. In ABM, a system is modelled as "a collection of autonomous decision-making entities called agents" (Bonabeau, 2002). By definition, ABM adopts a perspective at the level of the system's constituent units, its agents, rather than at an aggregate level (Bonabeau, 2002). This perspective does not match this research for two reasons. First, the goal of this research is to model a longer-term transition with a high abstraction level. Second, no model-based approach for evaluating policy interventions specifically in the naphtha cracking industry has been developed yet. Therefore, there is still limited information about the system's behavior, let alone the behavior of individual system constituents. Consequently, adopting a aggregate level perspective is suitable (Borshchev & Filippov, 2004).

Moreover, modelling methods such as SD the impact of policy interventions can be evaluated in quantitative terms. Current studies focusing on electrification in the naphtha cracking industry (e.g. van Kranenburg et al. (2016)) outline roadmaps and make suggestions for policy interventions but have not actually modelled them. Existing scenario analyses - such as the Energy Transition Model, or ETM, developed by Quintel Intelligence and used by Berenschot (Quintel Intelligence, n.d.) are static and do not take into account the dynamic characteristics of sustainability transitions. Hence, the application of SD could deliver an important contribution to evidence-based decision-making for both industrial actors as well as the government.

Lastly, SD fits well within the RDM framework chosen for this research. When complemented with Exploratory Modelling & Analysis (EMA) SD can be used for the analysis of the impact of uncertainties and the resulting vulnerabilities of policy interventions. EMA is explained in more detail in the next section, Section 3.2.4 (Kwakkel et al., 2015).

3.2.4 Exploratory Modelling & Analysis

Exploratory Modelling & Analysis (EMA) is a methodology to analyze complex systems characterized by deep uncertainty (Bankes, 1993). Unlike SD, it is not a modelling method but rather "a particular way of developing and using models to support decision-making under deep uncertainty" (Kwakkel et al., 2015). EMA is especially suited for the development of robust policy and hence, fits well within the RDM framework (Kwakkel et al., 2015). In contrast to predictive modelling, where a single model is designated as representative for a certain system, EMA recognizes that such a model does not exist since the modeller never has complete knowledge of the system that he/she is modelling. Instead, EMA acknowledges that the system is best represented by a series of models. By combining these models, the system's behavior can be understood better than by a single model (Bankes, 2002; Kwakkel et al., 2015). This implies that instead of using a model to make predictions, it should be used to perform experiments based on multiple hypotheses (Kwakkel et al., 2015).

The idea of using a model to conduct experiments relates to the notion of using the model as a function $M = f(X, L)$, also known as the XLRM framework (Lempert, 2003), visualized in Figure 4. In the XLRM framework, R represents the simulation model, which in this case is an SD model. L represents the policy levers or policy options aimed at influencing the system's behavior. X represent the exogenous uncertainties, which lead to different plausible future scenarios. With EMA one samples over this series of plausible futures, yielding different system behaviors and different results. The performance of different policy options L against multiple plausible futures are analyzed and evaluated based on M, the performance metrics which follow from the stakeholders' objectives and criteria (Lempert, 2003; Bankes et al., 2016; Kwakkel, 2017b).

Hence, instead of in predictive modelling where just one model $M = f(X, L)$ is obtained, EMA results in multiple models $M_{11} = f(X_1, L_1)$, $M_{12} = f(X_1, L_2)$, ..., $M_{1n} = f(X_1, L_n)$, $M_{2n} = f(X_2, L_n)$, ..., $M_{mn} = f(X_m, L_n)$.

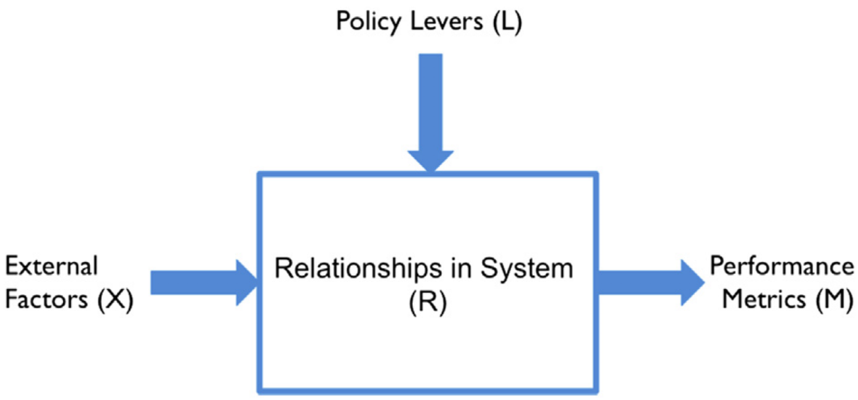

Figure 4: The XLRM framework. Source: Kwakkel (2017b)

3.3 Description of research phases

In section each of the research phases formulated in Section 3.1 will be outlined in more detail. The research phases will be illustrated by means of a simple example. For each research phase and subphase will be described what data is needed to answer the subquestion, which research methods will be used to gather that data and which data analysis tools will be applied.

3.3.1 Phase 1. System description

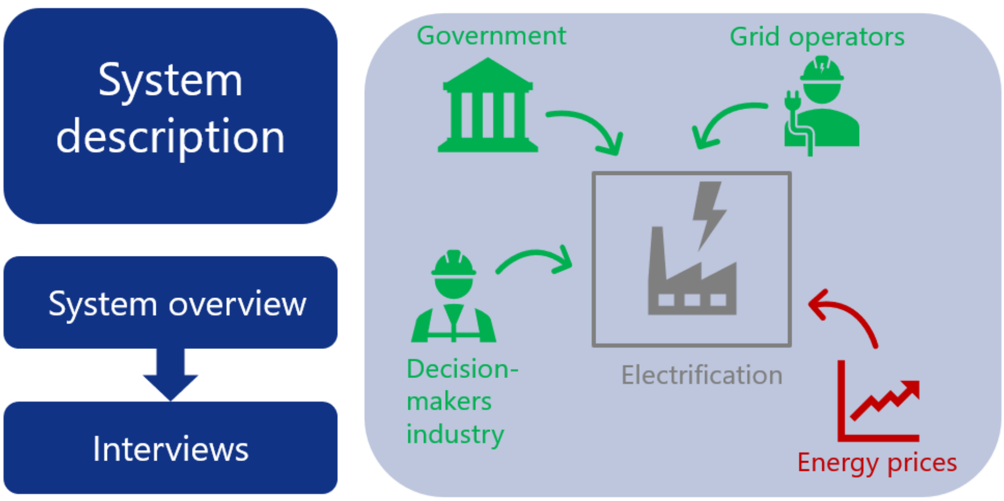

Figure 5: Illustration of the system description phase. This phase involves outlining an initial understanding of the system, including the identification of the actors and external factors that influence investment decisions in the naphtha cracking industry and a qualitative description of relationships between system components.

Through a review of literature and interviews with representatives from the naphtha cracking industry, it will be elicited which actors influence investment decisions in the naphtha cracking industry. Also, relationships between system components will be studied. Moreover, it will be identified which uncertain external factors currently pose barriers for the industry to invest in electrification. Some uncertainties were already described in Section 2.1.5. Moreover, through interviews with the Ministry of Economic Affairs and Climate policy options will be identified and described.

3.3.2 Phase 2. System dynamics modelling

In this phase, the system dynamics (SD) simulation model will be built. This will be done based on the system relationships that follow from the semi-structured interviews with actors in the system. Furthermore, literature such as reports belonging the MIDDEN (Manufacturing Industry Decarbonisation Data Exchange Network) database (e.g. Wong & van Dril (2020)) will be used that contain technical specifications of industrial installations and electric alternatives, e.g. electricity demand, feedstock demand, investment costs and greenhouse gas emissions. The SD modelling software Vensim will be used for model conceptualization, model formalization and verification & validation of the resulting model.
As outlined in Section 3.1 this phase will consist of four steps.

1. **System boundary setting**

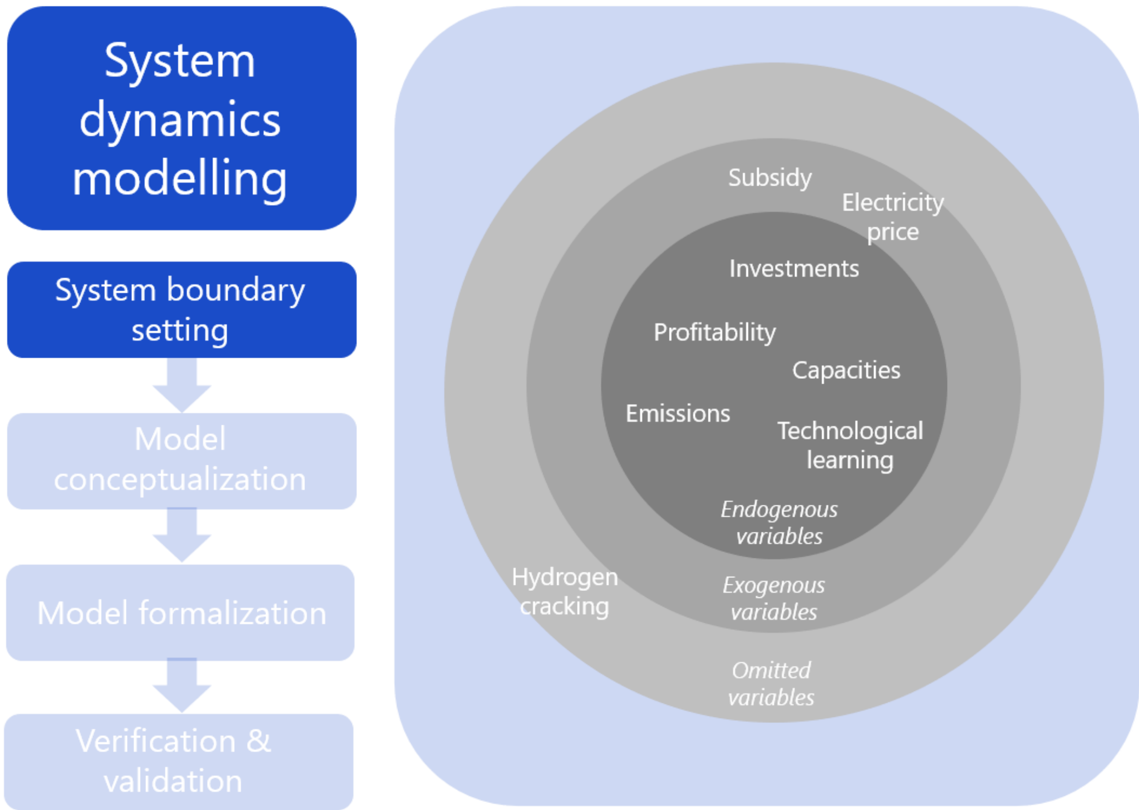

Figure 6: Illustration of the system boundary setting subphase. This phases involves determining which variables are considered endogenous to the system, which are exogenous and which are emitted entirely.

System boundary setting is about determining which variables are modelled endogenously, i.e. variables considered internal to the system under consideration. Other variables are modelled as external factors (or modelled exogenously). Yet other variables are omitted from the system because they are either considered out of scope or not influential on the system (Sterman, 2000). Figure 6 provides an illustration of the system boundary setting. In this example, profitability, investments, capacities, etc. are all considered internal variables. On the other hand, subsidy (policy option) and the electricity price (external factor) are modelled exogenously. Hydrogen cracking (replacing natural gas by hydrogen in naphtha cracking plants) is considered out of scope of this research as only electrification is studied.

2. **Model conceptualization**

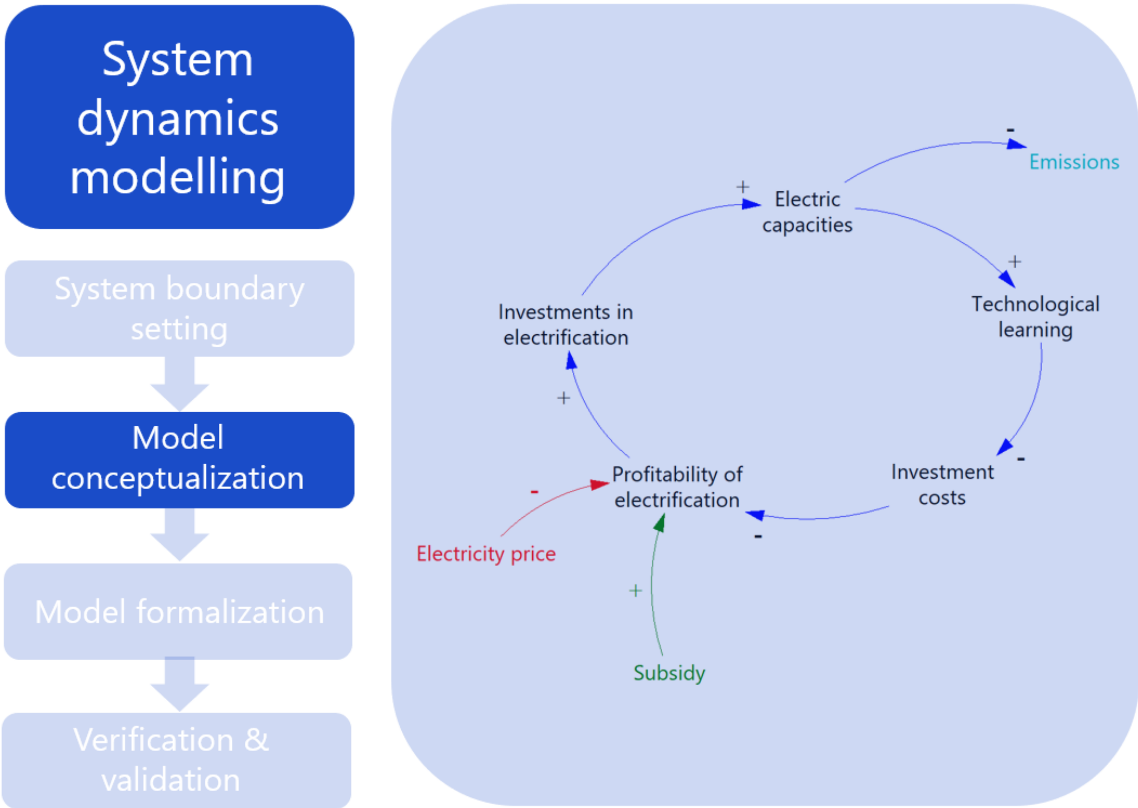

Figure 7: Illustration of the model conceptualization subphase. The output of the model conceptualization is a causal loop diagram (CLD). This example CLD features a positive (or reinforcing) feedback loop: higher investments lead to more installed capacities, which increase technological learning as a consequence of the learning effect, in turn reducing the required investment costs, fostering investments. The CLD features two input parameters which affect the profitability of electrification: *subsidy* (a policy lever) and *electricity price* (an external factor). *Emissions* form the model's output variable, by which the system's performance is measured.

Based on the system description and system boundary, a dynamic hypothesis is formulated that govern the structure of the model. This model structure consists of feedback loops, stock and flow variables and time delays. To conceptualize the model, a causal loop diagram (CLD) will be constructed, a highly aggregated qualitative model of the causal relationships within the system. These causal relationships in a CLD are indicated by either a + (a positive relationship: one variable leads to an increase in another variable) or a − (a negative relationship: one variable leads to a decrease in another variable).

A simple example of a CLD is given in Figure 7. This CLD shows how the profitability of electrification fosters investments, leading to an increase in electric capacities. A positive (reinforcing) feedback loop can be observed as a higher amount of electric capacities leads to more technological learning, reducing the required investment costs, improving the profitability. Two input parameters further act on the profitability of electrification: *subsidy* (a policy option) and *electricity price* (an external factor). *Emissions* form the model's output variable, by which the system's performance is measured.

3. **Model formalization**

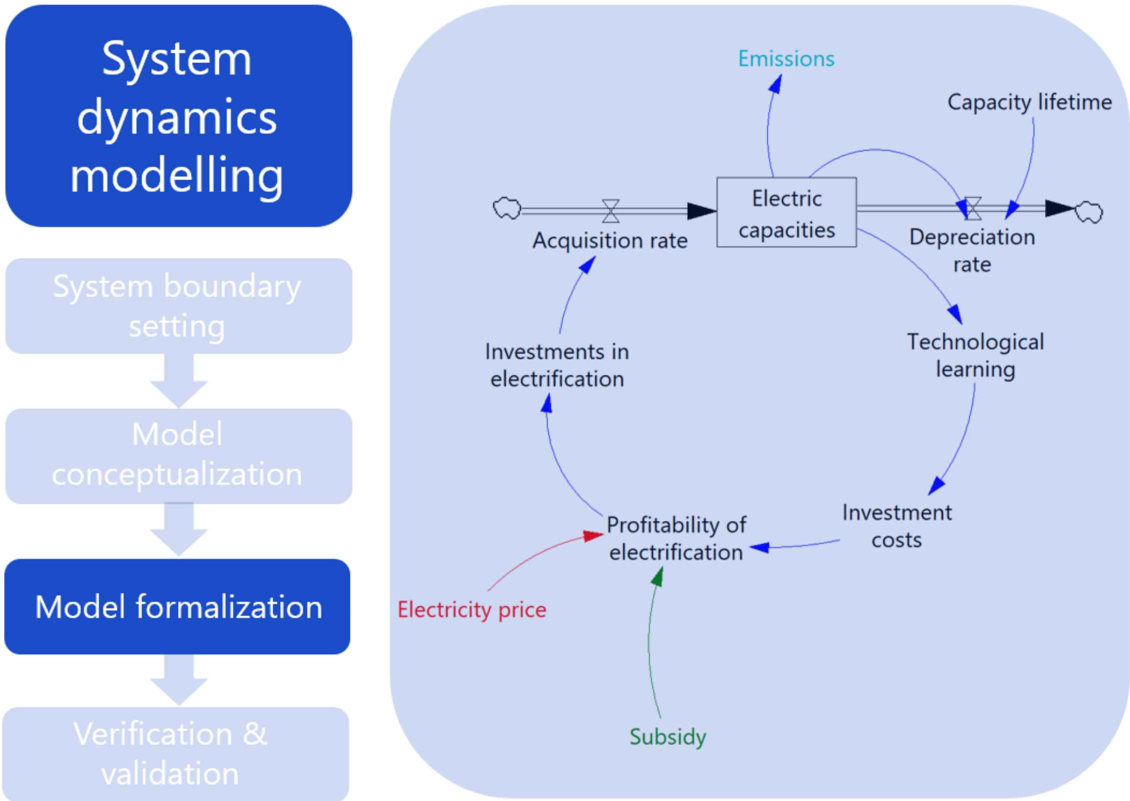

Figure 8: Illustration of the model formalization subphase. The output of the model formalization is a stock-flow diagram (SFD). This example SFD represents the same dynamics as Figure 7 but now showing how capacities (a stock variable) increase due to acquisition and decrease to depreciation (flow variables).

Based on the CLD, a stock-flow diagram (SFD) will be developed. The SFD can then be used to develop a detailed quantitative model containing stock variables representing the state of the system and flow variables representing changes in the system state resulting from actions based on the discrepancy between the system's current state and its desired state. Mathematically, the SFD can be viewed as a set of differential equations (Lane, 2000). The SFD can be simulated to show the system's behavior (Bala et al., 2017). Simulation in this context means numerical integration of the differential equations contained in the model. An example of an SFD is given in Figure 8.

4. **Verification & validation**

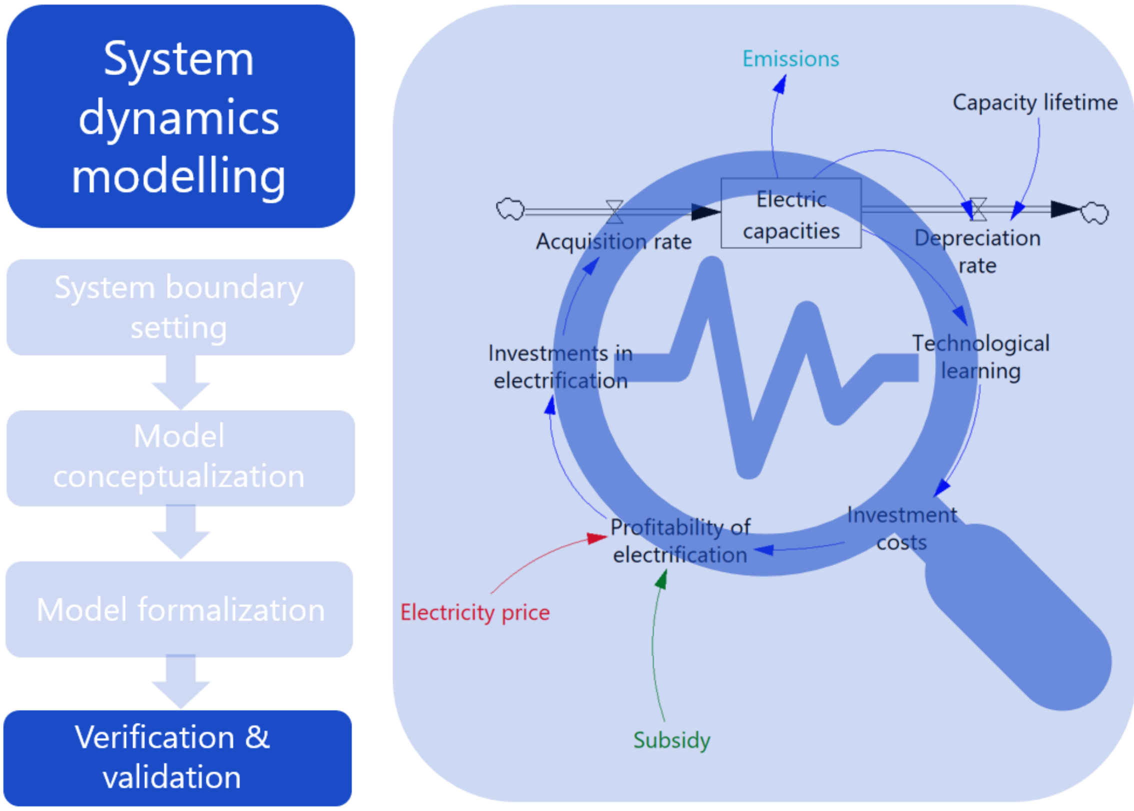

Figure 9: Illustration of the verification & validation subphase. During this phase the stock-flow diagram (SFD) is subjected to various tests to determine whether it is fit to study the formulated research objective.

The verification & validation subphase, illustrated in Figure 9 concerns testing the SD model to determine whether it is appropriate for studying the formulated research objective (Sterman, 2000). Verification means that the model is tested to check whether it is able to reproduce the reference mode. A reference mode is a "pattern of behavior over time" of key system variables (Vensim Documentation, n.d.-b) which can either be historical or hypothesized behavior (Vogstad, 2004; Vensim Documentation, n.d.-b). As this research concentrates on the future development of electrification the reference mode is one of hypothesized behavior. It is produced using a "base case" containing projected values for external factors and policy options. Verification in the context of this research involves determining whether the produced reference mode behaves according to our expectations. Concerning example SFD shown in Figure 9 verification would imply assessing whether the emissions behave as expected under a certain reference subsidy and reference electricity price.

Validation involves testing the model for e.g. extreme values of certain exogenous uncertainties (electricity prices in the case of our example) to see if it produces the expected behavior. If unexpected behavior arises, possibly extra model variables have to be included. Testing may also lead to certain variables being omitted or included in the model as exogenous factors. In SD terminology, these tests are to examine whether the system boundary established in step 1 is adequate (Vogstad, 2004; Vensim Documentation, n.d.-b).

3.3.3 Phase 3. Exploratory Modelling & Analysis

In phase 3 the SD model developed in phase 2 is subjected to Exploratory Modelling & Analysis (EMA). The EMA workbench developed by Jan Kwakkel, an open-source Python library for EMA (Kwakkel, 2017b), provides toolboxes for performing the steps of EMA. The EMA workbench also provides an interface with the SD modelling software Vensim. EMA consists of the following steps.

1. **Performing experiments**

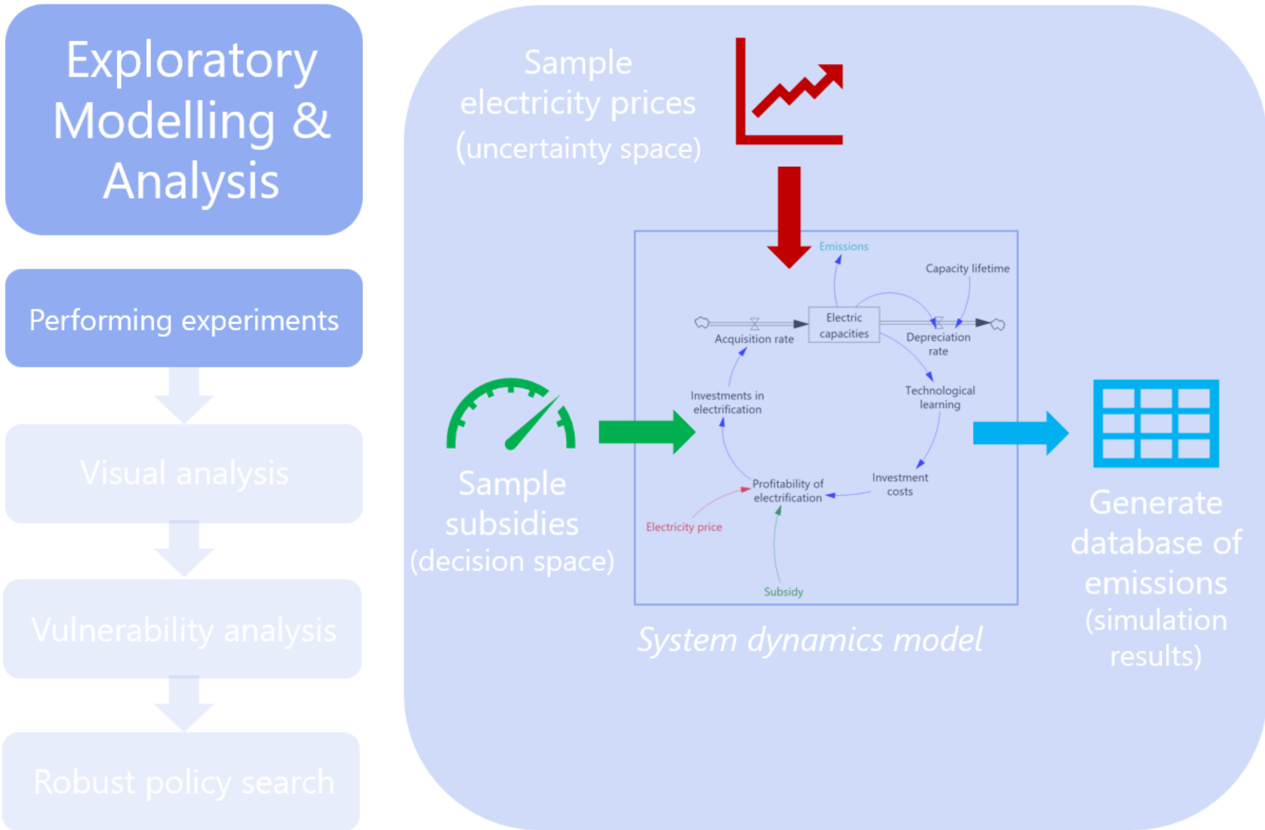

Figure 10: Illustration of the performing of experiments. By sampling the decision space different *subsidy* values are generated. By sampling the uncertainty space different values for the *electricity price* are generated. Every combination of a *subsidy* value and an *electricity price* value called an *experiment*. In this way the input parameters *subsidy* and *electricity price* are varied across the experiments. Each experiment produces an emissions time plot; this is the simulation result. Multiple experiments are performed which together form a database of emissions time plots.

In this subphase, experiments will be performed on the SD model developed in phase 2. Each experiment represents a combination between a *scenario* and a *policy*. According to Kwakkel (2018): "a scenario is understood as a point in the uncertainty space, while a policy is a point in the decision space." In the case of our example model the *uncertainty space* is the range of possible values the electricity price can attain. Hence, in this case the uncertainty space is one-dimensional and each scenario comprises a different electricity price value. If more external factors are identified, the uncertainty space becomes multi-dimensional. That is: two external factors yield a two-dimensional uncertainty space, three external factors a three-dimensional uncertainty space, etc.
The same logic applies to the decision space. As only one policy option, subsidy, is considered, the decision-space is also one-dimensional. The more policy options, the more dimensions the decision space will have.

In each experiment both the uncertainty space and the decision space are sampled so different combinations of scenarios and policies are obtained. Imagine the electricity price can attain a value ranging from 40 euro/MWh to 60 euro/MWh. Hence, the uncertainty space spans 40 euro/kWh to 60 euro/kWh. The subsidy can attain a value ranging from 10 euro/MWh to 20 euro/MWh. Hence the decision space spans

10 euro/kWh to 20 euro/kWh. Both uncertainty space and the decision space are sampled twice. This yields four experiments as follows:

- Experiment 1: electricity price = 39 euro/MWh, subsidy = 15 euro/MWh
- Experiment 2: electricity price = 39 euro/MWh, subsidy = 11 euro/MWh
- Experiment 3: electricity price = 55 euro/MWh, subsidy = 15 euro/MWh
- Experiment 4: electricity price = 55 euro/MWh, subsidy = 11 euro/MWh

Each time the SD model is subjected to a different experiment, it yields a different emissions time plot: this is the simulation result. Hence, by performing these experiments a database of four emission time plots.

When the uncertainty and decision spaces are set, the EMA workbench provides support for constructing experiments using an experiment design method for, e.g. Monte Carlo sampling and Latin Hypercube sampling (Kwakkel, 2017a).

2. **Visual analysis**

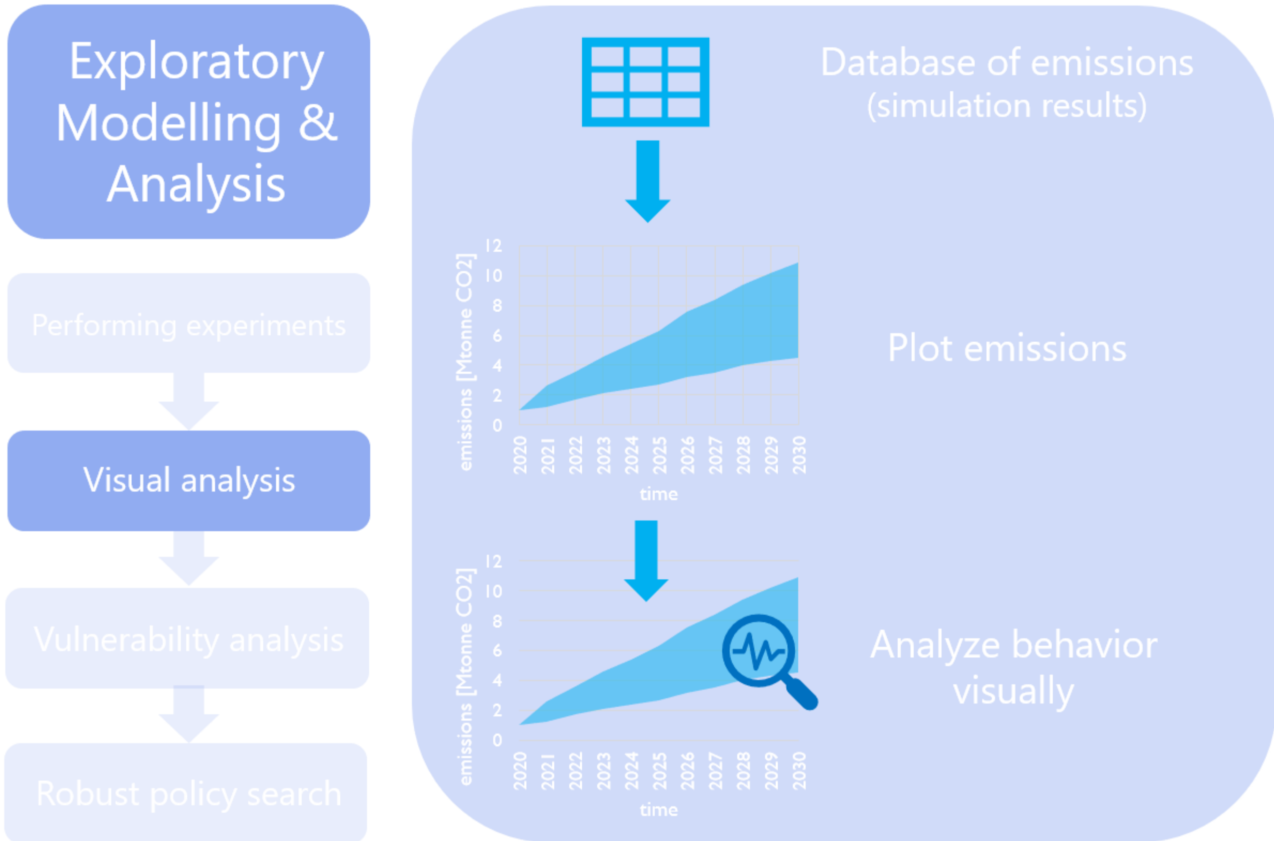

Figure 11: Illustration of the visual analysis subphase. The database of emissions time plots generated by the performing of experiments is plotted. In this way, the behavior of emissions under different scenarios and policies can be studied.

During the visual analysis subphase, illustrated in Figure 11 the database of simulation results is plotted. The EMA workbench provides several tools for performing visual analysis. With the plots the behavior of the simulation results under different combinations of scenarios and policies can be analyzed visually. In the case of the example introduced before, emissions are plotted. The plot shows a bandwidth of results as each experiment generates a different emissions time plot. Using visual analysis the different regions in this bandwidth are explored.

3. **Vulnerability analysis**

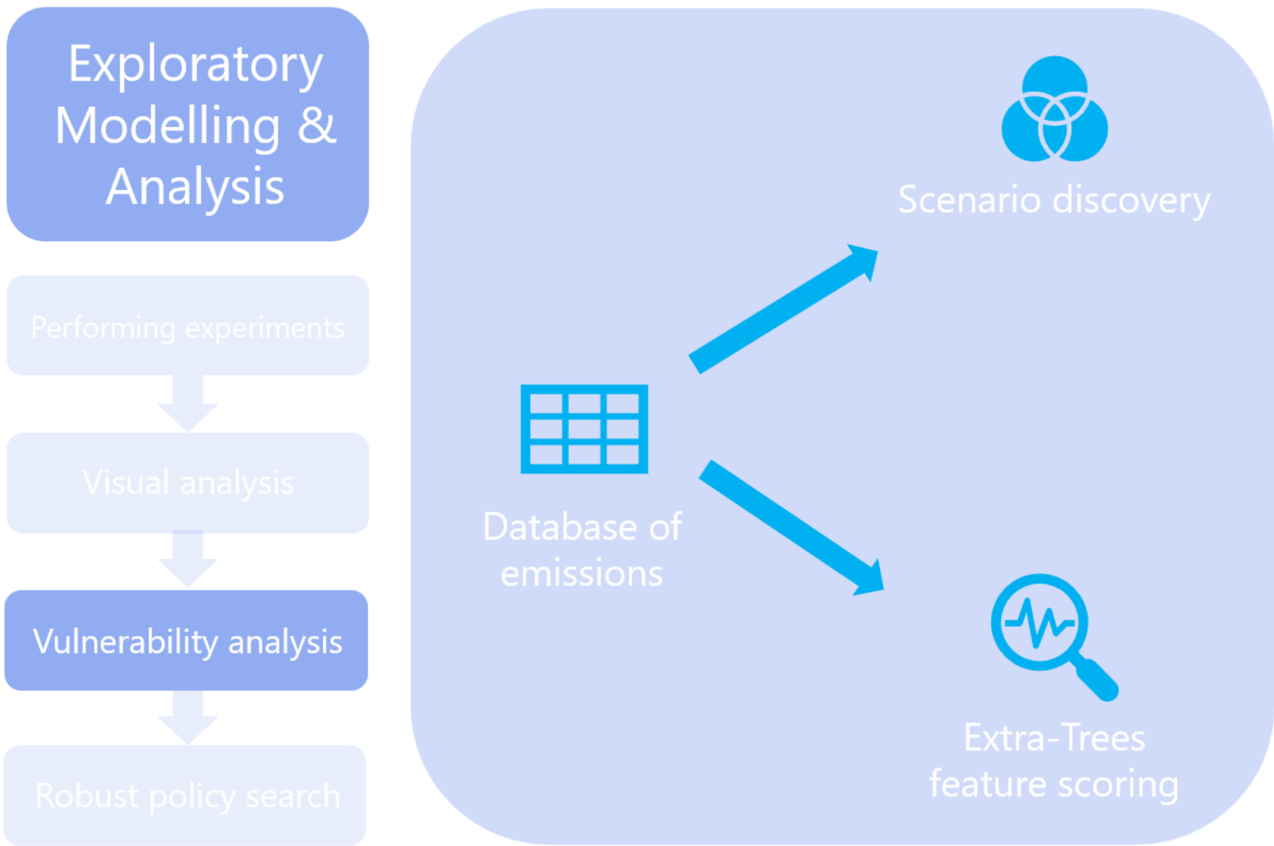

Figure 12: Illustration of the vulnerability analysis subphase. During this phase the database of emissions time plots (the simulation results) are subjected to more advanced analysis. Two analyses are performed: (1) scenario discovery, which aims at characterizing regions of interest within the simulation results and (2) Extra-Trees feature scoring, which is a machine learning alternative to global sensitivity analysis.

After the visual analysis we dive a little deeper. With the vulnerability analysis (illustrated in Figure 12) we seek to understand why the simulation results (emissions in the case of the example) behave as they do. Specifically, vulnerability analysis aims at identifying the influence of input parameters on the simulation results. Two different methods will be used in this regard: (1) scenario discovery (Bryant & Lempert, 2010) and (2) Extra-Trees feature scoring (Geurts et al., 2006). The EMA workbench provides support for both methods.

Scenario Discovery, originally introduced by Bryant & Lempert (2010) is a statistical method that seeks to characterize regions of interest within the simulation results. In the example these are the regions that feature low emissions. Scenario Discovery identifies the combinations of values in the input parameters (policy options L and external factors X) that are most strongly predictive of this subset of results. Scenario Discovery often employs visualization and data analytics to explore and characterize vulnerabilities (Lempert et al., 2008; Lempert, 2019).
In the context of the example scenario discovery would be used to identify which combinations of *subsidy* and *electricity price* are most predictive of low *emissions*.

Feature scoring is a family of machine learning techniques that is used to determine the relative influence of individual input parameters on the simulation results. In this sense, it is a machine learning alternative to global sensitivity analysis (Kwakkel, 2018). In this research Extra-Trees (short for extremely randomized trees) feature scoring developed by Geurts et al. (2006) is used.
In the case of the example Extra-Trees feature scoring determines the relative influence of *subsidy* versus *electricity price* on *emissions*.

4. **Robust policy search**

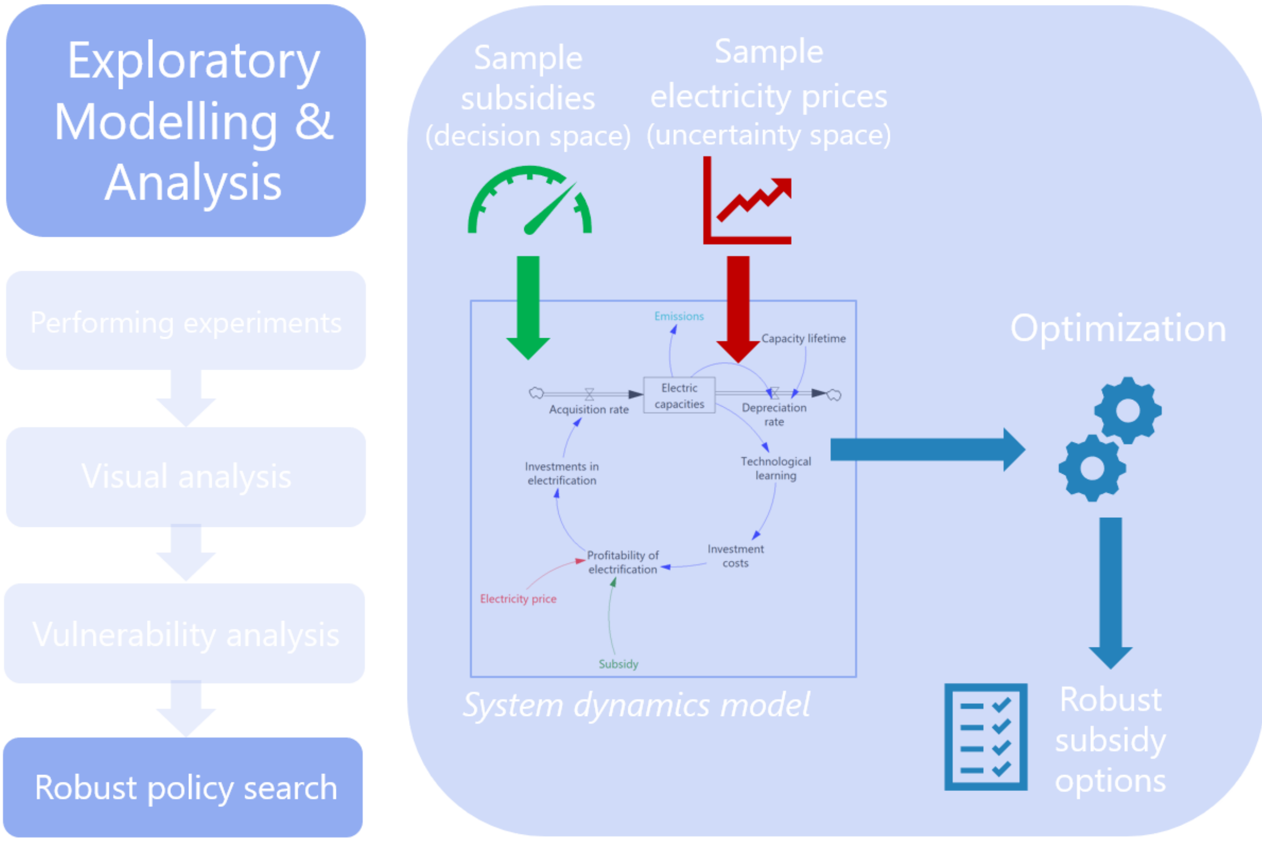

Figure 13: Illustration of the robust policy search subphase. The SD model is subjected to an optimization algorithm that seeks subsidy options that minimize emissions across the range of electricity price. These subsidy options are called *robust*.

In this final step, illustrated in Figure 13 the SD model is subjected to an optimization algorithm that identifies robust policies: policies that maximize system performance across a range of plausible futures (Walker et al., 2013b). For this purpose the same experiment design as used in subphase 1 (*Performing experiments*) is used.
In the case of the example the objective of the optimization is to find subsidy options that minimize emissions over the range of electricity prices.

Robustness can be defined in different ways. Thus, defining metrics to operationalize robustness is also part of this subphase (Lempert, 2019).

4 System description

In this chapter an initial understanding of the socio-technical system of electrification in the naphtha cracking industry is outlined. Section 4.1 starts with a system overview. In this section technical aspects of the system are explored and an overview of actors in the system and their interests are outlined.
In Section 4.2 results of the semi-structured interviews held among representatives from the industry and the Ministry of Economic Affairs & Climate are presented. These serve to gain a deeper understanding of actors' objectives, their potential actions and the influence of uncertainties on their actions. Four industry representatives were interviewed in one-on-one interviews and one representative from the Ministry of Economic Affairs & Climate. Because the interviewees have been anonymized, they are cited as Interviews (2021) and Interview Min. EA&C (2021), for the industry interviews and the interview with the ministry representative, respectively.

4.1 System overview

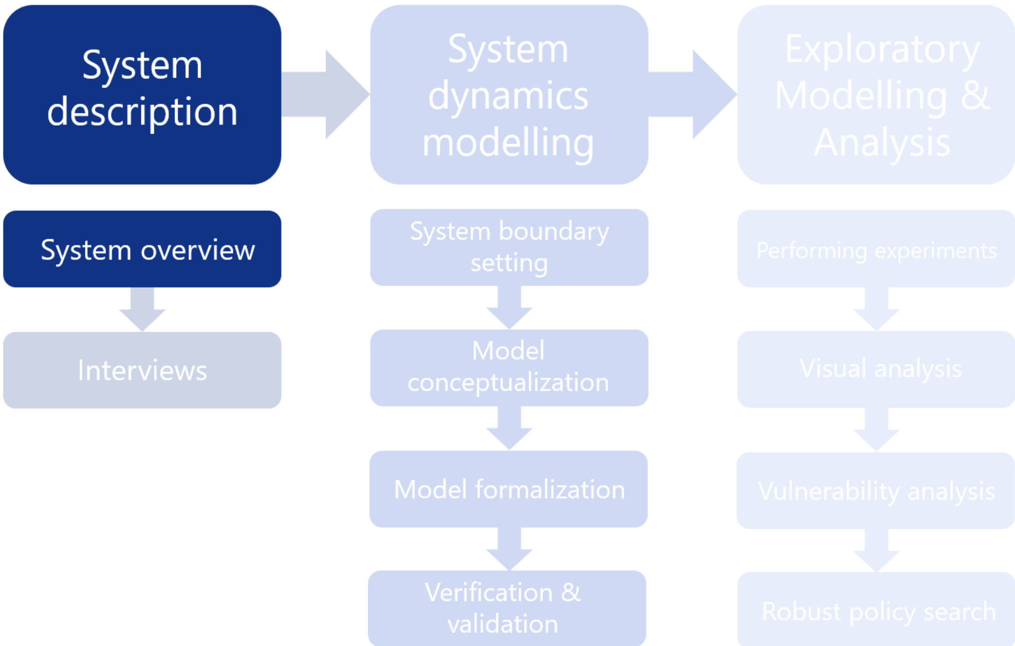

Figure 14: Position of the system overview step in the research roadmap.

This system overview starts with technical aspects of the system. This includes some background information on ethylene and propylene production (Section 4.1.1). Second, an overview of the naphtha steam cracking process will be given in Section 4.1.2. Third, decarbonization options are outlined in Section 4.1.3.
Subsequently, based on a complex socio-technical systems perspective, general characteristics of the system will be described in Section 4.1.4. Finally, the relevant actors and their interests will be discussed in Section 4.1.5.

4.1.1 Cracking for ethylene and propylene production: background

Cracking is a process by which large organic molecules or hydrocarbons are broken down into smaller chemical compounds that can be used as building blocks for the production of various materials and products. Whereas ethane and natural gas (methane) are the main feedstock for cracking in the United States and the Middle East, in Europe and Asia-Pacific mainly naphtha, a mixture of various hydrocarbons produced from crude oil, is used (Godini et al., 2014; Haribal et al., 2018). The main methods for cracking are *catalysis*, i.e. using a catalyzer to crack molecules and *pyrolysis*, i.e. cracking through the application of high temperatures. Throughout Europe, pyrolysis through steam cracking is the most common cracking approach. Steam cracking implies that the naphtha is first diluted with steam before it is subjected to high temperatures. In the Netherlands, six steam crackers are operated: three in Terneuzen (Dow Chemical), two at the Chemelot site in Geleen (SABIC) and one in Moerdijk (Shell) (Wong & van Dril, 2020).

Steam cracking is mainly applied for the production of ethylene and propylene. Ethylene is the most-produced compound in the chemical industry (Wong & van Dril, 2020). About 60% of the ethylene produced in Western Europe is used as a building block for polyethylene, the world's most widely used plastic (Geyer et al., 2017), which is used for food packaging, housewares and plastic bottles, among other purposes. Other applications of ethylene include PVC pipes, antifreeze for cars, clothing, contact lenses, tires and insulation materials (ACC, 2004).
Propylene is also a mass-produced chemical compound, globally ranking second only to ethylene (Wong & van Dril, 2020). Steam crackers produce 70% of the propylene demand worldwide (Falcke et al., 2017; Boulamanti & Moya, 2017a). For the most part, propylene is used for the production of polypropylene and propylene oxide, which are applied in the production of e.g. textiles, packaging and pipes. Other applications of propylene include coatings, nylon fibers, vehicle components and toys (ACC, 2017).

4.1.2 The naphtha steam cracking process

The steam cracking process consists of multiple phases, see Figure 15. In the first phase, naphtha enters the convective section of the furnace where naphtha is pre-heated, evaporated and mixed with steam. This gaseous mixture is then further heated to 500-600°C. The mixture then enters the natural gas-fired radiant section of the furnace, where temperatures of 750-900°C result in cracking of the hydrocarbons. This process requires extremely high energy inputs. The cracked gas that exits the furnace is then cooled to 230°. During the cooling process, steam is produced which is used for power generation, e.g. driving the compressors at later stages in the process (Haribal et al., 2018; Wong & van Dril, 2020).
The cracked gas is further cooled before entering the primary fractionation phase, where heavy components (tar and oily components) are removed from the cracked gas. The remaining lighter components are separated into gas and liquid streams. The gaseous stream is first cooled to near-ambient temperature before it is compressed in a steam turbine-driven multistage compressor (compressor 1), dried and then fed into a cryogenic cooler where it reaches -50°. The gas is then subjected to several subsequent separation processes in distillation columns. By subjecting the distillates to hydrogenation reactions finally ethylene and propylene are produced (Haribal et al., 2018; Wong & van Dril, 2020).
Ethylene and propylene are also used at the plant for refrigeration at several stages in the process. Propylene refrigeration is used to cool the cracked gas before it enters the primary fractionation phase while ethylene refrigeration is utilized in the cryogenic cooler. Both refrigeration cycles feature a multi-stage compressor (compressor 2 and 3) (SABIC, 2005; Mafi et al., 2009; de Santana et al., 2017; Harvey, 2017).
In addition to ethylene and propylene, the distillation train produces crude C_4, which is distilled to produce butadiene, and heavy components which are sent to the BTX recovery section for benzene extraction. Moreover, methane-rich gas is produced, which is fed back to the furnace and boilers as fuel gas, and ethane and propane, which are recycled as cracker feedstock (Haribal et al., 2018; Wong & van Dril, 2020).
As steam is required as input in multiple phases in the process but is also produced at various stages within the process, naphtha cracking processes feature a steam cycle system. As mentioned, part of the steam (∼60%) is produced during the cooling of the cracked naphtha. The remaining ∼40% is produced in steam boilers at a utilities facility (Wong & van Dril, 2020; Interviews, 2021). The steam system features four distinct steam grids (SABIC, 2005; Wong & van Dril, 2020):

- HHP grid (extra high-pressure steam): 110 bar/510°C. This grid is fed in part by the steam resulting from the cooling of cracked gas. The remainder is provided by steam boilers. The steam is used to dilute the naphtha stream entering the furnace and to drive the turbine of the cracked gas compressor (compressor 1).
- HP grid (high-pressure steam): 37 bar/370°C. HP steam is generated by steam boilers and the extraction steam from the cracked gas compressor turbine; it is used to drive other compressors onsite.
- MP grid (medium-pressure steam): 18 bar/300°C. The MP steam grid is fed mainly by the extraction steam of various turbines. MP steam is used, inter alia, to provide heat to the distillation columns and to drive various turbines.
- LP grid (low-pressure steam): 3.5 bar/150°C-200°C. The LP steam grid is fed by the extraction steam of various turbines and by waste flows from the HP steam grid.

4.1.3 Decarbonization options for the naphtha steam cracking process

Decarbonization in steam cracking can be achieved in various ways. One is energy efficiency improvements, which are expected to reach 14-21% in 2030 and 23-34% in 2050 (CEFIC, 2021). However, in order to achieve

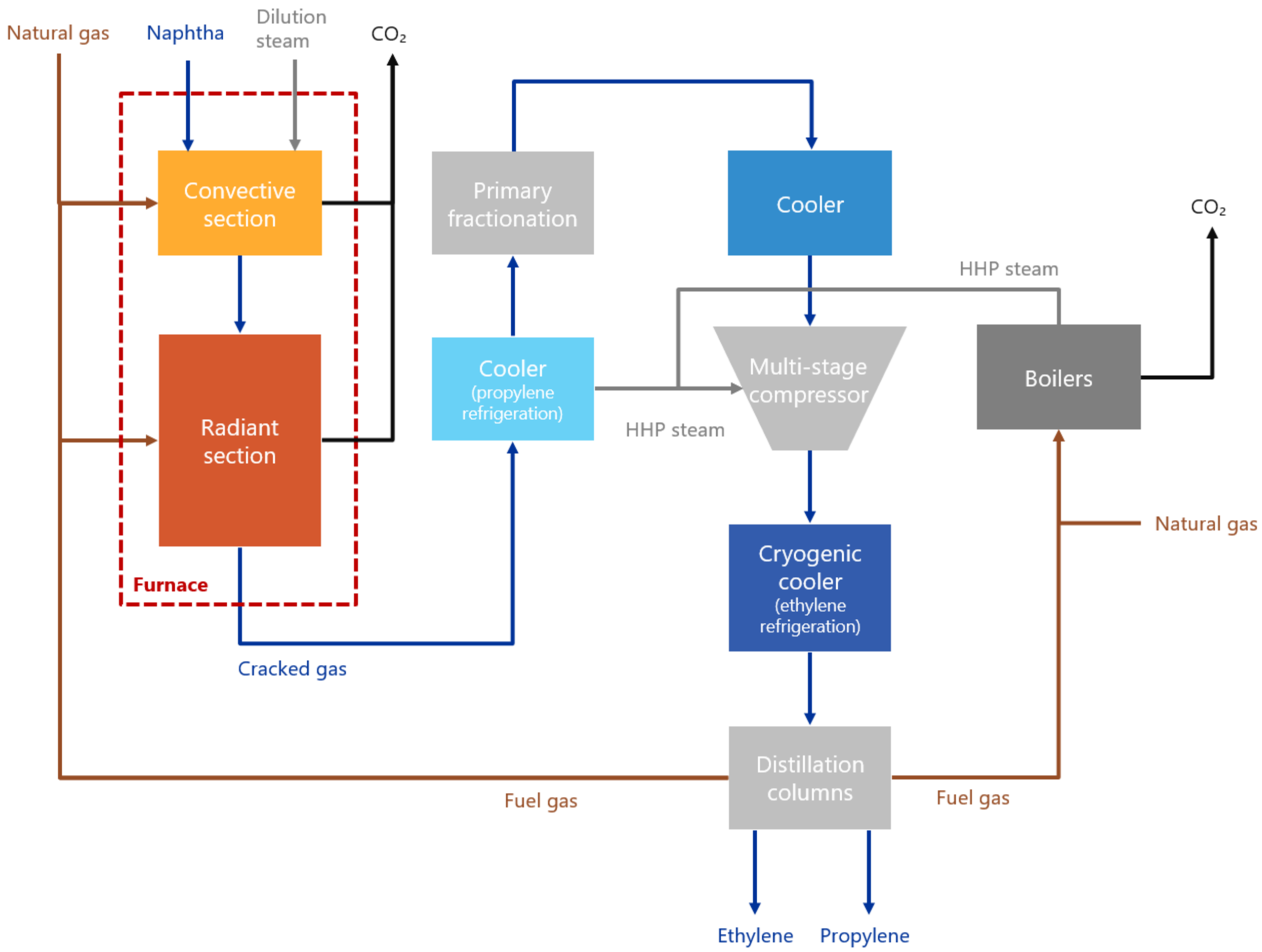

Figure 15: Schematic overview of the naphtha steam cracking process. The process stream is denoted by the blue arrows. Note that *multi-stage compressor* is described in the previous as *compressor 1* while compressors 2 and 3 are contained in the refrigeration cycles that provide the chilling duty for two of the coolers displayed in the overview. Furthermore, it should be noted that the boilers are not part of the main process but of the utilities section. Source: adaptation of Spallina et al. (2017).

deep decarbonization additional measures will be needed, such as replacing natural gas by low-carbon hydrogen, substituting feedstocks or processes and CCS (Wong & van Dril, 2020).
Electrification is yet another decarbonization strategy. The following electrification options are considered in this research:

- Electric furnaces. Instead of a natural-gas fired furnace electric heating technology can be applied to perform the pyrolysis. Because of the furnace's high energy and emission intensity it offers an important CO_2 abatement potential. The cracker furnace at Shell Moerdijk alone is responsible for 2.5% of the Dutch industrial emissions. Extrapolating this figure to the total of six furnaces, their combined emissions could well be as large as 15% of the Dutch industrial emissions (NEa, 2019; Wong & van Dril, 2020). However, as furnaces have a power of 350-500 MW, electric furnaces will require enormous amounts of electricity. This means that large investments are needed to upgrade the electricity grid. Moreover, required investments are in the order of 150-200 million euros per furnace (Interviews, 2021). As of today, electric furnaces still have a low technology readiness level and are only expected to enter the market by 2030. Industrial-scale application of electric furnaces is expected only by 2050 (Wong & van Dril, 2020). In June 2020, Shell and Dow announced they will be cooperating on the development of electric cracking technology, with the goal of reaching a "technologically and economically feasible solution" (Shell, 2020).

- Electric motors to replace steam-driven compressor turbines. The three compressors in the steam cracking process - one 40-50 MW cracked gas compressor and two ~20 MW refrigeration compressors - are currently driven by steam turbines but these could be replaced by electric motors. At some sites, several experiments have already been conducted by replacing smaller turbines of a few MW by electric motors (Wong & van Dril, 2020; Interviews, 2021). In the electrification of naphtha cracking processes this will most likely be the first step. However, challenges remain, stemming e.g. from the highly integrated steam cycle. If compressors are electrified steam production in the steam boilers may be reduced but at the same time there will be less exhaust heat available downstream. Hence, electrification of turbines require an adjustment of the steam cycle (Wong & van Dril, 2020). Moreover, representatives from the industry highlight that it is unlikely that all compressors will be electrified because steam will always be produced from the cooling of cracked naphtha (Interviews, 2021).

- Electric boilers. Instead of gas-fired boilers, electric boilers could be implemented, which produce steam through electric heating. However, only for the production of LP and MP steam electric alternatives exist. For the production of HP and HHP steam electric boilers are not suitable yet because with the current state of technology they cannot reach the required heat duty (Interviews, 2021).

- Flexible electrification of steam production or boiler hybridization. Flexible electrification (see Section 2.1.3) could be applied to steam production to utilize low electricity prices when renewable energy is abundant. During low electricity prices, steam is produced using electric boilers while steam is produced using conventional gas boilers during the rest of the time. An electric boiler is already operated at one of the sites (Interviews, 2021).

4.1.4 The naptha cracking industry as a complex socio-technical system

If the naphtha cracking industry sector is viewed as a system it can be concluded that it is a complex socio-technical system. It is complex because it is composed of many different components of technical, social and economic nature - production installations, management boards, governments, electricity and carbon markets, among many others - which interact through e.g. ownership, communication and material flows (Ladyman et al., 2013; Moallemi, Aye, et al., 2017). Moreover, it is characterized by *distributed control*, which means the development of the system does not rely on a single actor. Instead, complex systems evolve as a result of the decisions of multiple actors (Chappin, 2011; Ladyman et al., 2013). These decisions are in turn influenced by all kinds of developments, such as innovation and competition. These characteristics allow for information feedbacks to emerge (Chappin, 2011).
The system can also be regarded as socio-technical because the aforementioned technical, social and economic components should be studied in relation to each other (Chappin, 2011). They form separate, though interdependent subsystems. Improvement of the system's performance - e.g. an increase in the electrification rate and a reduction in carbon emissions - can only occur if these subsystems are jointly evaluated. Another feature of socio-technical systems is *equifinality*, which means system goals can be attained in a variety of ways (Badham et al., 2000; Baxter & Sommerville, 2011). This is reflected in the different decarbonization pathways that exist for the naphtha cracking industry (see Appendix A for an overview of the different decarbonization pathways for the chemical industry) and the different electrification strategies.

4.1.5 Overview of actors and their interests

Actions undertaken by actors may change the state of the system and influence its performance. Therefore, it is important to consider the relevant actors and their roles in the system. An overview of actors and their interests is given below. They are schematically displayed in Figure 16.

- **Naphtha cracking industry**. First of all, the industry is interested in further electrification because of the potential opportunities it offers to reduce costs. Electric installations require lower operational and maintenance costs and feature longer technical lifetimes. Second, electrification offers an opportunity for innovation. For example, with Power-to-Specialties (P2S) new chemicals can be developed. A third driver is sustainability. The motivation for becoming more sustainable is both extrinsic, because of the targets set in the Climate Agreement, as well as intrinsic: sustainability is increasingly associated with corporate social responsibility (den Ouden et al., 2018).

- **Energy sector**. The energy sector consists of energy suppliers and grid operators. Due to the increasing supply of renewable energy, aligning supply and demand is becoming ever more important to ensure a stable electricity grid. Through electrification, the chemical and other industries can provide flexible capacity either by storing energy when supply is high or by bringing down demand when supply is at a low. Moreover, by aligning supply and demand the grid is used more "smartly" and peaks in the energy supply are levelled, reducing the need to expand the grid to accommodate for these peaks. Hence, certain investments in the grid become unnecessary (van Kranenburg et al., 2016; den Ouden et al., 2018).

- **Government**. For the Dutch government, reaching the carbon reduction targets set in the Climate Agreement is paramount. Accounting for 34% of all industrial CO_2 emissions (CBS, 2019) decarbonization of the chemical industry offers a major CO_2 reduction potential. Moreover, electrification contributes to higher energy efficiency and circularity by e.g. heat upgrading through Power-to-Heat (P2H). Moreover, the Dutch government strives to create a competitive fossil-free economy (van Kranenburg et al., 2016).
- **Equipment suppliers** develop the technologies that enable electrification (van Kranenburg et al., 2016).
- **End markets**. For businesses and consumers, the naphtha cracking industry needs to uphold the quality and market price conformity of its products. Moreover, there is a demand for sustainable and innovative products (van Kranenburg et al., 2016).
- **New market players**. New players may emerge to play a role in the socio-technical system. These include Energy Service Companies (ESCOs): third-party companies to which the naphtha cracking industry can outsource the operation of flexible electrification. For instance, ESCOs invest in the electrification technology, selling the output to a contracted industry or engage in a joint venture together with the industry to enable investments (den Ouden et al., 2018).

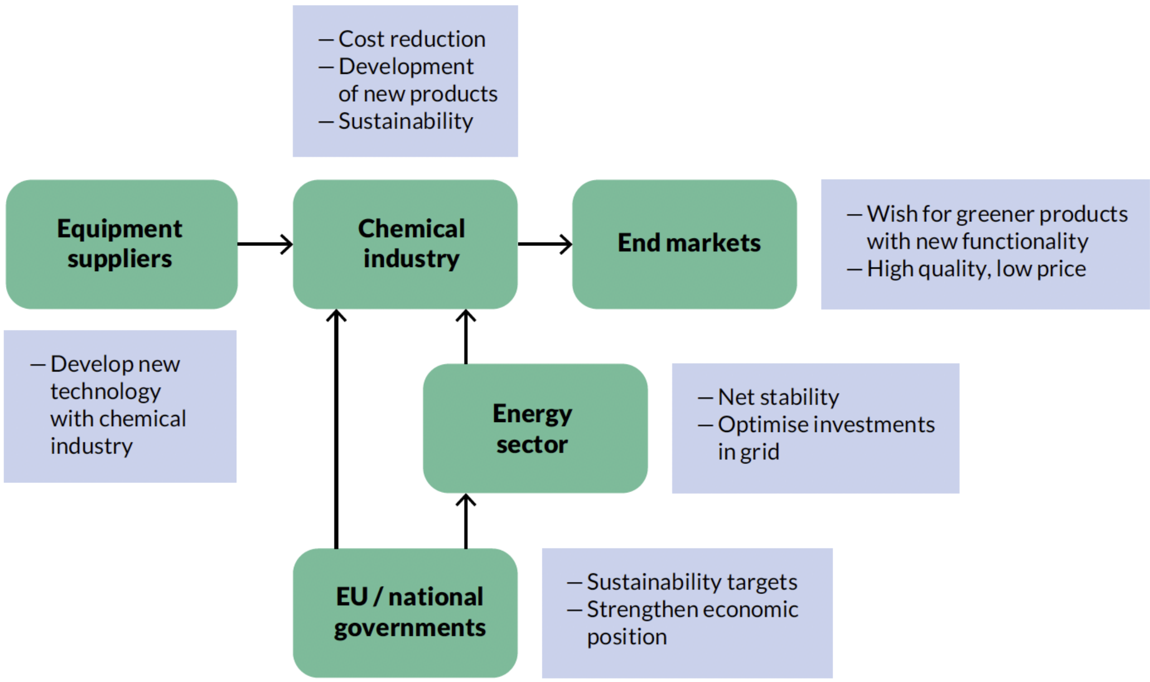

Figure 16: Schematic overview of actors in the naphtha cracking industry's environment, including their interests and interactions. Source: van Kranenburg et al. (2016).

4.2 Actor perspectives: results from the interviews

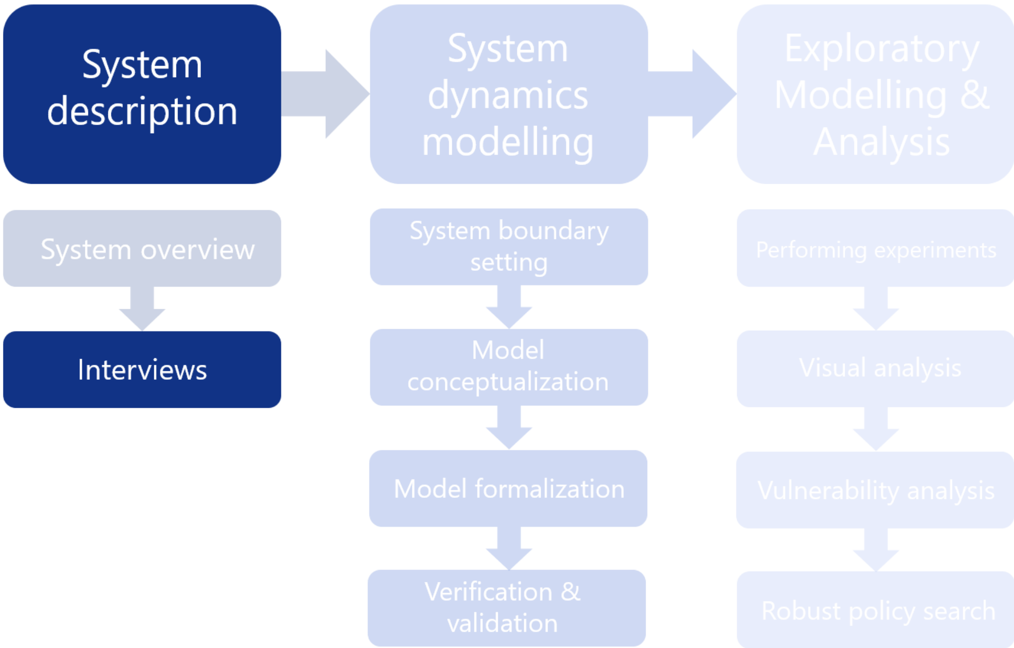

Figure 17: Position of the interviews step in the research roadmap.

As was introduced in Section 3.2.1 semi-structured interviews were held among relevant sectors: four representatives from the naphtha cracking industry and one representative from the Ministry of Economic Affairs and Climate. These were all one-on-one interviews of approximately one hour. Through analysis of these interviews a picture of the system has been sketched by means of a system diagram, displayed in Figure 18. The full analysis from the interviews, which will elaborate the relations presented in the system diagram, is presented below.

4.2.1 Naphtha cracking industry

Four interviews were held among representatives from the industry and service companies operating in the industry. Due to confidentiality, the interviewees and their companies have been anonymized and their comments have been aggregated into one section. Therefore, in the rest of this thesis, they are simply cited as Interviews (2021).
Below, first a summary is given of the interviews. Subsequently, the results from the interviews are discussed in more detail by topic.

Summary of the interviews

All of the interviewees recognize that the electrification of naphtha cracking processes is a potentially important option in the decarbonization of the naphtha cracking industry. Although electrification offers potential economic opportunities to the industry as well, investment decisions regarding electrification depend on various factors.
Electrification concerns enormous amounts of energy - dozens of PJ's per year for an individual plant - and requires hundreds of millions of euros in investments. This makes the deployment of electrification is highly sensitive to external developments. In fact, due to the current emission factor of electricity, fundamental uncertainties, lacking policy, among other issues, electrification does not yet offer a commercial advantage to the industry.

For instance, the success of electrification is dependent on the availability of renewable electricity because without it, electrification does not result in an emission reduction. Uncertainties also exist concerning the capacity of the electricity grid, which has to be upgraded to accommodate electrification. The intermittency of renewable energy poses an additional challenge since naphtha cracking processes require a stable baseload provision of electricity.

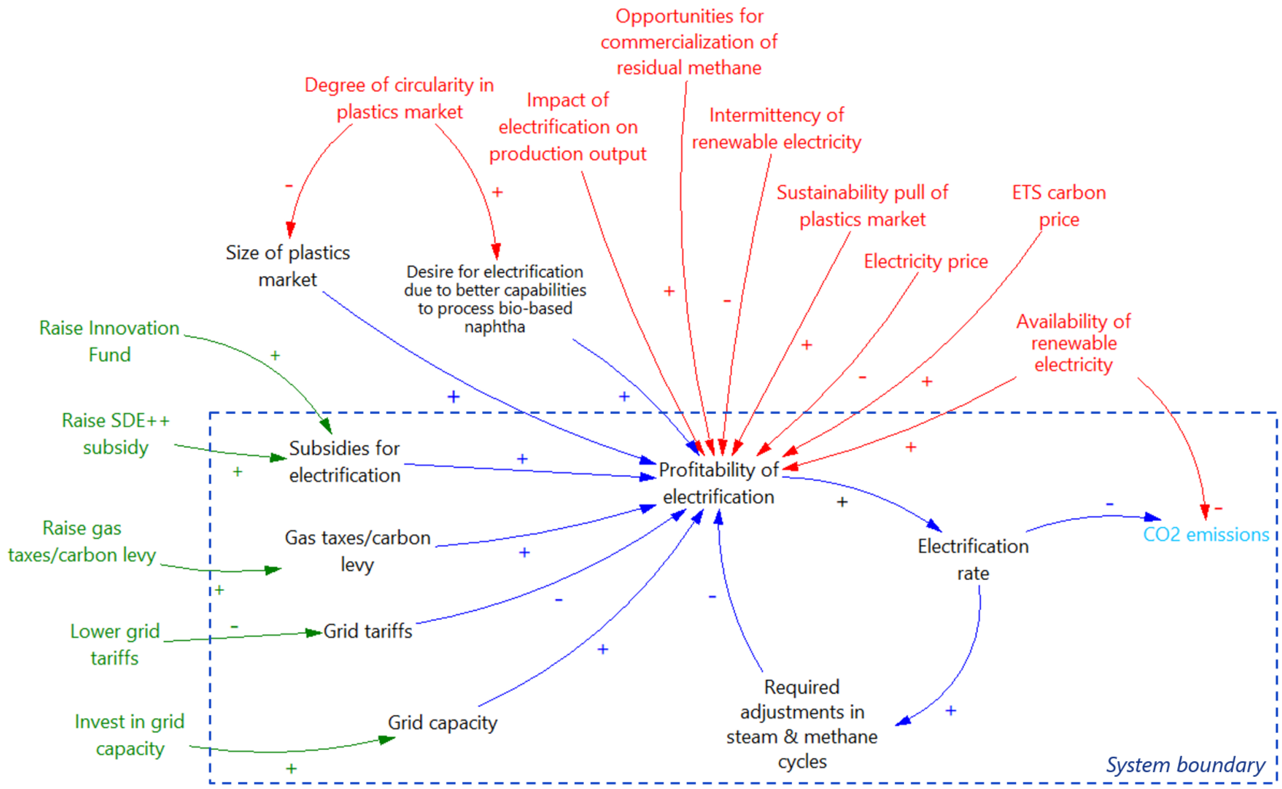

Figure 18: System diagram of electrification in the naphtha cracking industry. The diagram is sketched from the perspective of the industry. As such, the industry can implement electrification through investments. In turn, the profitability of electrification is determinant for the industry's behavior. CO_2 emissions is the criterion against which the system's performance is measured. In red are the exogenous factors of influence to the system. In green are the potential actions taken by the relevant actors: the EU, the the Government of the Netherlands (denoted by *NL Govt*) and grid operators (denoted by *GO*).

Furthermore, the development of electrification is impacted by other sustainable developments. One example is green hydrogen, as hydrogen cracking is a potential competitor to electric cracking.
Government policy has the potential to resolve many of these challenges but is currently lacking according to the industry. The interviewees argue that a paradigm shift is required within the government towards stable and long-term policymaking.

Next to external developments, certain characteristics of naphtha cracking processes also make electrification challenging. One is the high degree of integration between systems onsite. As a consequence, electrification of certain parts of the process require adjustments in other systems and cycles. An example is the methane cycle. Methane is produced during the process and is fed back into the cracker as fuel. However, electrification of the furnaces implies this methane can no longer be usefully applied. Moreover, electrification is accompanied by operational challenges. Naphtha crackers have turnaround frequencies of 6-7 years, meaning that every 6-7 years the plant is shut down for 6-7 weeks window to perform maintenance and replacement operations. For some projects it may be difficult to respect this turnaround window, with the financial consequences that entails. Whatever the case, electrification requires extensive project planning.

One interviewee summarizes the challenges as follows. First and foremost, certain boundary conditions need to be fulfilled: there should be (1) an adequate electricity infrastructure, (2) sufficient availability of renewable electricity and (3) opportunities for the commercialization of residual methane. Once these preconditions are met, there should be a viable business case for electrification.
In the following, the opportunities and challenges with regard to electrification are discussed in more detail.

Opportunities for electrification

The interviewees agree that the electrification of compressor turbines will be the first step in electrification.

At several sites, pilot projects have been run with smaller electric motors. The interviewees mention the large efficiency gain as an important advantage: current condensing steam turbines have thermal efficiencies of 30-35% while electric motors are 95% efficient or more. Moreover, the steam production in boilers can be reduced by about 50%, reducing gas consumption by the gas-fired boilers. However, one interviewee highlights that steam will still be generated in the cracking process (during the cooling of cracked naphtha) so some compressors will remain steam-driven. Otherwise, the steam produced in the cracking process will be lost. For that same reason, the electrification of compressors is ideally combined with the electrification of furnaces as electric cracking produces less steam.

The electrification of the steam production poses a more significant challenge due to the highly integrated steam cycle and the different steam grids (see Section 4.1.1). While the boilers producing MP steam could be electrified using electric boilers, electric boilers that are capable of producing HP and HHP steam do not exist yet. However, one interviewee foresees that by electrifying compressors and implementing steam saving measures, steam production by the boilers will become entirely redundant and therefore, it will not be necessary to install electric boilers for the production of HP and HHP steam.

Provided that electricity is largely renewable, the employment of electric furnaces results in a major emission reduction as furnaces will no longer rely on natural gas, all interviewees agree. However, once a technologically and economically feasible solution is available, the electrification of furnaces will be a logistically challenging operation. It is expected that it will be at least 10 years before the first electric furnace is taken into operation; a cracker typically employs 10 or more furnaces, depending on the site.

Requirements for grid capacity and availability of renewable electricity

The electrification of cracking processes requires an update of the grid capacity. Furthermore, a sufficient availability of renewable electricity is paramount for electrification to actually lead to an emission reduction. In fact, with the current emission factor of electricity (0.53 tonne_{CO_2}/MWh (PBL, 2020)) electrification will not result in an emission reduction.

The power requirements for naphtha cracking are extremely high: 350-600 MW for electric cracking (depending on the number of furnaces) and 20-50 MW for compressor turbines (depending on the type of turbine). For comparison: the maximum power of a modern wind turbine amounts to 2-5 MW (Vattenfall, n.d.). Consequently, the electricity infrastructure around the sites should be upgraded by means of a 380 kV power line (a high-voltage power line). This upgrade requires a considerable investment. Moreover, such infrastructure upgrades feature project lead times of 6 to 10 years.

Even with a sufficient grid capacity, industrial decision-makers remain faced with uncertainties regarding the future availability of renewable energy. The availability of green energy is essential since with the current, largely fossil, energy mix, electrification would cause an overall emission increase rather than a reduction, as one interviewee emphasizes. Several interviewees are rather pessimistic about the availability of renewable energy, given the large amounts of electricity required by electric cracking processes and the increasing reliance of the rest of society on renewable energy.

Another challenge arises from the intermittency of renewable electricity. As cracking requires a baseload energy input, a stable provision of electricity should be sufficiently assured in order for electric cracking to become possible. On the other hand, electric furnaces offer opportunities for better process regulation. Compared to conventional furnaces, electric furnaces are better geared towards being ramped up and down, though the extent to which this is possible remains limited. One interviewee also highlights that nuclear energy is a potential gamechanger since it could offer the baseload energy required by cracking.

Another development that could resolve the challenges of intermittency are international cables that connect electricity grids of individual countries in the EU. Multiple cables already connect the Netherlands to Norway and Germany but these interconnections still have limited capacity. Therefore, expanding the interconnection capacity can increase the security of supply of renewable electricity.

Impact of other sustainable developments

Other sustainable developments also impact the prospects for electrification. For instance, the current development of a (green) hydrogen economy is accompanied by a strong lobby. As hydrogen cracking, i.e. using hydrogen instead of natural gas to fire the furnaces, could be an alternative to electric cracking this development is delaying electrification. According to one of the interviewees, this is a reason why decisions about updating the electricity grid are being suspended. All of the interviewees strongly prefer electric cracking to hydrogen cracking. They underline that burning hydrogen for heat is associated with considerable energy losses. Moreover, like conventional crackers, hydrogen cracking still produces residual energy in the form of flue gas. This residual energy could be reused to drive compressors for instance but overall integral electrification is more efficient.

Moreover, due to developments in circularity, the quality of the cracker feedstock may also change. Currently, the cracker continuously receives large batches of naphtha with a stable quality. In the future, the shares of bio-based naphtha or naphtha produced from recycled plastic may increase, causing more and more frequent quality variations in the feedstock. This poses an uncertainty for industrial decision-makers. On the other hand, it provides an opportunity for electric cracking, since electric cracking is better equipped to deal with such issues.

The ethylene and propylene-based plastics market

The ethylene and propylene-based plastics market are also of concern to the business case for electrification. In the current market, the revenue may already not be sufficient for a viable business case for electrification. Moreover, some in the industry expect a drop in the future demand for ethylene and propylene. Although the global demand for these compounds is still growing by 3% annually (Interviews, 2021), developments in circularity may temper this growth. This poses an additional uncertainty for industrial decision-makers.
The revenue also depends on the demand for greener end products and the willingness to pay a higher price for these products. In the current market this willingness falls short, meaning that manufacturers cannot internalize the costs of decarbonization in the current market. Only once the market starts to "pull" and its willingness to pay a higher price for greener products increases, the industry can capitalize on its decarbonization "push".
In summary, in order for the naphtha cracking industry to provide a pull on renewable electricity and improve the business case for renewable electricity, a pull on the product side for plastics produced with a reduced carbon footprint appears helpful.

Challenges related to integration of systems onsite

Next to external factors, challenges are posed by the integration of systems onsite. As the processes at the cracker sites are all highly integrated, electrification of (parts of) the cracking process require adjustments in other systems at the site, such as the steam cycle. The interviewees have slightly different views on how to tackle this challenge. One interviewee suggests starting with the electrification of MP steam production and foresees the electrification of compressors will happen at a later stage. However, another interviewee argues that the steam demand will actually be reduced by the electrification of compressors and steam reduction measures. In this way, electrification of steam production becomes redundant entirely. However, in this case, the compressor should be electrified simultaneously with the implementation of electric furnaces.
By one interviewee it is also argued that some compressors will remain steam-driven as steam is still produced in the cracking process and would be lost otherwise. He foresees a hybrid situation at the site in which both steam and electricity will be used. This is already the case for pumps which run partially on electricity due to operational reliability reasons.

Another issue is the use of residual methane. In the distillation train methane is produced and fed back into the process to fire the cracker. If the furnace becomes electric, this methane stream does not have an application within the process anymore. This worries some of the interviewees as the future value of methane is uncertain. As the built environment is switching away from natural gas for the provision of heat and electrolysis is projected to be the most important production method for hydrogen in the future, it is doubtful whether methane will still have a useful application. Moreover, the usage of methane for heat production will still emit CO_2. However, other interviewees foresee a potential solution in the processing of methane for the production of chemicals through reforming. Also, they believe that methane will still remain valuable for the production of blue hydrogen. Another option mentioned is to convert methane to ethylene. In theory, this conversion would raise the efficiency of ethylene production to 100% given that currently 15% of the naphtha feedstock ends up as methane and is burned in the furnace, causing CO_2 emissions.

Financing and operational challenges

The electrification of furnaces and compressor turbines require large investments. For furnaces these investments are expected to amount to 150-200 million euros for replacing a furnace heat input and 300-400 million euros for building an entirely new furnace. Electrification of compressors are expected to require an investment in the order of 50 million euros, depending on the compressor power.

Moreover, because the cracker furnaces and compressors are at the core of the process, the financing of electrification will be very challenging unless the implementation of electric furnaces/turbines is scheduled when furnaces/turbines need to be replaced anyway due to end-of-life. Plants typically have a turnaround frequency of 6-7 years during which the process is shut down for 6-7 weeks. These operations feature long-term planning; maintenance activities are often planned 6 or more years in advance, making decision-making in this context rather complex. Through these kinds of maintenance operations current installations are continuously retrofitted with new technologies in order to extend their lifetimes. Therefore, most crackers are already 50 years old or more.
However, one interviewee mentions that the turnaround time window will be too short to replace a compressor turbine. Without doubt, electrification will feature a phase-wise implementation.
On the other hand, since decarbonization measures are regarded as a strategic investment, investments in electrification feature longer payback times of 5-7 years.

Impact of electrification on the production output

Because electric furnaces produce a different heat profile compared to conventional furnaces, furnace electrification affects the composition of the production output: that is, the share of each chemical in the total production volume. In this sense, electrification affects the industry's revenue. This effect can either be positive or negative; research is still being conducted into this phenomenon.
It should be mentioned that the conversion time of the installations also temporarily affects the production output, which should be accounted for in the costs and the business case.

Operational and maintenance costs

Operational and maintenance costs of the plant are impacted by electrification. Although electricity-driven turbines are more efficient compared to steam-driven turbines, electricity is still relatively expensive compared to producing steam. However, rising CO_2 prices are reducing the difference in energy costs and will make electric motors commercially viable in the future.
However, reduction of the steam demand may complicate the business case for electrification as steam that is not produced as a by-product may need to be generated in another way. Hence, once the compressors are electrified, the price paid for the remaining steam consumption may rise.

Policy requirements

The interviewees agree that the government's expectations of the industry committing to the emissions reduction target set in the Climate Agreement is not yet translated into adequate policy. Current policy does not sufficiently match the uncertainties faced by the industry when it comes to investments in electrification. The interviewees argue that a paradigm shift is required within the government that results in stable and long-term policymaking. This is deemed necessary to enable the large, long-term investments required for electrification. The government should adopt a more long-term perspective, they say.

This argument is illustrated by the norms set for the SDE++, the government's subsidy scheme for renewable energy production and sustainable technologies. The provision of SDE++ is dependent on the direct emission reduction achieved by a technology. However, electrification does not result in an emission reduction in the short term, because the electricity supply is not renewable yet. Hence, electrification is not evaluated on its potential to reduce emissions in the future.
Therefore, the industry argues for a more forward-looking SDE++ which takes into account the future development of the electricity supply, which is bound to become more renewable. Currently, the industry can only turn to EU innovation subsidies to finance investments in electrification.

Moreover, the interviewees argue that government policy should adopt a broader view to include the value chain of the industry. As such, it should concentrate on scope 3 emissions resulting from that value chain, instead of just scope 1 emissions (direct emissions) and scope 2 emissions (indirect emissions resulting from electricity, steam and heat consumption) (Greenhouse Gas Protocol, 2013).
In addition, a higher (EU) carbon levy is required because the carbon price in the EU ETS remains too low.

Furthermore, on an EU level recycling standards should be implemented.

4.2.2 Ministry of Economic Affairs and Climate

One interview was held with a representative from the Ministry of Economic Affairs and Climate. The interview was meant to gain more insight in the view of the ministry on electrification of the naphtha cracking industry and the policy options the ministry is considering. Like the previous interviews, the interview has been anonymized and is cited in the rest of this research as Interview Min. EA&C (2021).

General remarks

The interviewee regards electric cracking as a promising electrification option. Besides reducing emissions it also guarantees a continous and robust demand for renewable electricity; this benefits the business case for renewable electricity generation. However, he also has some reservations concerning electrification in the naphtha cracking industry. First, he emphasizes that it is paramount that the electricity supply is renewable; otherwise electrification will not lead to the desired emission reduction. Second, he argues that electrification of the energy supply does not change the naphtha cracking process in itself and therefore emissions originating from the naphtha feedstock remain. Therefore, the interviewee emphasizes that the focus should not only be on electrification but that also decarbonization of the feedstock should be considered. Electrification should fit in the bigger picture of a more sustainable industry.

The interviewee comments that the ministry strives to design policy such that energy-intensive industries stay in the Netherlands and are supported in their decarbonization. The ministry wants to avoid that energy-intensive industries move abroad because this results in carbon leakage: in that case companies would emit more CO_2 abroad. However, the ministry also realizes that certain industries are likely to shrink as a consequence of the energy transition.

Electricity infrastructure

The interviewee recognizes that the electricity infrastructure is crucial for electrification. In this regard the Netherlands has established the Trilateral Chemical Region together with the Belgian region of Flanders and the German state of North Rhine-Westphalia which aims to address the challenges related to infrastructure and innovation in the chemical industry.

SDE++ subsidy

The interviewee sees no limitations in applying the SDE++ subsidy to novel electrification options. However, the SDE++ calculations falls short when it comes to subsidization of so-called "scope 3 options": decarbonization options that focus on reducing emissions resulting from that value chain, such as chemical recycling.
The interviewee agrees that the SDE++ scheme cannot provide the industry with sufficient financial incentive to invest in electrification. He suggests developing a new subsidy instrument akin to the EU's Innovation Fund. This scheme is currently under development at the ministry.

Fiscal differentiation

Implementing a fiscal shift from gas to electricity seems logical to the interviewee. However, a complication arises from the fact that electricity is not fully renewable yet. Hence, an increasing consumption of electricity may cause an increase in emissions if not kept in check. Moreover, as gas is also used in the industry as a feedstock, this application of gas should be decoupled from the energetic use of gas if such a fiscal differentiation is implemented. Furthermore, such as a fiscal differentiation should keep pace with the technological developments in electrification.

5 System dynamics model

This chapter describes the rationale behind the *electrification model*, a system dynamics model, and its structure. First, in section 5.1 the system boundary is outlined. Section 5.2 gives an overview of the conceptual model and its assumptions. In section 5.3 the formal model is described. Finally, 5.4 describes the steps taken in the verification and validation of the electrification model.

5.1 System boundary

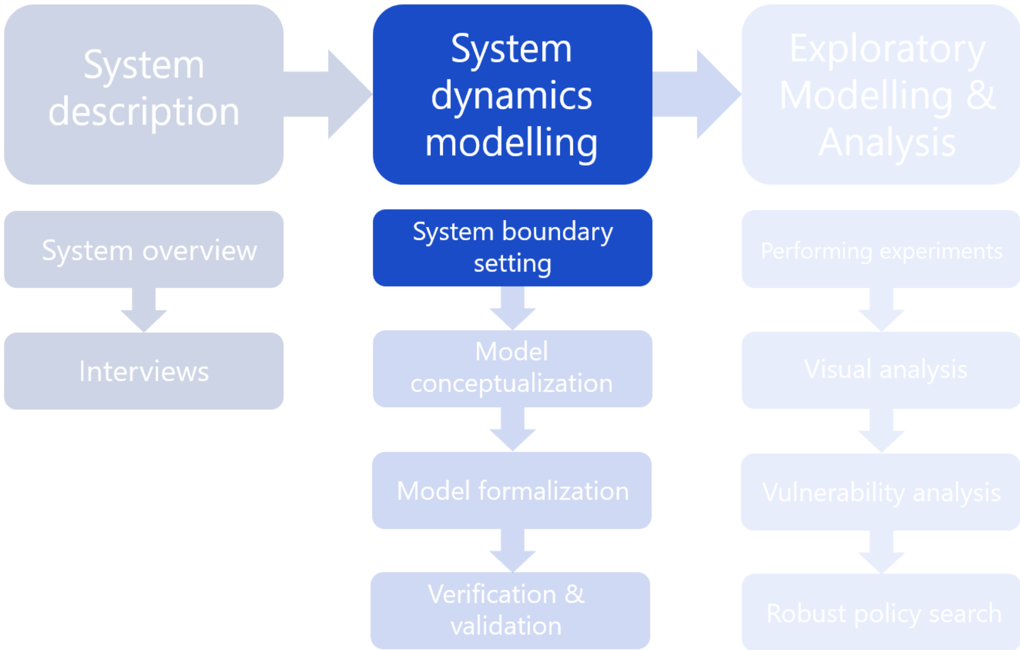

Figure 19: Position of the system boundary setting step in the research roadmap.

In the following, the system boundary will be outlined. Through system boundary setting it is determined which variables are endogenously modelled (being internal system variables) and which are exogenously modelled (being external factors). System aspects that are considered outside of the scope of this research are omitted.

Electric or conventional retrofit based on cost optimization. The electrification model concentrates on the question what the cost-optimal option for these retrofits is: electric technologies or conventional, gas-fired technologies. Though hydrogen-fuelled cracking using hydrogen is also an option to decarbonize the energy supply of crackers (Chang, 2021), it is not included in the model.

Investment decisions at the core of the model. Comparing the costs in the case of electrification relative to the case of conventional retrofitting determines whether the business case for electrification is an attractive one. In turn, the attractiveness of this business case determines the investment decisions regarding retrofitting. Hence, investment decisions are at the core of the electrification model as they form the connection between cost calculations which reflect the industry's expectations and capacity acquisition in the real world.

Stable production capacity. The electrification model assumes that the production capacity of the cracking industry will remain constant over time. This assumption is deduced from the perspectives in the industry: in the current economy building new cracker capacity is not opportune, also due to the high investments involved (Interviews, 2021). In Europe, no new cracker has been built for decades; currently one new cracker is being built by INEOS in Antwerp (T. Brown, 2021). Therefore, investments in the industry are intended for retrofitting existing capacity for the purpose of lifetime extension.
This implies the output capacities of the installations considered - furnaces (aggregated heat output) and compressor turbines (aggregated work) - are assumed constant. The exception is boilers because the steam demand depends on the capacity of the remaining compressor turbines operating on steam. Therefore, the boilers'

aggregated output capacity (measured in the energy content of the steam produced) declines in proportion to the electrified compressor turbine capacity.

Flexible electrification only an option for boilers. Currently naphtha cracking processes require a baseload supply of energy. Though some interviewees indicated that electric furnaces offer a limited potential for flexible electrification (see Section 2.1.3) others emphasized the baseload nature of operating furnaces and compressor turbines within the cracking process. Hence, the possibility of flexible electrification is not considered for furnaces and compressor turbines. Therefore, only retrofits are considered for these technologies with two options: a conventional retrofit or an electric retrofit (electrification).
For boilers the situation is different as an electric boiler can be placed next to an existing gas boiler. In this way, at any point in time either the gas boiler or the electric boiler can be operated based on the availability of renewable energy. Hence, the boiler capacity runs on gas and electricity in a hybrid fashion. In this manner, the baseload steam demand of the naphtha cracking process is not affected. Hence, for boilers both retrofits (i.e. replacing depreciated gas boilers by either gas or electric boilers) and hybridization are considered.

Focus on decarbonization of the energy supply. Only the decarbonization of the energy supply is considered. Hence, the decarbonization of the naphtha feedstock is out of the model's scope.

Divestment not considered. The possibility of the industry discontinuing its operations and thus divesting its capacity due to profit margins becoming negative has not been included in the model. Calculating profit margins would require a rather complete picture of costs and benefits associated to a site's operations, which is deemed outside of the scope of this study. Instead, when looking at the question of retrofitting, only those cost aspects need to be considered that are expected to change if electrification is implemented, i.e.: investment costs, energy costs (including taxes and subsidies), CO_2 costs and operations & maintenance costs. This makes the cost calculations more manageable and more in line with this project's scope.
A crucial factor of concern in this comparison is the availability of renewable electricity as it determines the emission intensity of electricity and hence, the CO_2 costs per unit of electricity consumed. A higher share of renewables in the electricity mix thus means there are lower costs involved with electrification.

No changes in the composition of the production output. Though interviewees within the industry have indicated that electric cracking may induce changes in the composition of the production output and therefore the revenues obtained may either increase or decrease(Interviews, 2021), this is not taken into account in the model. Because electric cracking is still in an experimental face, no valid assumption could be made about the order of magnitude of these changes.

No changes in feedstock due to electrification. It assumed that electrification does not require changes in the type or volume of the naphtha feedstock required. Hence, feedstock costs are not considered in the model as they are assumed equal between electric and conventional retrofits.

Sufficiency of grid capacity not taken into account. Though grid capacity is an important prerequisite for the electrification of steam cracking processes (Interviews, 2021) it is not included in the model. This is because, from the industry's perspective, it can be considered binary: the grid capacity is expected to be either sufficient or insufficient. As such, it does not influence the cost comparison; it does influence whether the decision to invest in electrification is ultimately taken or not. Moreover, whether or not the grid connection of a site has to be upgraded and how much the required upgrade is, is highly dependent on site-specific conditions. Furthermore, a grid connection could perhaps be shared with other plants in an industrial cluster.
Because of the foreseen difficulties in modelling the grid capacity, a reverse approach has been adopted in this research. Based on the expected rate of electrification following from the modelled business case dynamics conclusions can be drawn about the required grid capacity upgrade rather than it being an input to the model.

5.2 Model conceptualization

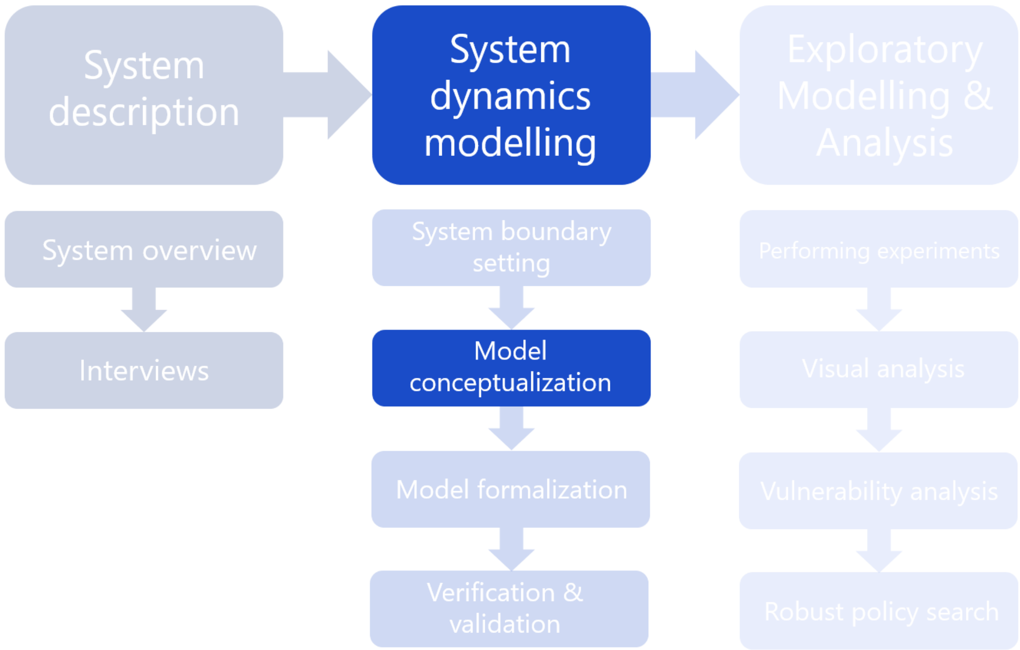

Figure 20: Position of the model conceptualization step in the research roadmap.

The goal of model conceptualization is to develop a causal loop diagram (CLD), a highly aggregated qualitative model of the causal relationships within the system. To this end the model components included in the model are outlined in Section 5.2.1, based on the system boundary set in Section 5.1. Second, the key performance indicators are listed in Section 6.1.2. This is important for determining the output of the model. Third, the exogenous factors and policy options are described in Section 5.2.3. Section 5.2.4 combines the model components, key performance indicators (output variables) and exogenous factors and policy options (input parameters) in a overview of model variables and parameters. Finally, the CLD is presented in Section 5.2.5.

5.2.1 Model components

Based on the system boundary defined in section 5.1, the model can be divided into the following components.

- **Costs**. This component reflects the expectations about the industry about the cost developments of certain technologies. It calculates different cost elements contributing to the expected operational expenditures (OPEX). The cost elements considered are: (1) energy costs, (2) carbon costs, (3) fixed operations & maintenance (O&M) costs and (4) grid connection costs.
  - Energy costs are in turn determined by (i) gas/electricity market prices, (ii) taxes, (iii) SDE++ subsidy and (iv) grid tariffs.
  - Carbon costs are in turn determined by the (i) EU ETS carbon price, (ii) the carbon levy and (iii) the availability of renewable electricity.
- **Investments**. Based on its expectations about costs, the industry makes an investment decision. These decisions are reflected by the *Investments* component. The investments in the model concern the investments required to extend the lifetime of existing installations by retrofitting. Only retrofitting of existing capacities is considered, not investments in new capacities or divestments. An exception are the boilers, for which also capacity hybridization is considered (see Section 5.1). The model allows for two methods of retrofitting: electrification or a "conventional" retrofit using gas-fired technologies. Whichever method the model chooses (the choice representing an investment decision) depends on the ratio of costs for electrification over the costs for a conventional retrofit. After adding the investment costs to the expected OPEX, the costs for the respective retrofit options can be compared and cost ratios can be calculated.

- **Capacities**. Following an investment decision, capacities are retrofitted. These capacities include the main installations relevant for the naphtha cracking process: furnaces, compressor turbines and boilers. Only the boilers capacity required for the production of steam for the furnaces and compressors is considered. Thus, boilers required for the steam demand of other processes onsite are excluded. Based on their respective lifetimes, the capacities are periodically retrofitted. However, it is assumed that retrofits are only executed during a turnaround, which occurs once every 6 years. This fact introduces a time delay in the model.
  The installation capacities and characteristics at Shell Moerdijk Lower Olefins (MLO) are used as a reference for the model. This is because this is the cracker site which features the largest availability of data through the MIDDEN project (Wong & van Dril, 2020). However, as the configuration at each site is different, the choice has been made not to extrapolate the installation capacities at Shell MLO in order for the model to represent the entirety of the six cracker sites. Rather, the electrification model considers a "reference plant" based on Shell MLO. Although the model does therefore not strictly represent the six cracker sites, the model behavior can be seen as representative for an individual cracker site.

5.2.2 Key performance indicators

To study the behavior of the model three key performance indicators are defined. First of all, we are interested in the CO_2 emissions of the naphtha cracker reference plant, which should be reduced. However, curbing CO_2 emissions may induce high production costs for the industry as well as high government expenditures for the required policy options. Hence, ideally CO_2 emissions reduced, while keeping production costs and policy costs limited. Hence, the selected key performance indicators are:

1. CO_2 emissions of the model naphtha cracking plant
2. Production costs of the model naphtha cracking plant (assuming a stable production volume)
3. Policy costs: costs of the combined policy options associated with the model naphtha cracking plant

5.2.3 Exogenous factors and policy options

The model components outlined in section 5.2.1 are impacted by various exogenous factors and policy options.

Exogenous factors. It is assumed that market prices are exogenous to the system and hence, outside of the system boundary. In other words: the industry's consumption of gas and electricity is assumed not to affect the market prices for these commodities. The exogenous factors considered in the model are the following:

- Electricity market price
- Gas price
- ETS price. The ETS price is the price paid per ton CO_2 emitted in the EU Emission Trading System.
- Investment costs for conventional retrofits. The investment costs for conventional retrofitting remain constant as these technologies have matured already. However, the investment costs for electrification are assumed to decrease over time due to technological learning. Hence, the investment costs for electric retrofits are modelled endogenously rather than exogenously.
- Technological learning. Learning effects reduce the costs of novel technologies over time. In this model it is also assumed that the costs of electric technologies will decrease over time according to a certain learning rate. In the model technological learning is assumed to be exogenous, that is technological learning is the result of global technological progress rather than upscaling. Endogenous learning due to upscaling is assumed only to occur on a larger geographical scale. This approach is in accordance with the approach employed in national energy models used by institutes such as PBL and TNO (Fattahi et al., 2020).
- Share of renewables. This factor denotes the share of renewable sources in the electricity mix. A higher share of renewables lowers the emission intensity of electricity, thus decreasing the carbon costs of electricity consumption.
- Efficiency improvements. It is assumed that conventional technologies will become more efficient over time, thus reducing the expected operational expenses for conventional retrofitting.

- Export value of residual gas. This factor reflects the uncertainty among the industry concerning the commercialization of surplus methane that results from electrification.

Policy options impact the cost comparison as they can make electricity cheaper than gas and thus improve the business case for electrification or vice versa. In the model only national-level policies are considered, not EU-level policies. Moreover, subsidies for pilots or demonstration projects such as the national DEI+ (*Demonstration Energy and Climate Innovation* subsidy) and the EU's Innovation Fund are not explicitly included in the model. Such subsidies would influence the costs for electrification more indirectly, as opposed to the SDE++ subsidy (see below). Incorporating these effects would require an in-depth understanding of innovation dynamics, which is deemed outside of the scope of this study. On the other hand, these subsidies can be regarded as having an impact on technological learning and therefore they can be seen as having been taken account implicitly through the exogenous factor of technological learning.
The following policy options are included in the model:

- SDE++. The Dutch *Stimulation Scheme for Sustainable Energy Production and Climate Transition* (SDE++) is a subsidy scheme aimed at stimulating the deployment of renewable energy sources in the electricity sector and the uptake of low-carbon technologies in the industry. It is an OPEX subsidy, meaning that it only lowers the operational costs of low-carbon technologies rather than lowering investment costs (PBL, 2021).

- Electricity taxes. Two different taxes apply to electricity: the electricity tax and the ODE (*Opslag Duurzame Energie* or Sustainable Energy Premium), which is an additional premium on energy consumption used by the government to finance energy transition measures such as the SDE++ (Government of the Netherlands, 2020a).

- Grid tariffs are costs charged by grid operators for maintaining a company's connection to the electricity grid and for the transport of electricity (Liander, 2020).

- Natural gas taxes. Like for electricity, companies pay both a "regular" tax and a ODE on their natural gas consumption.

- Carbon levy. The carbon levy (Dutch: *nationale CO_2-heffing*) is a CO_2 tax implemented by the government in 2021 to stimulate the industry to move away from fossil fuel. It starts at 30 euro/tonne CO_2 in 2021 and increases linearly up to 125 euro/ton CO_2 in 2030. Effectively, companies only pay a carbon tax if the carbon levy exceeds the EU ETS carbon price. In this case, the effective carbon tax is the difference between the carbon levy and the EU ETS carbon price. However, as long as the carbon levy remains lower than the EU ETS price, no carbon tax is levied (NEa, 2020).

- Number of dispensation rights (DPRs). The industry only pays the carbon levy tax on their avoidable emissions. That is, companies get a certain amount of free emissions rights called dispensation rights (DPRs) based on a industry-specific benchmark; this portion of their emissions is not taxed. 1 DPR is equivalent to 1 tonne CO_2. However, the amount of DPRs decreases linearly over time according to a certain reduction factor (NEa, 2020).

5.2.4 Overview of model variables and input parameters

Based on the system boundary defined in section 5.1, the model components defined in section 5.2.1 and the exogenous factors and policy options outlined in section 5.2.3 a bull's eye diagram visualizing the variables endogenous and exogenous to the model and the variables omitted in the model is shown in Figure 21.

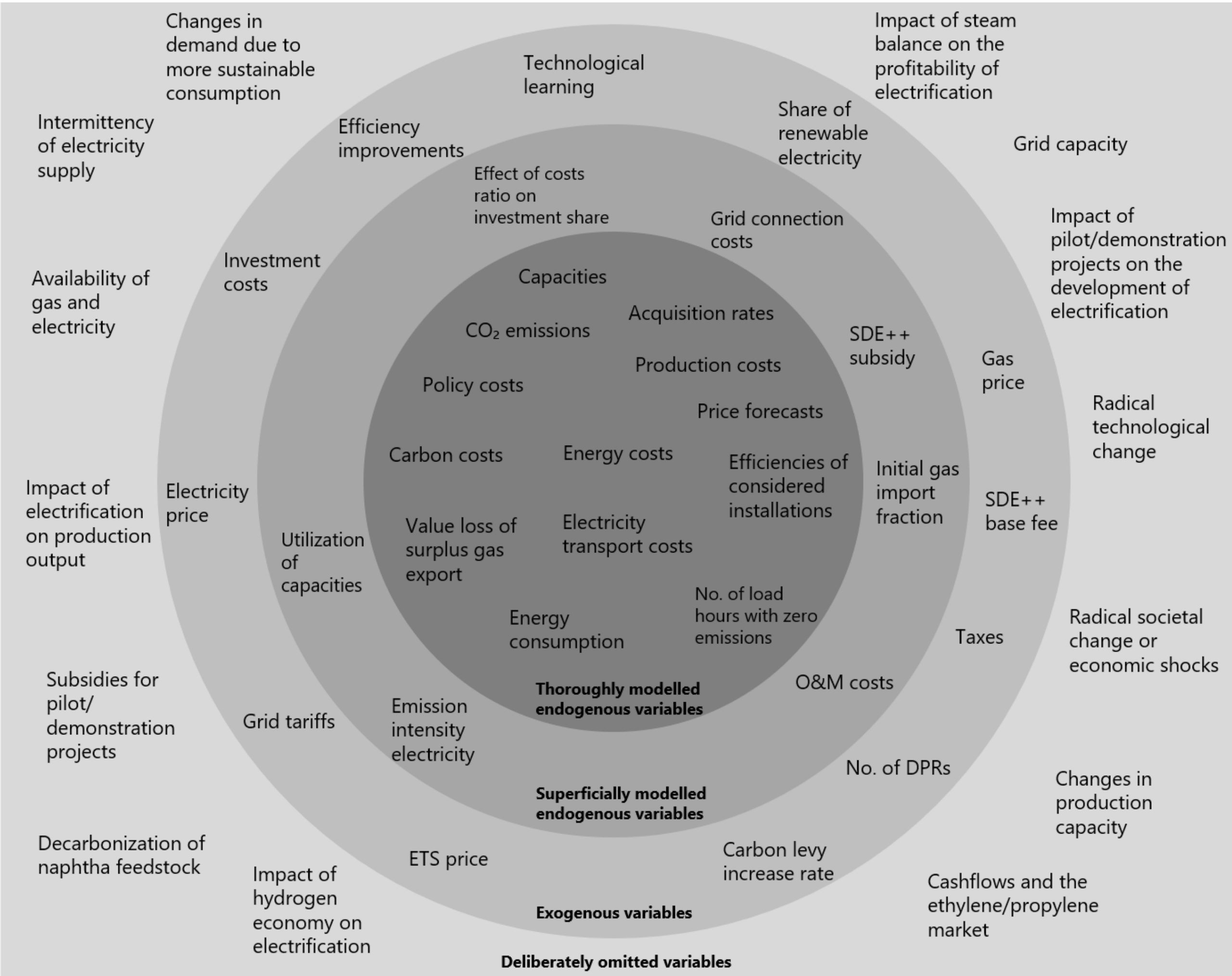

Figure 21: Bull's eye diagram of the variables included in and deliberately omitted from the model. Modelled after Moallemi, Aye, et al. (2017).

5.2.5 Causal loop diagram

In Figure 26 the causal loop diagram of the electrification model is shown. In the CLD in Figure 26 the following feedback loops can be identified.

1. Grid connection costs loop (reinforcing). Because of the high power requirements of electric furnaces and electric compressor turbines, installing this equipment requires a connection of the site to the High Voltage (HS) or Extra High Voltage (EHS) grid (Interviews, 2021; ACM, 2020). Grid operators recover the investment costs for implementing this connection from the site owner. Initially this costs form a barrier for electrification. However, with more electric capacity being added the marginal grid connections costs (i.e. the costs per MW of installed electric capacity) decrease. Therefore, a reinforcing feedback loop is involved. The grid connection costs loop is illustrated by Figure 22.

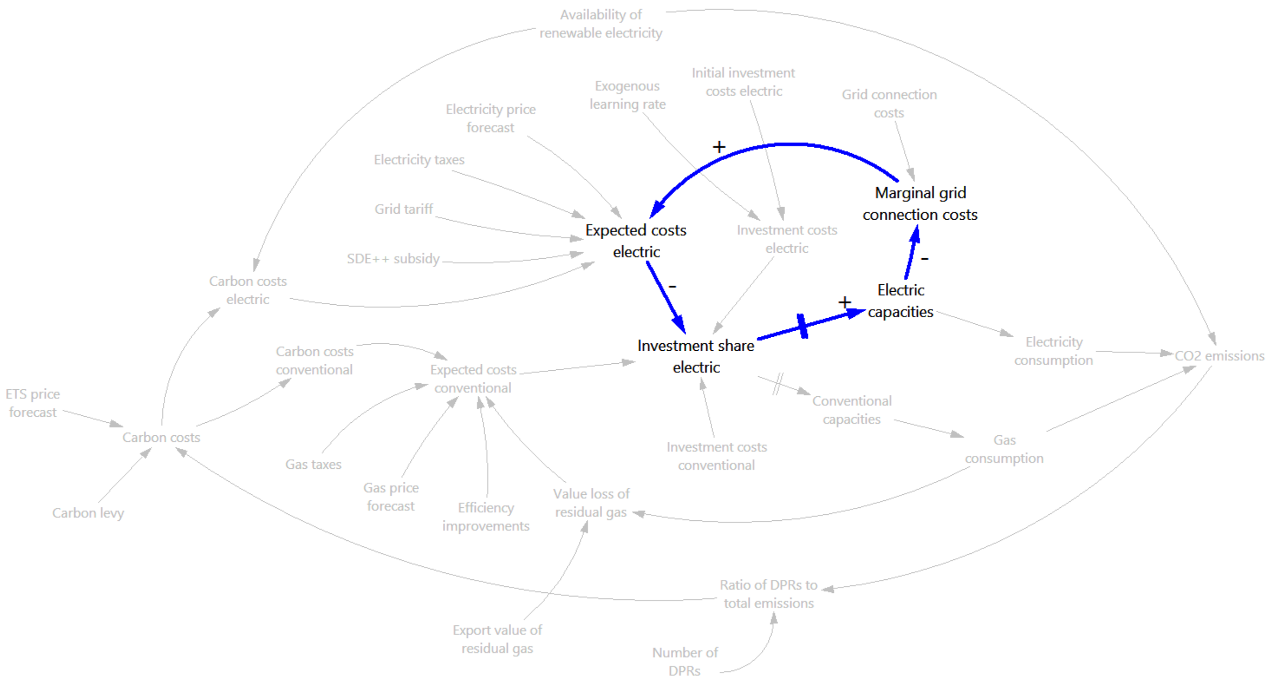

Figure 22: Illustration of the grid connection costs loop, a reinforcing loop. With increasing electric capacities, the marginal grid connection costs decrease. Arrows featuring an equal sign represent a time delay: it is assumed that capacity is only replaced during a turnaround.

2. Residual gas loop (balancing). Furnaces and boiler onsite require gas for their operation. Part of this gas demand is supplied by methane-rich gas that is produced in the naphtha cracking process itself. Hence, initially only 23% of the gas demand needs to be imported[1]. However, when electrification reduces the gas demand such that the demand drops below the amount of gas produced, there is a surplus of methane-rich gas. There exists uncertainty among the industry about whether this gas can be commercialized because the gas demand in society will decrease due to the energy transition (Interviews, 2021).
Suppose the residual gas has an export value of zero. In this case, if the gas consumption level drops below the gas production level as a consequence of electrification, this means any conventional retrofit will feature zero energy costs as the gas it will consume (originating from the gas production within the process rather than from gas imports) cannot be commercialized otherwise. Thus, the *Expected costs for a conventional retrofit* are reduced, decreasing the *Investment share of electrification*. Hence, this is a balancing feedback loop. The residual gas loop is illustrated by Figure 23.

[1]Based on gas consumption and production data for Shell Moerdijk Lower Olefins (MLO) published in Wong & van Dril (2020) the net gas import fraction has been calculated to be 23%. This number is used for the reference plant used in the electrification model.

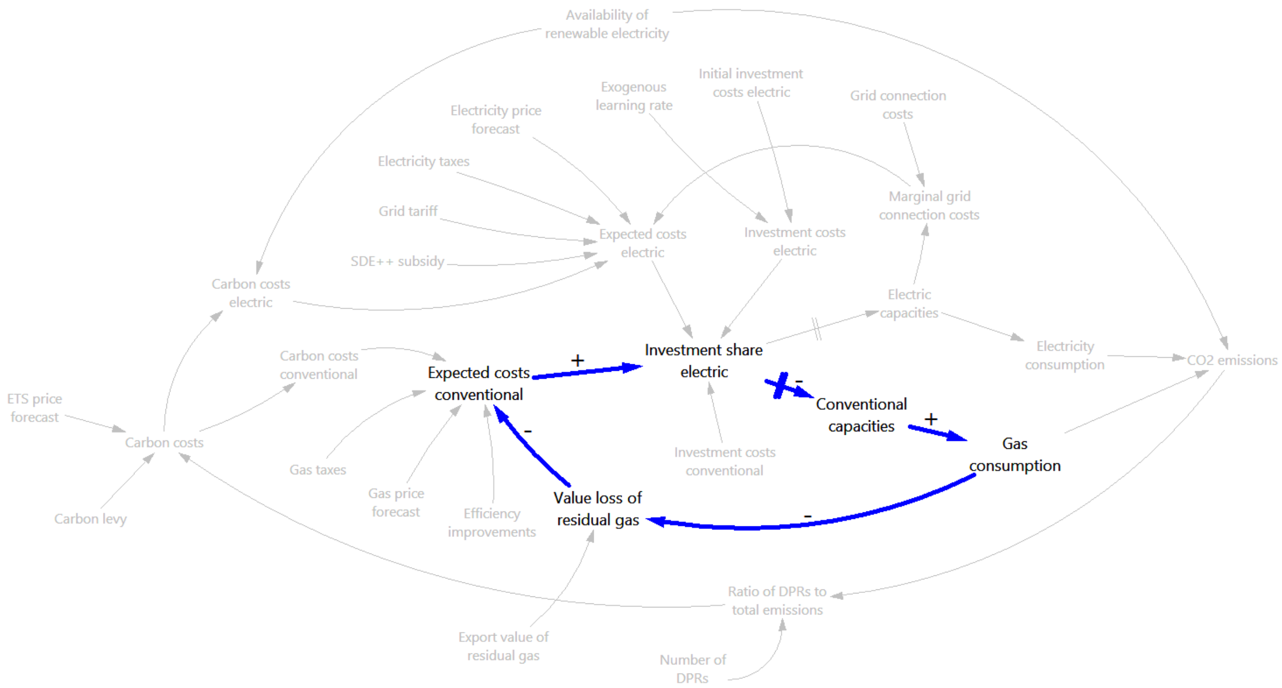

Figure 23: Illustration of the residual gas loop, a balancing loop. As gas consumption decreases due to electrification, while gas keeps being produced within the production process, there will be residual gas at some point. This residual gas will have a lower value than natural gas. Therefore, this residual gas represent a lost value. Arrows featuring an equal sign represent a time delay: it is assumed that capacity is only replaced during a turnaround.

3. Carbon costs electricity loops (one reinforcing and one balancing loop). As described in Section 5.1 the carbon levy features an allocation of free emissions rights to the industry. These rights - or exempted emissions - are called dispensation rights (DPRs). These dispensation rights are independent from the actual emissions but are determined by a benchmark based on a company's production output. Hence, if the site's emissions decrease the ratio of DPRs to total emissions increases, in turn decreasing the effective carbon tax paid (labelled *Carbon costs* in the causal loop diagram Figure 26). This ultimately increases the profitability of electrification. As long as electricity is not 100% renewable and thus the emission intensity of electricity is non-zero, electrification results in an increase in emissions, hence acting as a balancing feedback loop. On the other hand, less conventional capacities will be retrofitted, decreasing the gas consumption and thus, decreasing emissions; this is a reinforcing feedback loop.

4. Carbon costs gas loop (one reinforcing and one balancing loop). Due to the DPRs granted to the industry, two other feedback loops emerge. As the effective carbon tax decreases due to decreasing emissions, the expected costs for a conventional retrofit are also reduced, negatively affecting emissions. Therefore, this is a balancing feedback loop. On the other hand, as long as their is insufficient renewable electricity available, emissions due to electricity consumption are reduced; this is a reinforcing feedback loop.

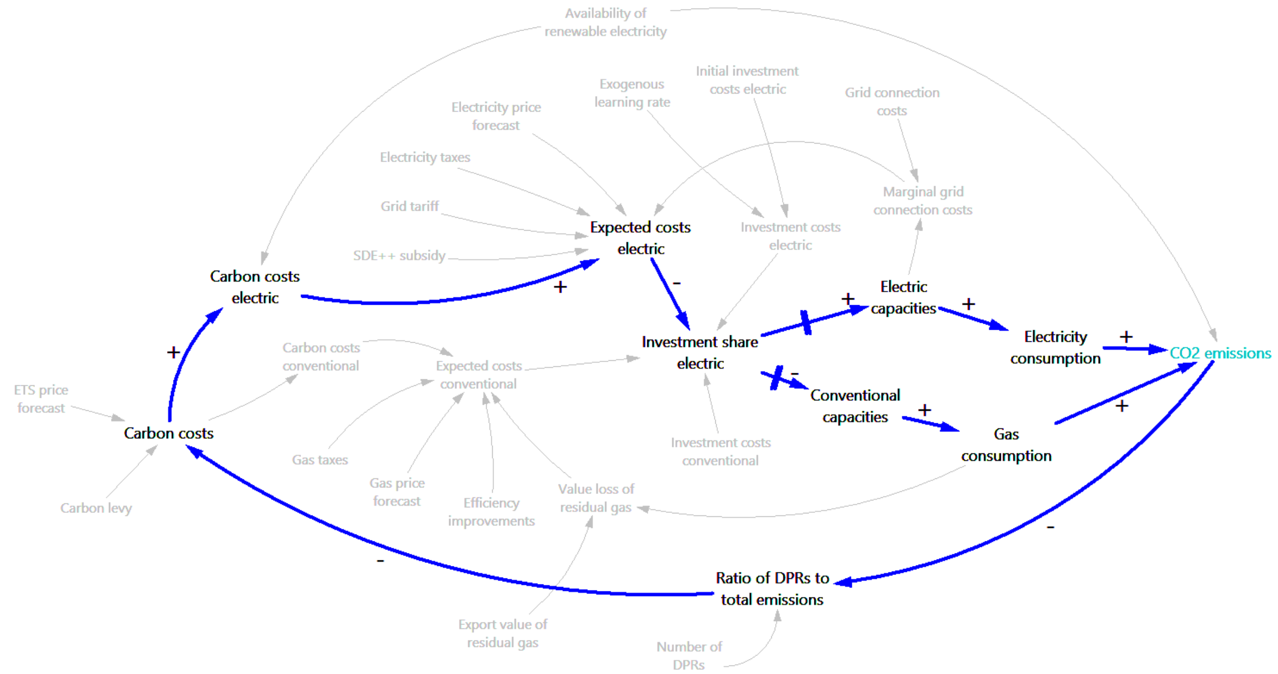

Figure 24: Illustration of the carbon costs electricity loops: one reinforcing and balancing loop. With decreasing emissions, the industry gains relatively more dispensation rights (DPRs). This reduces the expected costs for electric retrofits, causing more emissions due to electricity consumption but reducing emissions due to gas consumption.

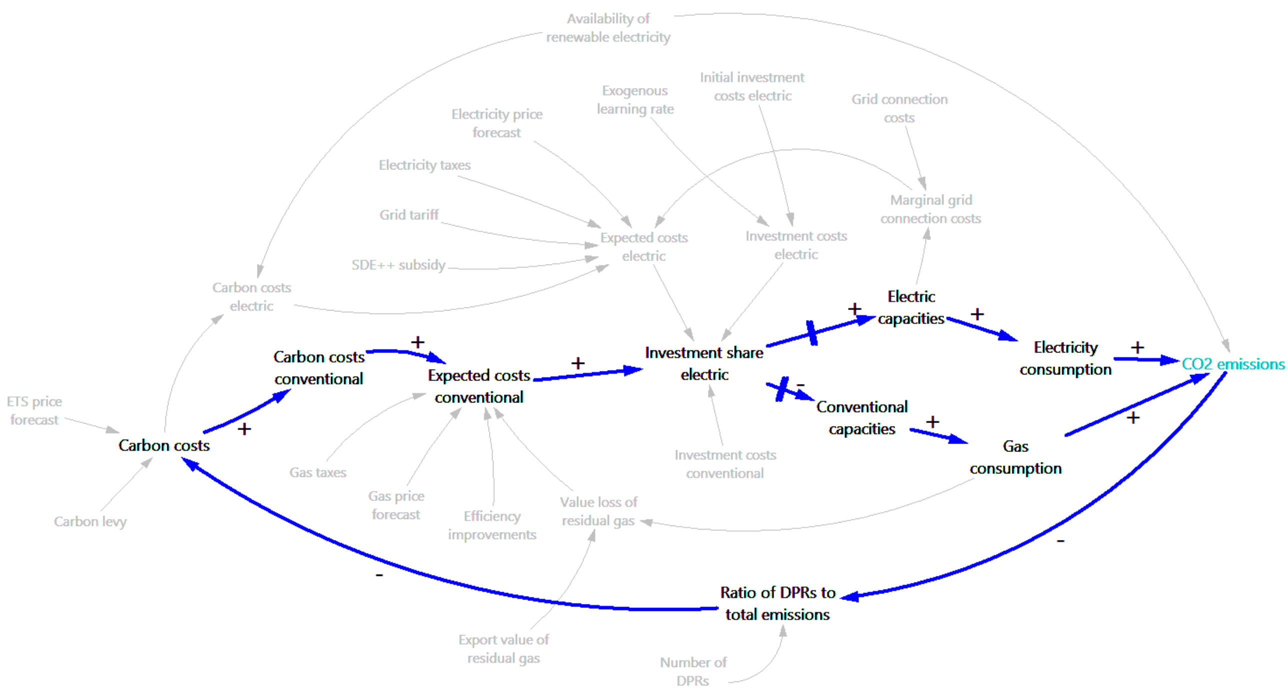

Figure 25: Illustration of the carbon costs gas loops: one reinforcing and balancing loop. With decreasing emissions, the industry gains relatively more dispensation rights (DPRs). This reduces the expected costs for conventional retrofits, causing more emissions due to gas consumption but reducing emissions due to electricity consumption.

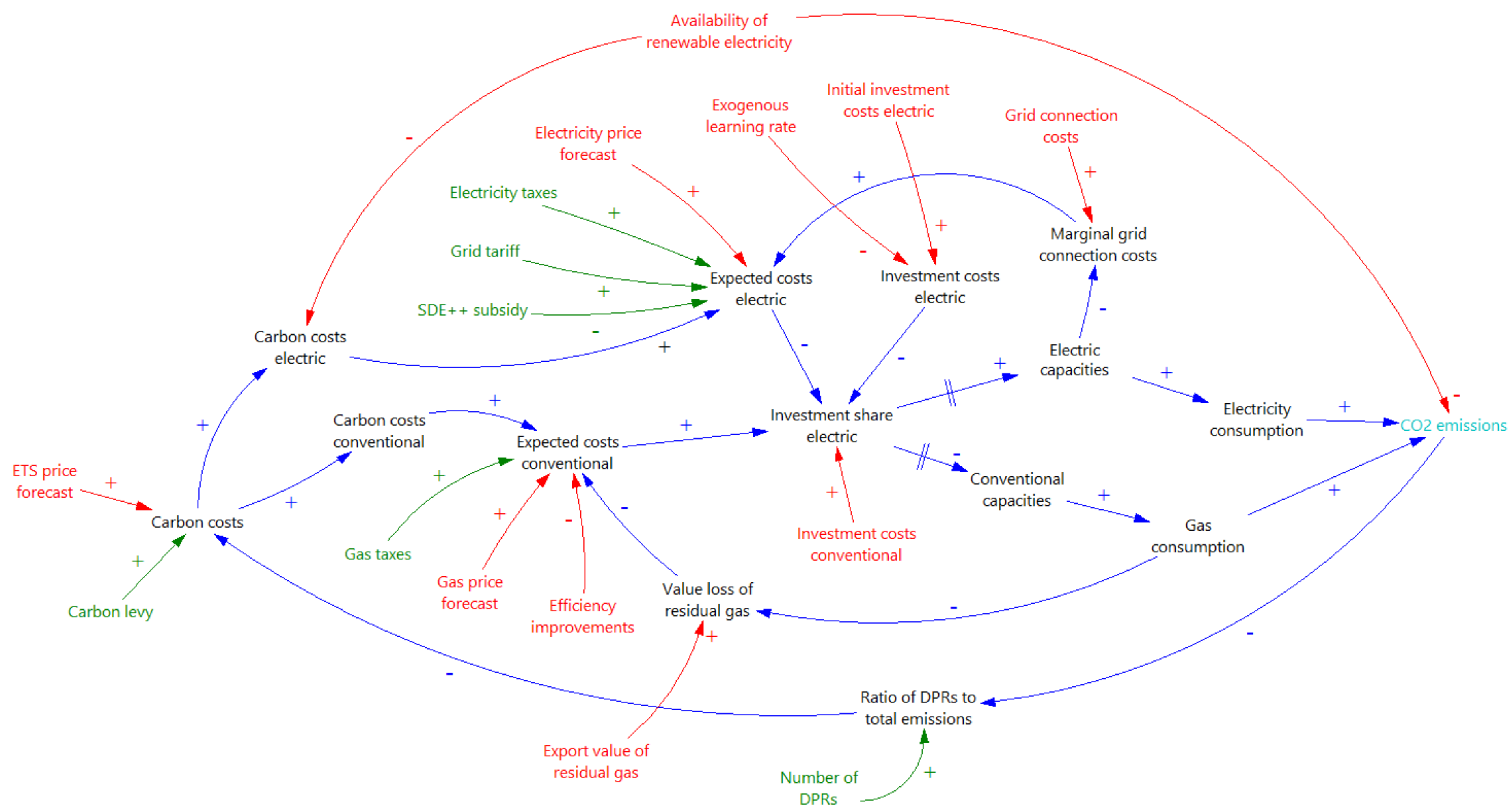

Figure 26: Causal loop diagram of the electrification model. The red-colored variables represent exogenous factors while the green-colored variables indicate policy levers. The arrow featuring an equal sign represents a time delay: it is assumed that capacity is only replaced during a turnaround.

5.3 Model formalization

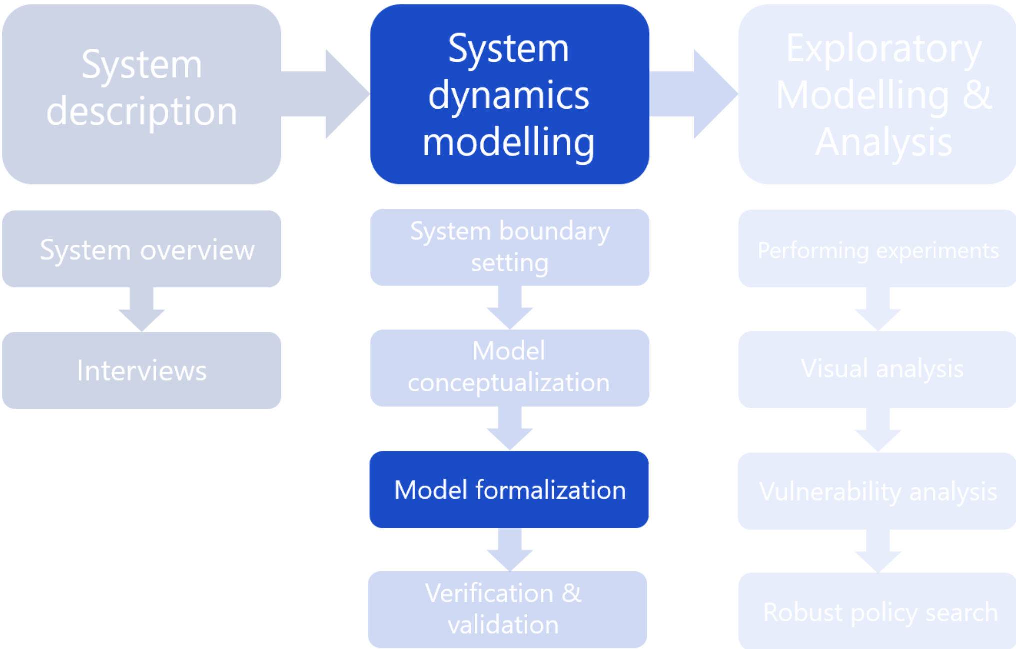

Figure 27: Position of the model formalization step in the research roadmap.

In the model formalization phase the causal loop diagram (CLD) developed in Section 5.2 is translated to a set of quantitative relationships. These quantitative relationships constitute a stock-flow diagram (SFD). As introduced in section 5.2.1 the model consists of three main components: *Costs*, *Investments* and *Capacities*. The role of each component is described below.

- **Costs**. In this component the expected operational expenditures (OPEX) are calculated for electric and conventional retrofits, respectively. The cost elements considered are: (1) energy costs, (2) carbon costs, (3) fixed operations & maintenance (O&M) costs and (4) grid connection costs.

- **Investments**. Based on its expectations about the costs of each technology, the industry makes an investment decision. These decisions are reflected by the *Investments* component. Investments are either channeled into electric or conventional retrofits. To determine the share of each option in the total investment sum the *present value* of each option is computed. The ratio of the present value of the electric retrofit option over the present value of the conventional retrofit option then determines the share of each option in the total investment sum, also called the "investment share".
Beside retrofits also the hybridization of the boiler capacity is considered. In this regard, a separate investment share is computed.

- **Capacities**. Following an investment decision, capacities are retrofitted, which is represented by *capacity acquisition* in the model. The *Capacities* component features a stock-flow structure where *capacites* are represented by a stock while *capacity acquisition* and *capacity depreciation* are represented by flow variables.
The capacities are periodically retrofitted. It is assumed that retrofits are only executed during a turnaround, which occurs once every 6 years. This fact introduces a time delay in the model. Based on their respective lifetimes, the capacities are also depreciated. However, the depreciation rate is linked to the investment rate so the overall capacity of each installation remains constant. An exception is the boiler capacity which changes based on the steam demand required by the conventional steam-driven compressor turbines. If the electrification rate of compressor turbines increase, the steam demand is reduced, lowering the overall boiler capacity.
The *Capacities* component also contains the calculation of the system's key performance indicators: CO_2 emissions, production costs and policy costs.

In the following, the three model components are outlined by means of simplified Vensim diagrams accompanied by the most important model equations. The detailed Vensim model can be found in Appendix C.

The variables in the simplified Vensim diagrams are color-coded as follows: endogenous model variables are colored ***black***, policy options are colored *green*, uncertain external factors are colored *red*, fixed external factors are colored *brown* and model outputs are colored *cyan*, following the categorization outlined in Section 5.2. Finally, the *gray* variables that occur in some components represent variables originating from other model components. These are known as *shadow variables* in Vensim terminology.

5.3.1 Costs component

In the *Costs* component of the model the expected operational expenses (OPEX) of each technology are calculated. That is: (conventional) furnaces, compressor turbines, boilers and their respective electric counterparts. As decision-makers in the industry plan their investments for the next turnaround, they formulate expectations about future prices, such as the electricity price, the price of natural gas and the EU ETS carbon price. In the model, these values are assumed to show a linear development based on their current value and their predicted future value in 2030 or 2050 depending on the variable. The reference year for the prices is 2019 as for this year PBL (Netherlands Environmental Assessment Agency) published its latest price report (PBL, 2020). In the model, it is assumed that decision-makers in the industry also assume the prices will increase linearly according to their current value and their predicted value. That is: the expected price 6 years from the current time instant in the model is equal to the actual price 6 years ahead.
It should be noted that this is a rather large assumption. In reality, decision-makers in the industry will likely base their price forecasts on analyses and reports such as the World Energy Outlook (IEA, 2021).
Besides price forecasts, policy options (the carbon levy and the SDE++ subsidy), the share of renewable electricity in the electricity mix and efficiencies are also forecasted. However, these forecasts are non-linear. For further details see Appendix C.
Other policy options (i.e. taxes and grid tariffs) are represented by constants.
Based on these forecasts, the OPEX for electric retrofit options (denoted as "OPEX electric") and for conventional retrofit options (denoted as "OPEX conventional") are calculated. These calculations are outlined below. The OPEX calculations include the following elements:

- Energy costs (gas or electricity)
- Carbon costs
- Taxes and ODE
- Efficiencies of each technology
- Fixed O&M (operations & maintenance) costs
- SDE++ subsidy (for electrification)
- Grid transport costs (for electrification)
- Grid connection costs (for electrification)

The carbon costs, which features in the calculations of both OPEX electric and OPEX conventional, are discussed separately.

OPEX electric

In Figure 28 a simplified structure of the calculation of OPEX electric is shown. This calculation includes the electricity price forecast of course, in addition to taxes, SDE++ subsidy, carbon costs and fixed O&M costs. Note that this component also features a feedback loop as discussed in Section 5.2.5. With increasing electric capacities, the grid connection costs can be divided over a larger amount of megawatts (MW's). Hence, the marginal grid connection costs (the per MW costs) decrease.
In the model, OPEX electric at each time instant t is calculated as follows. Note that this calculation is different for each technology (electric furnaces, electric compressor turbines or electric boilers) depending on its efficiency, fixed O&M costs and grid tariffs.

$$OPEX_{el} = EC_{el} + O\&M_{el} + MGCC \tag{1}$$

where $MGCC$ represents the marginal grid connection costs and EC_{el} represent the energy costs, which are in turn calculated as follows:

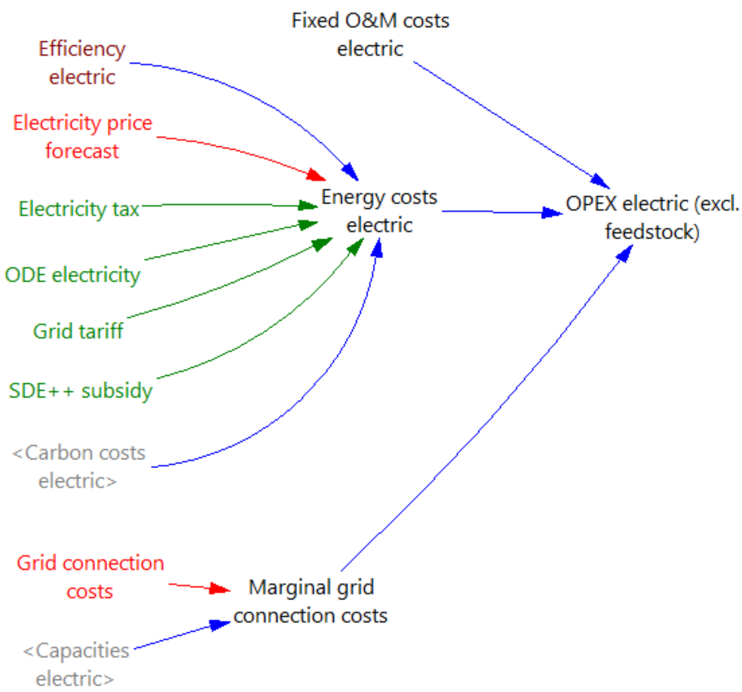

Figure 28: Simplified representation of the calculation of the OPEX (operational expenses) for electric retrofits in the model.

$$EC_{el} = \frac{electricity\ price + tax_{elec} + ODE_{elec} + carbon\ costs_{elec} + grid\ transport\ costs - SDE}{efficiency_{el}} \tag{2}$$

Note that the efficiency is considered fixed for electric technologies. Electric technologies already feature efficiencies of 95% or more. Electric boilers even feature efficiencies of 99% (Marsidi & Lensink, 2020a). Hence, it is assumed no further efficiency improvements occur in electric technologies.
The calculation of the SDE++ subsidy is further outlined in Appendix D.1.

OPEX conventional

In Figure 29 a simplified structure of the calculation of OPEX conventional is shown. This calculation features the gas price forecast of course, in addition to taxes, carbon costs and fixed O&M costs.
For conventional retrofits the OPEX is calculated as follows:

$$OPEX_{con} = EC_{con} + O\&M_{con} \tag{3}$$

where EC_{con} equals:

$$EC_{con} = \frac{v \cdot gas\ price + tax_{gas} + ODE_{gas} + carbon\ costs_{gas}}{efficiency_{con}} \tag{4}$$

where v represents the value of gas, details about which can be found in Appendix D.2.
In contrast to electric technologies, conventional technologies are assumed to see efficiency improvements over time. These efficiency improvements are further explained in Appendix D.3.

Carbon costs

The structure of the carbon costs calculation is shown in Figure 30. The carbon costs differ between electric and conventional technologies as the emission intensity of gas consumption is different from the emission intensity electricity consumption. The emission intensity of gas consumption is considered fixed and based on the net calorific value of gas (Wong & van Dril, 2020; Zijlema, 2020). However, the emission intensity of electricity changes over time according to the share of renewable electricity in the electricity mix. The calculation

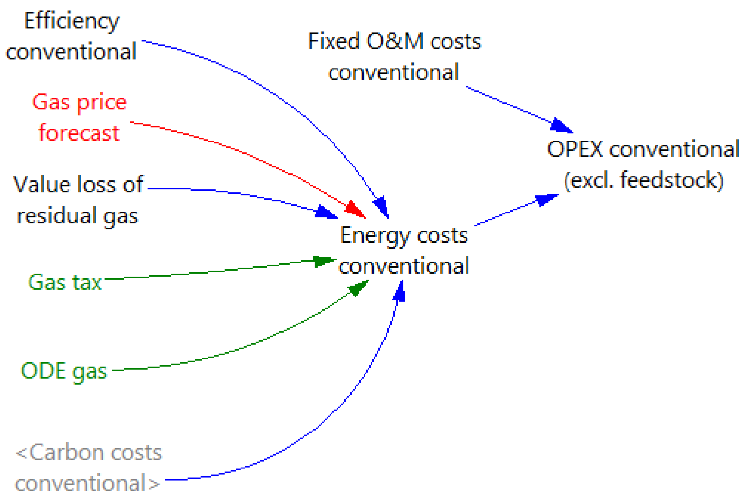

Figure 29: Simplified representation of the calculation of the OPEX (operational expenses) for conventional retrofits in the model.

of the share of renewable electricity and the emission intensity of electricity is further explained in Appendix D.5.

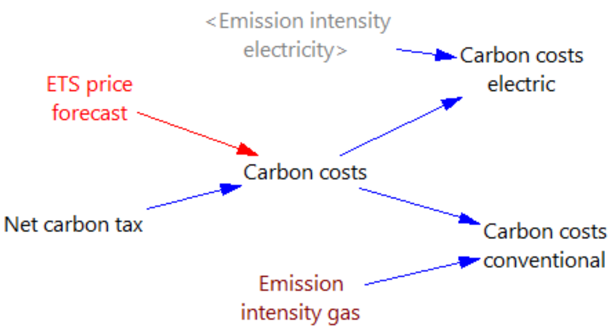

Figure 30: Simplified representation of the calculation of carbon costs in the model.

The carbon costs for electric and conventional technologies, respectively, can be represented by the following equations:

$$carbon\ costs_{el} = carbon\ costs \cdot emission\ intensity_{elec} \tag{5}$$

$$carbon\ costs_{con} = carbon\ costs \cdot emission\ intensity_{gas} \tag{6}$$

where:

$$carbon\ costs = ETS\ price + net\ carbon\ tax \tag{7}$$

Here, $ETS\ price$ is the carbon price paid by the industry in the EU Emission Trading System (ETS). The $net\ carbon\ tax$ is levied on the industry by the government and features a separate calculation, which is outlined in Appendix D.6.

5.3.2 Investments component

In the *Investments* component, the OPEX of each technology, along with its investment costs, are translated to a *present value* for each technology. The ratio of the present values then determines which share of each investment sum is channeled towards electric retrofits and to conventional retrofits. The structure of the *Investments* component can be represented by a simplified diagram shown in Figure 31.

In the following, the calculations of the present value and the investment share are discussed in more detail. The investment share for boiler hybridization involves a separate calculation, which is discussed at the end of this section.

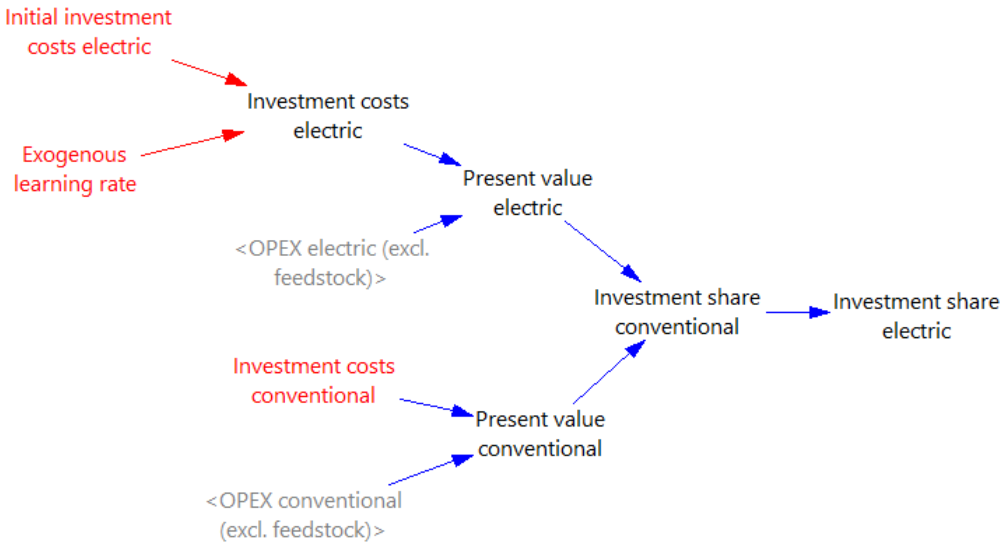

Figure 31: Simplified representation of the calculation of investment shares for electric and conventional retrofits in the model.

Present value calculations

The *present value* (PV) is the current value of a sum of future cash flows (Moyer et al., 2011). The current value of a future cash flow is lower than its future value because future cashflows are discounted according to the discount rate. The higher the discount rate, the lower the present value. Moreover, the further in the future the cashflow, the lower its present value. The PV is calculated as follows:

$$PV = \sum_{t=1}^{n} R_t \cdot D_t \tag{8}$$

where R_t is the cashflow's future value, t=*1* is the start of the time period considered, n is the number of time periods and D_t is the discount factor. In turn, the discount factor D_t depends on the discount rate d as follows.

$$D_t = \frac{1}{(1+d)^t} \tag{9}$$

where d is the discount rate and t is the time instant considered in the time period t=*1, ..., n*.

In investment decisions, the *net present value* (NPV) is ofted used to determine whether a potential investment is profitable or not (Interviews, 2021; Verbeek, 2021).

$$NPV = \sum_{t=1}^{n} (X_t - Z_t) \cdot D_t - I_0 \tag{10}$$

Here, X_t is the cash inflow at time t, Z_t is the cash outflow and I_0 is the initial investment sum. However, in the case of this model, only cash outflows are considered, i.e. OPEX and investment costs. Hence, we adhere to the term *present value* rather than *net present value* because cash inflows are not considered.

Hence, the equation used in the formal model is:

$$PV = \sum_{t=T+1}^{n} \frac{OPEX_t}{(1+d)^t} + I_T \tag{11}$$

where n is equal to the economic lifetime. Normally the NPV is considered over the entire (technical) lifetime of an installation. However, in reality investments are required to generate a return faster than the technical lifetime. Therefore, the economic lifetime is considered an appropriate time frame for the NPV calculations (Schure, 2021a). T is the length of the time interval between consecutive turnarounds. As the industry looks 6 years ahead for its investment, T=*6* in the reference case. Hence, also the investment cost is discounted (Verbeek, 2021):

$$I_T = \frac{I_0}{(1+d)^T} \tag{12}$$

Investment shares electric and conventional

Once the present values of the costs for a conventional retrofit and the costs for an electric retrofit are calculated based on Equation 11, the model calculates the ratio between the costs for the respective options:

$$r = \frac{P_{el}}{P_{con}} \tag{13}$$

where P_{el} represents the present value of the costs for an electric retrofit and P_{con} represents the present value of the costs for a conventional retrofit. The model then translates r to a share of each option in the investment rate for retrofits using a logistic function, also called an S-curve (Kucharavy & De Guio, 2011; Lotfi et al., 2014). According to Vogstad (2004) behavior patterns of capacity development "typically exhibit s-shaped diffusion curves for technologies." As in this model only retrofits are considered, the upper limit of the S-curve is 1, i.e. the maximum investment rate is equal to the depreciation rate. Furthermore, the S-curve reflects the expectation that the industry will already channel part of its investments towards electrification when decision-makers expect that electrification will become profitable in the near future.
Thus, the investment shares for conventional retrofits and electric retrofits are computed as follows:

$$i_{con} = \frac{1}{1+e^{-k\cdot(r-1)}} \tag{14}$$

$$i_{el} = 1 - i_{con} \tag{15}$$

where k is the steepness of the S-curve. Note that at $r = 1$: $i_{con} = i_{el} = 0.5$. This reflects the assumption that if the costs for an electric retrofit P_{el} equal the costs for a conventional retrofit P_{con} the industry invests 50% in electrification.

Investment share boiler hybridization

Boiler hybridization is different from retrofitting as it involves placing an electric boiler next to an already operating gas boiler. The two boilers then operate in hybrid fashion, each running part of the time. The effective output capacity (measured in PJ steam per time unit) remains the same. As it is assumed to not affect the continuation of the onsite processes, boiler hybridization can be implemented independent of the turnaround times. Hence, the investment decision is of a different nature as hybridization of the boiler capacity concerns *flexible electrification* while electric retrofits (of furnaces, compressor turbines and boiler) concern *baseload electrification* (see section 2.1.3).

In the case of boiler hybridization the investment decision concentrates on the question: are the costs of continuing the current operation of a gas-fired boiler higher than the costs of operating a gas-fired boiler and an electric boiler in hybrid fashion plus the investment costs of a new electric boiler? Mathematically: is the present value of continuing the operation of an existing gas boiler greater than the present value of a hybrid configuration: $P_{gas\ boiler} > P_{hybrid}$?

The structure of the investment share for hybrid boilers can be found in Figure 32.

The OPEX for a hybrid boiler configuration depends on the number of load hours N_{load} that an electric boiler in hybrid configuration is allowed to operate. It is assumed that this number equals the number of hours per

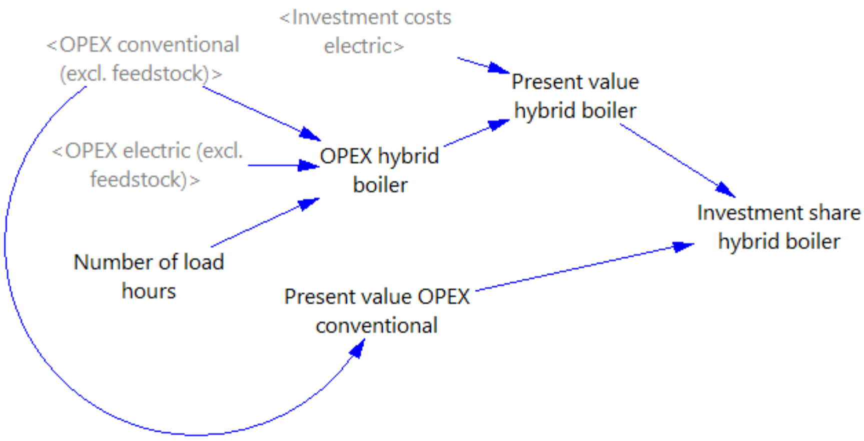

Figure 32: Simplified representation of the calculation of investment share for boiler hybridization in the model.

years in which renewable electricity is available. Hence, the number of load hours depends on the availability of renewable electricity. The calculation of this number is detailed in Appendix D.7.
Operating during these hours may mean that the electricity market price is lower. However, according to Elzenga & Lensink (2020), this effect is cancelled out by the increasing grid transport costs per MWh for a lower number of load hours.
Hence, the OPEX for a hybrid boiler is computed as follows:

$$OPEX_{hy} = \frac{N_{load}}{N_{tot}} \cdot OPEX_{el} + \left(1 - \frac{N_{load}}{N_{tot}}\right) \cdot OPEX_{con} \tag{16}$$

where N_{tot} is the total number of operating hours per year (which depends on the utilization rate of the plant).
The present value for a hybrid boiler is then calculated as:

$$P_{hybrid} = \sum_{t=1}^{n} \frac{OPEX_{t_{hybrid}}}{(1+d)^t} + I_{0_{e-boiler}} \tag{17}$$

Note that, as it is assumed that boiler hybridization does not adhere to the turnaround frequency, the start period of the present value calculation is $t = 1$ rather than $t = 7$.
To determine whether boiler hybridization is profitable P_{hybrid} should be compared to the present value of continuing operations with the current gas boiler, $P_{gas\ boiler}$, which is calculated as follows:

$$P_{gas\ boiler} = \sum_{t=1}^{n} \frac{OPEX_{t_{gas\ boiler}}}{(1+d)^t} \tag{18}$$

Note that $P_{gas\ boiler}$ does not include an investment cost component as it is based on the operations of an already existing gas boiler.

According to equations 13, 14 and 15 the investment share for hybridization i_{hybrid} is calculated.

5.3.3 Capacities component

In the *Capacities* component, investments are translated to capacity acquisitions for each technology. Based on these acquisitions, the model can simulate the development of capacities over time. This affects gas and electricity consumption, which in turn determines the CO_2 emissions of the plant, the production costs and the policy costs: the model output variables. In the following, the computation of capacity acquisition in the model is detailed, followed by the model output variables.

Capacity acquisition

In Figure 33 a simplified stock-flow diagram of capacity acquisition in the model is shown. Note that each element contains multiple variables. In Vensim terminology, they are "subscripted". For example, the *Capacities* stock contains the capacities of all technologies considered: conventional and electric furnaces, conventional and electric compressors, etc.

The investment shares calculated in the *Investments* component form the input for the *Investment rates*. The investment rates also depend on the *Expected depreciation rates*. The *Expected depreciation rates* are the sums of the depreciation rates of the electric and conventional capacities for each technology as, following the assumption of a stable production capacity, the total output capacity of each installation should remain equal. As the model only considers retrofits, the investment shares are multiplied with the expected depreciation rates to obtain the investment rates. This process can be clarified with the following example. Consider an initial conventional furnace capacity of 100 MW and an initial electric furnace capacity of 0 MW. The depreciation rate is 5 MW/year. At timestep 0 the investment share for conventional furnaces is 60% and the investment share for electric furnaces is 40%. Hence the investment rate for conventional furnaces in timestep 0 is 3 MW/year and the investment rate for electric furnaces is 2 MW/year. Hence, after a delay incurred by the turnaround the capacity of conventional furnaces decreases by 2 MW while the capacity of electric furnaces increases by 3 MW.

However, as boiler hybridization does not involve retrofitting, the investment share for hybrid boilers is not multiplied with the expected depreciation rate to obtain the investment rate. Instead, it is multiplied with a set maximum percentage of the boiler capacity to become hybrid per year, based on the expectation that a maximum of 5 MW per year could be subject to boiler hybridization in the current configuration (Schure, 2021a). Hence, in Figure 33 a direct relationship between *Capacities* and *Investment rates* can be observed.

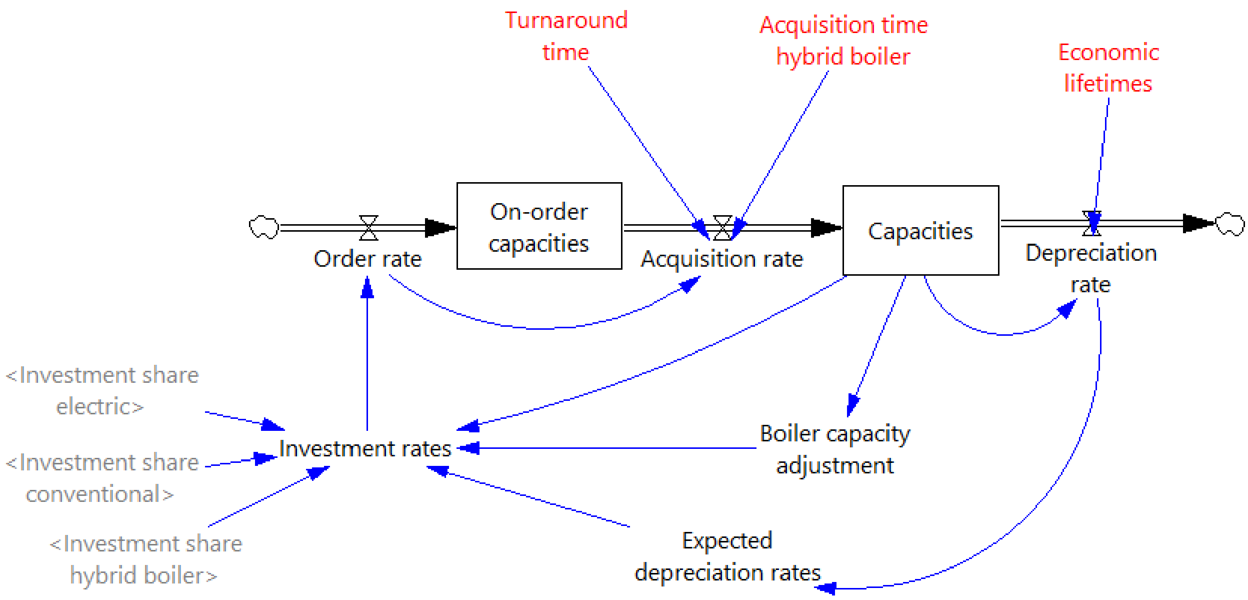

Figure 33: Simplified stock-flow diagram representing capacity acquisition in the model.

In the following, the model equations are detailed.

The *Investment rates* are calculated as follows:

$$investment\ rate_{con} = i_{con} \cdot EDR \tag{19}$$
$$investment\ rate_{el} = i_{el} \cdot EDR \tag{20}$$

where EDR is the expected depreciation rate. The *Expected depreciation rates* are the sums of the depreciation rates of electric and conventional capacities for each technology. The depreciation rate for each technology is equal to:

$$depreciation\ rate = \frac{capacity}{economic\ lifetime} \tag{21}$$

For boilers the calculation is slightly different as the expected depreciation rate rate is corrected for by *Boiler capacity adjustment* (see Appendix D.4 for further details). This adjustment is needed because if the number of conventional compressor turbines decreases due to electrification, the steam demand decreases and hence, a lower boiler capacity is required. Therefore, not all depreciated boilers need to be replaced or retrofitted. Hence:

$$investment\ rate_{con_{boiler}} = i_{con_{boiler}} \cdot DIR_{boiler} \tag{22}$$

$$investment\ rate_{el_{boiler}} = i_{el_{boiler}} \cdot DIR_{boiler} \tag{23}$$

DIR_{boiler} represents the desired investment rate for the boiler capacity. In turn, DIR_{boiler} is computed as follows:

$$DIR_{boiler} = \begin{cases} EDR_{boiler} + CA_{boiler}, CA_{boiler} > -EDR_{boiler} \\ 0, CA_{boiler} \leq -EDR_{boiler} \end{cases} \tag{24}$$

where EDR_{boiler} is the expected depreciation rate of the boilers and CA_{boiler} is the capacity adjustment of the boilers, which is based on the steam demand of the (remaining) steam-driven compressor turbines. The investment rate is not allowed to be negative, so if the CA_{boiler} decreases such that the sum $EDR_{boiler} + CA_{boiler}$ becomes zero, the desired investment rate becomes 0.

Once capacity retrofits have been ordered, it takes time before they are actually added to the capacities. This is because retrofits are only performed during a turnaround. This causes a third-order delay in the model according to *Average waiting time until turnaround* (Sterman, 2000). Boiler hybridization does not obey the turnaround time and hence in the case of capacity acquisition of hybrid boilers, the delay is based on an acquisition time, which represents the time required for construction etc.

Finally, the capacities of each installation k is calculated in the model as the time-integral of the acquisition rate minus the depreciation rate:

$$capacity_k = \int_t (acquisition\ rate_k - depreciation\ rate_k)\ dt \tag{25}$$

CO_2 emissions

The simplified structure of the CO_2 emissions calculation is shown in Figure 34.

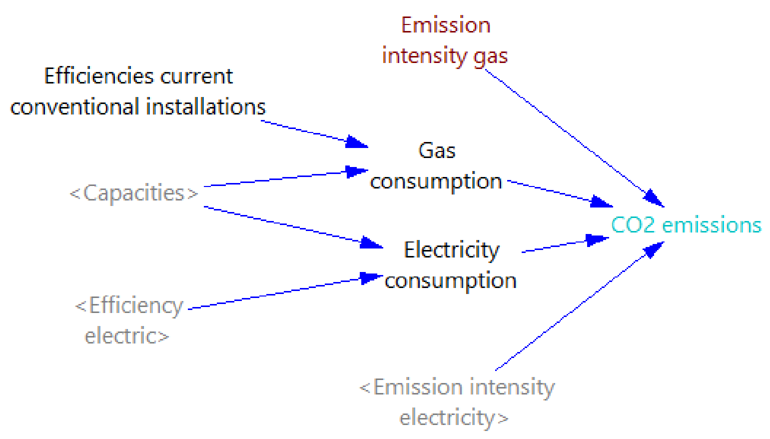

Figure 34: Simplified representation of the calculation of CO_2 emissions in the model.

CO_2 emissions are calculated as follows:

$$emissions_{CO_2} = C_{gas} \cdot EI_{gas} + C_{elec} \cdot EI_{elec} \tag{26}$$

where C_{gas} is the total amount of gas consumed by conventional installations, EI_{gas} is the emission intensity of gas (a constant), C_{elec} is the total amount of electricity consumed by electric installations and EI_{elec} is the emission intensity of electricity. EI_{elec} varies over time according to the availability of renewable electricity. More details can be found in Appendix D.5.

In turn, C_{gas} and C_{elec} are computed as follows:

$$C_{gas} = \sum \frac{capacity_{con_k}}{efficiency_{con_{k_{tot}}}} \tag{27}$$

$$C_{elec} = \sum \frac{capacity_{el_k}}{efficiency_{el_k}} \tag{28}$$

where $capacity_{con_k}$ represent the capacity of each conventional installation and $capacity_{el_k}$ represents the capacity of each electric installation. Not the difference in summation sign between the two equations. The efficiency of current electric capacities is constant as it is assumed no efficiency improvements occur in electric technologies. Hence, to obtain the electricity consumption per electric installation, its capacity is simply divided over the efficiency. However, the efficiency of conventional installations $efficiency_{con_k}$ changes over time (see Section 5.3.1). Hence, newly acquired capacities with higher efficiencies change the aggregate efficiency $efficiency_{con_{k_{tot}}}$ of the combined conventional installations. Therefore, an overall efficiency $efficiency_{con_{k_{tot}}}$ is calculated. This calculation is detailed in Appendix D.8.

Production costs

In Figure 35 the simplified structure of the calculation of production costs is shown. Its equations are further detailed below.

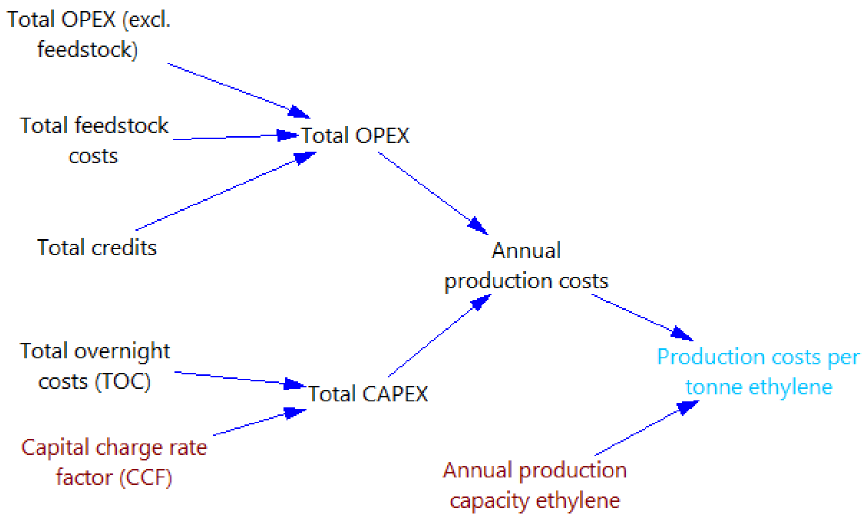

Figure 35: Simplified representation of the calculation of production costs in the model.

Following Spallina et al. (2017) the production costs per tonne ethylene are calculated as follows[2]:

$$production\ costs_{eth.} = \frac{annual\ production\ costs}{\dot{m}_{eth.}} \tag{29}$$

where $\dot{m}_{eth.}$ is the annual ethylene production capacity and *annual production costs* equals:

$$annual\ production\ costs = OPEX_{tot} + CAPEX_{tot} \tag{30}$$

In turn, $OPEX_{tot}$ is computed as follows:

$$OPEX_{tot} = OPEX_{excl.\ feedstock} + OPEX_{feedstock} + \sum OPEX_{credits} \tag{31}$$

[2] In Spallina et al. (2017) the numerator in the production costs equation also contains the fixed O&M (operations & maintenance) costs. However, in the model these costs are already included in the OPEX. Hence, they are left out of Equation 30.

where $OPEX_{feedstock}$ are the costs of naphtha feedstock, $OPEX_{excl.\ feedstock}$ is the sum of energy costs, carbon costs and grid costs and $\sum OPEX_{credits}$ is the sum of the revenue of chemical co-products, such as propylene. For the calculation of $OPEX_{feedstock}$ and $\sum OPEX_{credits}$, see Appendix D.9.

Following Spallina et al. (2017) $CAPEX_{tot}$ is computed as follows:

$$CAPEX_{tot} = CCF \cdot TOC \tag{32}$$

where CCF is capital capital charge rate factor, which "defines a characteristic unit cost of the plant over the life of the plant accounting for all expenditures that occur in different periods on a common value basis" (Spallina et al., 2017). For a naphtha cracking plant this value has been estimated to be 0.1 (Spallina et al., 2017). TOC stands for total overnight costs, which is the sum of the contingencies and owner's costs (COC) and engineering procurement and construction costs (EPC). The TOC is estimated to be equal to 2.4 times the bare equipment costs (BEC) of a plant, which is the sum of plant components, on-site facilities and infrastructure supporting the plant (Wong & van Dril, 2020). For some plant components an estimation of the TOC could be made directly from values reported by industry representatives (Interviews, 2021) and technology datasheets, e.g. Jansen et al. (2019). In other cases, an estimation of the TOC was made based on the BEC of common naphtha cracking plant components published by Spallina et al. (2017).

Policy costs

The policy costs are the sum of subsidies granted to the industry minus the sum of taxes (electricity taxes, gas taxes and carbon taxes) levied on the industry. Figure 36 shows the simplified structure of the calculation of policy costs in the model.

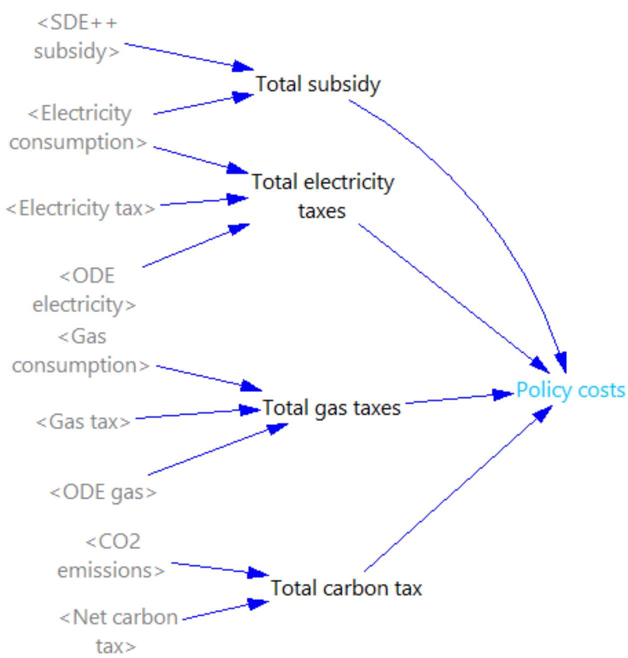

Figure 36: Simplified representation of the calculation of policy costs in the model.

The policy costs are calculated as follows:

$$policy\ costs = subsidy_{tot} - (taxes_{el,tot} + taxes_{con,tot} + tax_{carbon,tot}) \tag{33}$$

The individual elements of Equation 33 can be represented by the following equations:

$$subsidy_{tot} = C_{elec} \cdot SDE \tag{34}$$

$$taxes_{el,tot} = C_{elec} \cdot (tax_{elec} + ODE_{elec}) \tag{35}$$

$$taxes_{con,tot} = C_{gas} \cdot (tax_{gas} + ODE_{gas}) \tag{36}$$

$$tax_{carbon,tot} = emissions_{CO_2} \cdot net\ carbon\ tax \tag{37}$$

where C_{gas} and C_{elec} are calculated using Equations 27 and 28, respectively. CO_2 emissions are represented by Equation 26. The calculation of the SDE++ subsidy is detailed in Appendix D.1 and the calculation of the net carbon tax can be found in Appendix D.6.

5.4 Verification & validation

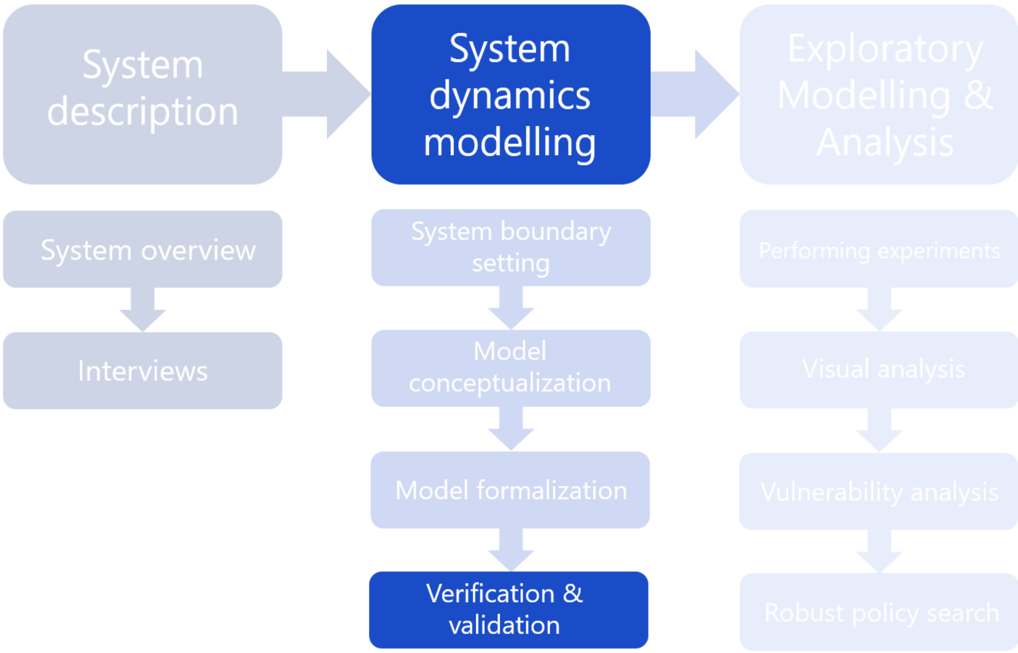

Figure 37: Position of the verification & validation step in the research roadmap.

Verification & validation is about testing the formal model to determine whether it is appropriate for studying the formulated research objective (Sterman, 2000). Hence, verification & validation serves to Verification & validation comprises different tests:

1. Reference mode (Section 5.4.1): an analysis of the behavior of performance indicators in a reference simulation
2. Boundary adequacy (Section 5.4.7): an evaluation of the system boundary set in Section 5.1
3. Dimensional consistency (Section 5.4.2): an assessment of the correctness of the units of input parameters and model variables
4. Integration error and time step (Section 5.4.3): verification of the insensitivity of the simulation results to the choice of time step or integration method
5. Extreme conditions tests (Section 5.4.4): an assessment of the model's behavior under extreme values of the input parameter
6. Sensitivity analysis (Section 5.4.5): an assessment of the model's output variables to changes in the input parameters
7. Face validation (Section 5.4.6): a test in which an expert judges on the structure and behavior of the model

5.4.1 Reference mode

The reference mode is a display of the behavior over time of key system variables. The reference mode can either be historically observed or hypothesized (Vensim Documentation, n.d.-b). Because this model concerns future development of electrification, the reference mode (see 3.3) is one of hypothesized behavior. The system variables that have been selected are: (1) output capacities of the installations considered, (2) annual CO_2 emissions, (3) production costs per tonne ethylene and (4) annual policy costs.
The reference mode for the electrification model is represented by the simulation results of a base case. In this base case, exogenous factors in the model are set to values published in several projections or based on assumptions or estimations. The base case is a "policy-rich" scenario, meaning that it contains policy options based on current, adopted and proposed government policy. For the full list of input parameters see Table 3 in

Appendix E.

For the base case, the development of capacities is displayed in Figure 38. Figure 39 is Figure 38 zoomed in to only show compressor turbines and boilers. It can be observed that no electrification happens for furnaces: the capacity of conventional furnaces remains stable at 600 MW, while the capacity of electric furnaces remains 0. This can be explained by the high expected initial investment costs for electric furnaces, which make the future business case for electric cracking unattractive.
By contrast, for compressor turbines, rapid and far-reaching electrification occurs. As a result, compressor turbines are almost entirely electric by 2050. This can be expected as compressor turbines feature a rather lower efficiency (32% gas-to-work) compared to furnaces (82% gas-to-heat). These results are also in line with the interviews held among the industry. The interviewees agreed that the electrification of compressor turbines will be the first step in the electrification of the naphtha cracking industry. Among the electrification options, this is also the most mature technology. At several sites, pilot projects have been run with smaller electric motors. The large efficiency gain was also mentioned as an important advantage by the interviewees. On the other hand, the interviewees emphasized that it is unlikely that all compressors will be electrified because the cooling of cracked naphtha will keep producing steam (Interviews, 2021). However, this has not been accounted for in the model.

As a consequence of the electrification of compressor turbines, the overall the boiler capacity decreases because the steam demand is reduced due to a higher share of electric compressor turbines. Therefore, though the capacities of electric and hybrid boilers increase initially, they start to decrease again around 2030. Before 2030 considerable electrification and hybridization of the boiler capacity occurs. These high degrees of electrification may be optimistic as from the interviews it became evident that the electrification of the steam production is challenging due to the highly integrated steam cycle and the different steam grids (see Section 4.1.1). Moreover, electric boilers that are capable of producing HP and HHP steam at an industrial scale are yet to be developed, as opposed to electric boilers for MP steam (Interviews, 2021).

In general, it is questionable whether the grid capacity can accommodate the rather fast electrification rates of compressor turbines and boilers projected in the reference mode. The grid capacity has not been included in the model but was described by the industry as an important precondition for electrification (Interviews, 2021). A recent report published by CE Delft (Scholten et al., 2021) showed that the required upgrades in the electricity grid to accommodate electrification can feature very long lead times up to 10 years or more. Thus, the reference mode confirms the concerns of the industry regarding the grid capacity as it shows that the business case for electrification may well outpace the grid capacity. Hence, the grid capacity may prove a limiting factor to electrification (Interviews, 2021).

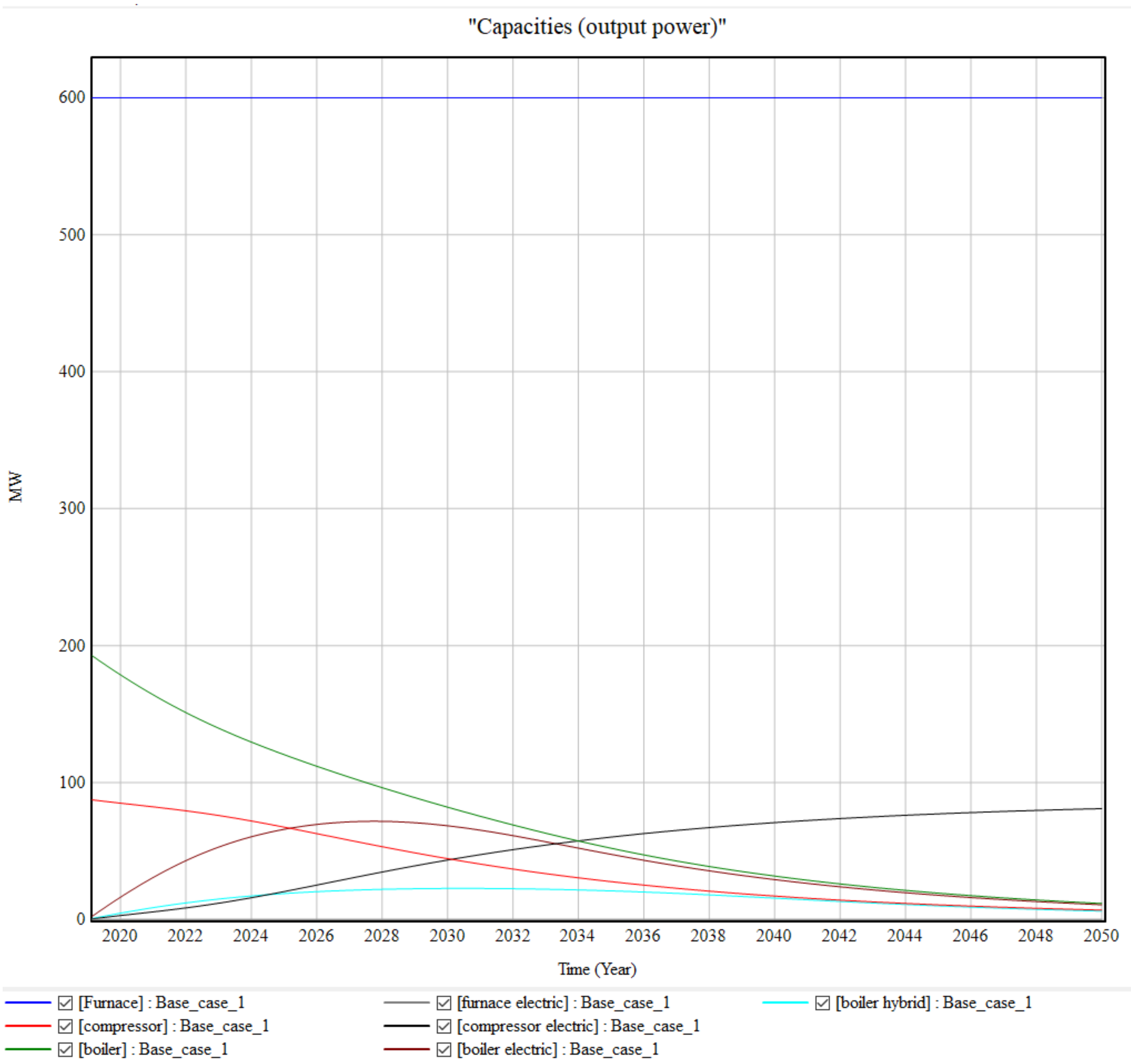

Figure 38: Base case: simulation of the installed capacities [MW] of gas-fired furnaces, compressor turbines, boilers, electric furnaces, electric compressor turbines, electric boilers and hybrid boilers (electric boilers that run part-time) in the electrification model.

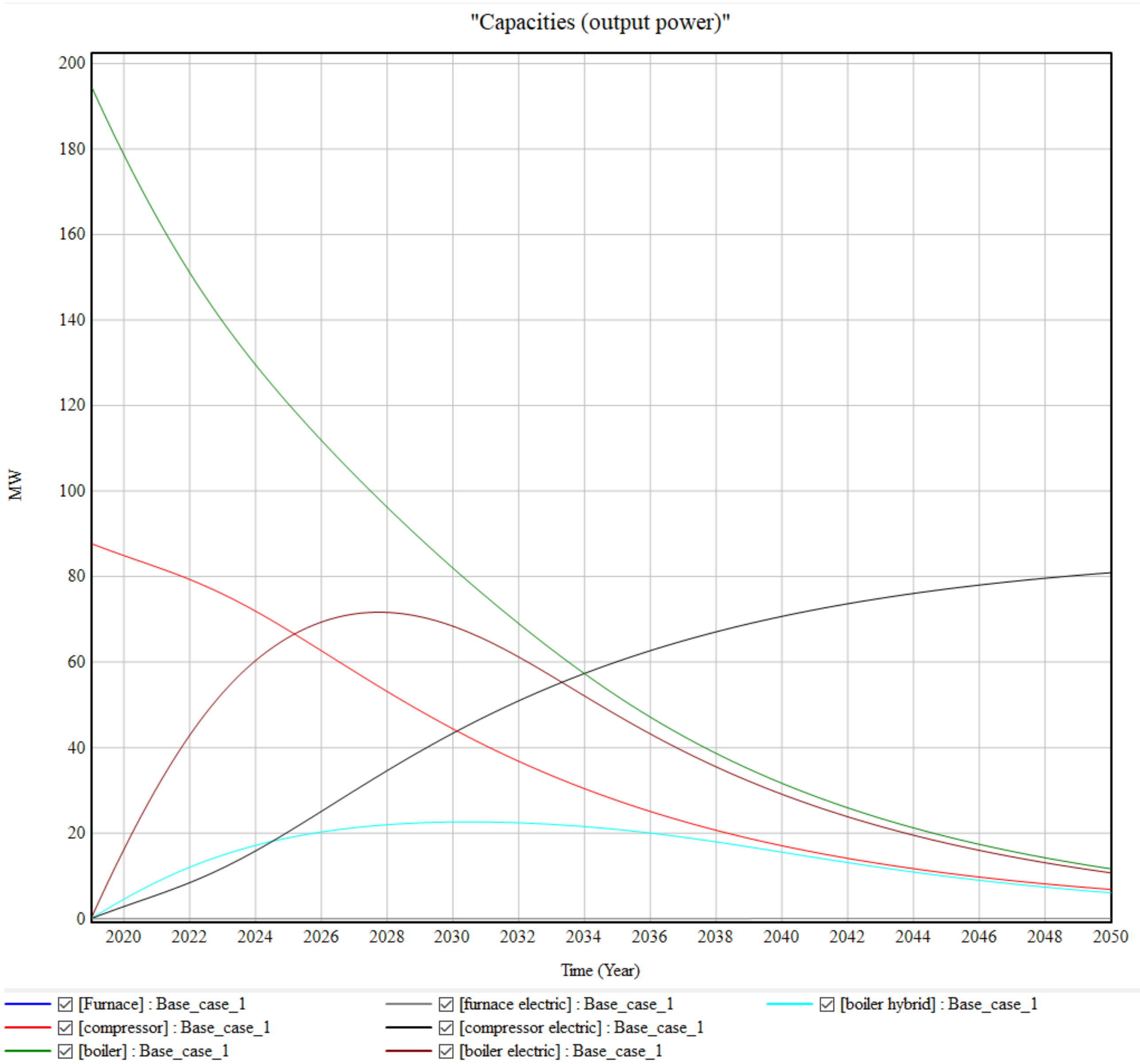

Figure 39: Base case: simulation of the installed capacities [MW] of installations in the electrification model, zoomed in to only show compressor turbines and boilers.

In Figure 40 the annual CO_2 emissions related to cracking are displayed. The initial value of 1569 kftonne/year corresponds to the value reported in Wong & van Dril (2020): 1210 kton/year for steam cracking and 662 ktonne/year for utilities (which includes the boilers). Summing these values yields an annual emissions of 1872 ktonne/year. However, as only part of the utilities serve the cracking process it is expected that the emissions as calculated in the model turn out lower.

It can be observed from Figure 40 that the emissions increase first before decreasing. This is line with e.g. Koelemeijer et al. (2018) who state that "electrification can lead to extra emissions in the short term".

From the model's perspective, this can be explained by the fact that electrification of compressor turbines and boilers already pose an attractive business case, resulting in rapid electrification as can be seen in Figure 39. However, the emission intensity of electricity is initially still higher than the emission intensity of gas due to the low share of renewable electricity in the electricity mix. Therefore, electrification initially leads to an increase in emissions as installations switch from gas to electricity. However, as the share of renewable electricity gains momentum, electrification starts having a beneficial effect on emission reduction.

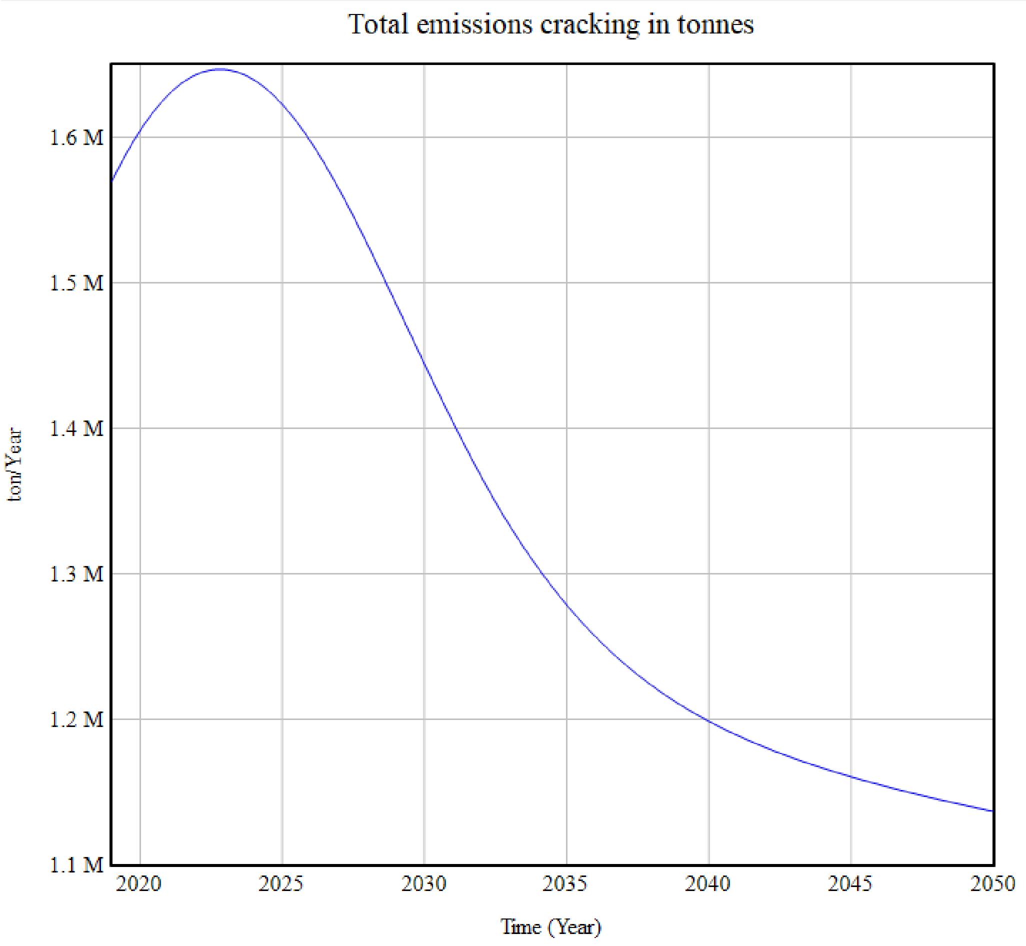

Figure 40: Base case: simulation of emissions [tonnes CO_2 per year] in the electrification model. Note that the value at each time instant represents the emissions at that time instant extrapolated to the entire year.

In Figure 41 the development of the production costs per tonne ethylene over time is shown. The production costs initially start at 920 euro/tonne ethylene. This is considerably higher than the value reported by Spallina et al. (2017) (835 euro/tonne on the European market) but does not seem unreasonably high. The production costs increase up to over 1040 euro/tonne ethylene in 2050. Note that the current market price of ethylene amounts to 1004 euro/tonne (PBL, 2021). This result confirms the concerns among the industry about the future profitability of ethylene and propylene. According to industry representatives interviewed, the profit margin of ethylene and propylene production may already be insufficient for a viable business case for electrification (Interviews, 2021).

The abrupt changes in the production costs curve can be attributed to the development of the carbon levy (see Section 5.2.3 for its principle and Appendix D.6 for its calculation). In 2026, the carbon levy exceeds the

ETS price and hence, the effective carbon tax becomes non-zero. This causes a rather sharp increase in the production costs. However, in 2030 the slope of the production costs curve decreases as the carbon levy remains stable at 125 euro/tonne$_{CO_2}$ from 2030 onwards. On the other hand, the number of dispensation rights (DPRs) granted to the industry keep decreasing, causing the slope to increase over time. After 2042 the production costs decrease. From this point onwards the the number of DPRs is has reached 0. Therefore, the carbon levy after reduction of DPRs remains stable (as the gross carbon levy has already been stable since 2030). At the same time, the ETS price keeps rising, reducing the difference between the carbon levy and the ETS price, causing the net carbon tax to fall. Hence, the production costs decrease as well.

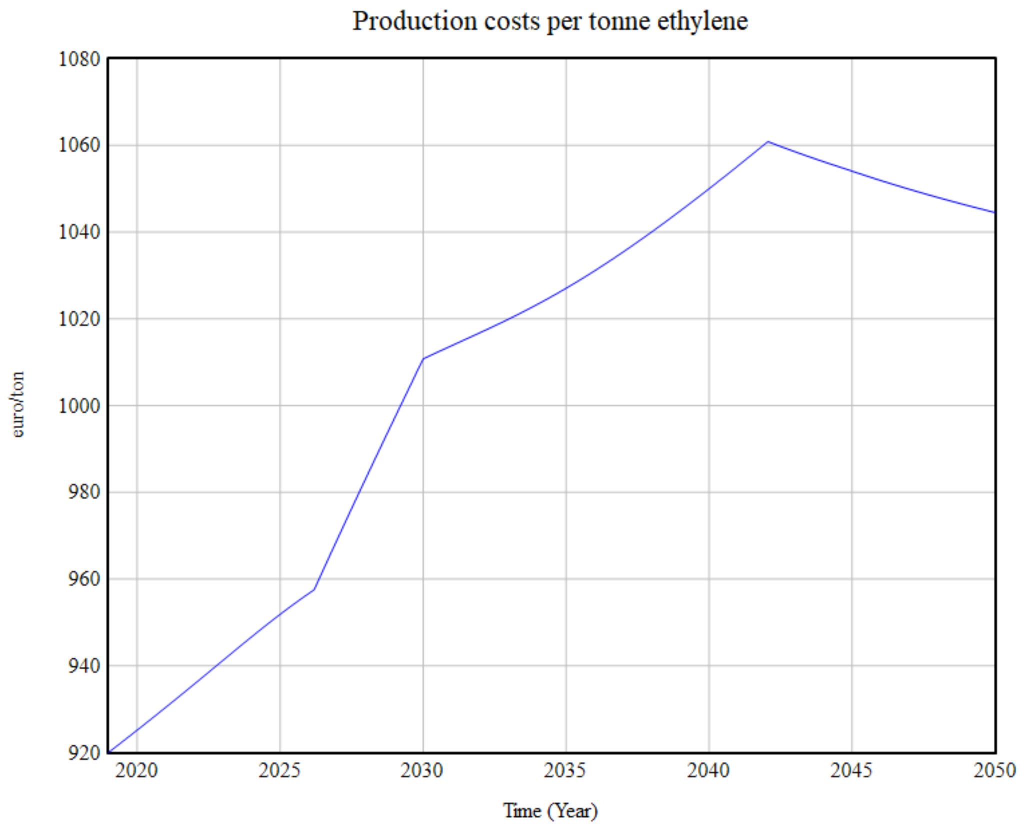

Figure 41: Base case: simulation of the production costs per tonne ethylene.

Figure 42 shows the development of policy costs in the base case over time. The policy costs remain negative, implying that the total amount of taxes levied remains larger than the SDE++ subsidy granted for electrification. Like in Figure 41, the abrupt changes in the curve can be attributed to the development of the carbon levy. The policy costs first rise due to the increasing SDE++ subsidy granted but then decrease due to the increasing net carbon tax. After 2042 the policy costs start to increase again as the net carbon tax drops.

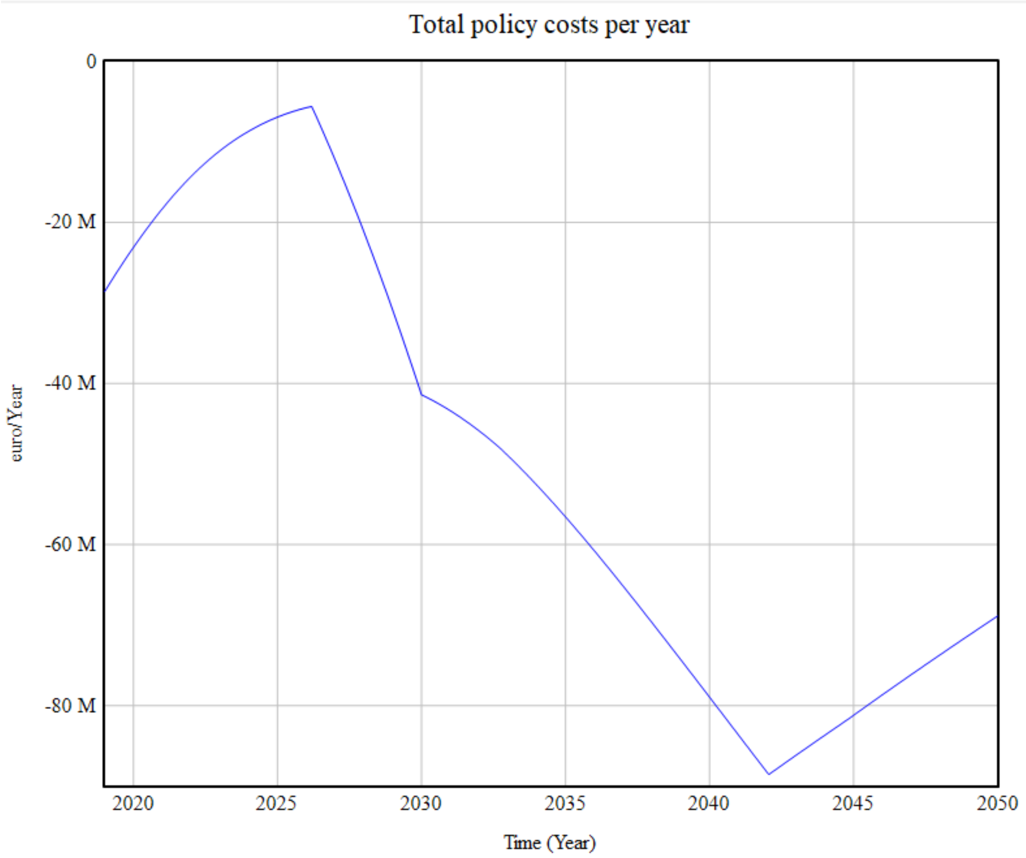

Figure 42: Base case: simulation of the annual policy costs.

5.4.2 Dimensional consistency

By means of a dimensional consistency test the modeller examines whether the units match on both sides of each model equation. By performing this test the internal validity of the model can be ensured (Schwaninger & Groesser, 2011). The units of the model's input parameters can be found in Table 3.
Vensim contains a functionality for performing a dimensional consistency test automatically for all equations. It then reports possible issues.
Using this functionality it was checked whether any dimensional inconsistencies were found. None were reported and hence the model is established to be dimensionally consistent.

5.4.3 Integration error and time step

System dynamics models are continuous-time models and use numerical integration. Hence, the selected integration method and time step should be such that the continuous dynamics are approximated with sufficient accuracy. The selected time step is 0.125 years as this is deemed a sufficiently small time step. The selected integration method is Runge-Kutta 4 Auto; this is a highly accurate integration method which also detects possible inaccuracies (Vensim Documentation, n.d.-a).
Simulation results should be insensitive to the choice of time step or integration method. Halving the time step is therefore a way to check for integration errors in the model (Sterman, 2000).
When halving the time step of the integration (to 0.0625 years), no changes in the output variables of the model are observed. Hence, it is concluded that no integration errors occur in the model.

5.4.4 Extreme condition tests

According to Sterman (2000) "extreme condition tests ask whether models behave appropriately when the inputs take on extreme values such as zero or infinity."
For the electrification model the following extreme conditions tests have been executed:

1. Electricity price set to 0

2. Electricity price set to an extremely high value (10^{10} euro/MWh)

3. Gas price set to 0

4. Gas price set to an extremely high value (10^{10} euro/m^3)

5. ETS price set to an extremely high value (10^{10} euro/tonne CO_2)

6. Investment costs conventional retrofit set to an extremely high value (10^{10} euro/MW)

7. Investment costs electric retrofit set to an extremely high value (10^{10} euro/MW)

The full analysis of the extreme conditions tests can be found in Appendix F.1. Only the main conclusions are listed below.

As expected, electrification is faster in extreme conditions 1, 4, 5 and 6 compared to the base case. In fact, the results for tests 1, 4, 5 and 6 are equal: from the start of the simulation all investments are channelled towards electrification, resulting in a high electrification rate for the three installations considered.
In all four cases, the short-term increase in emissions show a higher peak than in the base case. This is explainable, since due to its attractive business case in all four extreme conditions, electrification occurs even though electricity is not 100% renewable yet, temporarily resulting in higher emissions.

By contrast, no electrification occurs in extreme conditions 2 and 7, as could be expected. As a consequence, the only emission reduction originates from the decreasing boiler capacity, which is reduced due to efficiency improvements. Contrary to the expectations, some electrification does occur in boilers in extreme condition 3. This indicates that the rising carbon costs would still provide a good business case for electrification, even if the gas price were 0. However, in 2033 electrification comes to a halt and investments start to be channeled toward gas-fired boilers again due to the rising electricity price.
Remarkably, in extreme condition 3 the rate of boiler hybridization is similar to the base case. This can be attributed to the costs ratio $P_{hybrid}/P_{gas\ boiler}$ (see section 5.3.2) which decreases in this extreme condition, resulting in a higher investment share for hybridization. Second, due to the low electrification speed resulting from the low gas price there remains a higher steam demand as the compressor turbines remain largely steam-driven. Hence, there remains a larger hybridization potential.

In summary, the extreme condition tests generally lead to outcomes that could reasonably be expected. Only the higher rate of boiler hybridization in extreme conditions test 3 proved unexpected. However, upon inspection, this behavior could also be explained.

5.4.5 Sensitivity analysis

Through sensitivity analysis it is examined to what extent the simulation results change when parametric assumptions are varied over plausible ranges of uncertainty (Sterman, 2000). Because in this study the system dynamics model is used for vulnerability analysis in the context of Robust Decision-Making, the model's input parameters subjected to the sensitivity analysis are not varied over their full uncertainty ranges. Instead, they are varied over a bandwidth of -10% to +10% with respect to their base case values (see Appendix E Table 3). The full results of the sensitivity analysis can be found in Appendix F.2.

The input parameters subjected to the sensitivity analysis are chosen such that a range of subcomponents is represented in the analysis. Both certain (fixed) and uncertain input parameters are chosen. See Appendix E Table 3 for the full list of input parameters. CO_2 emissions are selected as the performance indicator in the sensitivity analysis as it provides a good indication of the overall degree of electrification. In this manner, we avoid looking at the capacities of the individual installations.
The following input parameters are varied in the analysis:

1. Electricity market price projection 2030

2. Gas market price projection 2030

3. Exogenous learning rate

4. Initial investment costs per MW: electric furnace, electric compressor turbine & electric boiler

5. Retrofit investment costs per MW: furnace, compressor turbine and boiler

6. Net calorific value gas
7. Response speed of investment share to costs ratio
8. Renewables share projection in 2030
9. Cracker production output (ethylene and propylene)
10. Base fee SDE++

The simulation results in the sensitivity analysis generally behave as expected. In Section 5.4.1 CO_2 emissions were identified to behave according to a increasing-decreasing pattern: electrification initially leads to an increase in emissions due to the emission intensity of electricity being initially higher than the emission intensity of gas, while it leads to a decrease of emissions in the long term. Therefore, input variations that benefit electrification were expected to amplify this pattern while input variations that counteract electrification were expected to have a dampening effect. These expectations are reflected by the simulation results.

It should be noted that the input variations of -10% and +10% do not induce changes in the capacities of furnaces and compressor turbines. Hence, only the boiler capacities are impacted. The electrification of furnaces remains 0 in all cases while the compressor turbines feature fast and complete electrification in all cases. This suggests that electrification of compressor turbines already provide a good business cases, while the electrification of furnaces requires more radical changes in the input parameters to yield a good business case.

In terms of sensitivity, the electricity price projection for 2030 has the largest impact on the CO_2 emissions of the input parameters included, followed by the SDE++ base fee and the projected renewables share in 2030.

5.4.6 Face validity test

In a face validity test, experts assess how closely the model resembles the real-world system (Qudrat-Ullah, 2005). In this research, the model has been assessed by Klara Schure, senior consultant at Berenschot, in an interview with the author. This interview has been cited as: Schure (2021b). The full results of the face validity test can be found in Appendix F.3, a summary is provided here.
The face validity test concentrates on three aspects (Shreckengost, 1985; Sterman, 2000): (1) model structure, (2) model boundary and (3) model behavior.

In all three aspects the model is generally concluded to be valid. However, the model could be improved in some aspects. Regarding the model structure, the SDE++ subsidy subcomponent could be strengthened by adhering more closely to PBL's calculation methods. This includes linking the subsidy to the avoided emissions of electric technologies in the model.
Concerning the model boundary, one important concept that is absent from the model is the role of the product side of the industry, i.e. the developments in the ethylene and propylene market and the effect of electrification on the production output. These aspects also emerged from the interviews held among the industry (Interviews, 2021). Moreover, including the lead times for grid capacity upgrades would have made the model outcomes more realistic. Finally, it would have been relevant to include national costs as an output parameter. National costs, a common concepts in policy studies done by PBL, represent the balance of costs and benefits of certain policy for society as a whole (Koelemeijer & Strengers, 2020).
Finally, there are limits to what purposes the model can be used for. The model should be used at a macro-level and not at a micro-level, e.g. as a choice model for electrification.

5.4.7 Boundary adequacy assessment

Boundary adequacy test are used to evaluate whether the model's structure is suited to dealing with the formulated research objective. As such, these test assess whether the model features the suitable level of aggregation and includes all relevant structural element such as feedback loops. Boundary tests sometimes involve adding or removing certain components to/from the model to examine whether the model behavior changes (Sterman, 2000; Schwaninger & Groesser, 2011). In this part, only a qualitative boundary adequacy assessment is conducted.

Upon consideration of model's level of aggregation, it can be concluded that most concepts relevant to studying the studying electrification in the naphtha cracking industry are included in the model. Price forecasts, carbon costs and the emission intensity of electricity, factors that drive the business case for electrification, have all

been modelled endogenously (see also Figure 21). The system's key performance indicators, i.e. CO_2 emissions, production costs and policy costs are also endogenous to the model.
The effect of the costs ratios of electric retrofits with respect to conventional retrofits on investments have also been modelled endogenously, though superficially. In reality, industrial decision-makers dedicate a certain investment sum to a discrete amount of capacity acquisition. However, due to the continuous nature of SD models, in the model capacities rather accumulate MW by MW. Therefore, the height of investments in electrification is determined by an investment share rather than a discrete investment sum (see also Section 5.3.2). Hence, the effect of costs ratios on investments as included in the model represents a highly aggregated version of reality and a modelling choice motivated by the continuous nature of the model.

On the other hand, a potentially important aspect omitted from the model is the grid capacity. As explained in Section 5.1 this choice has been made for several reasons: (1) it does not influence the business case but rather acts as a prerequisite for electrification, (2) whether or not the grid connection has to be upgraded is highly site-specific and (3) a grid connection may be shared between various industrial plants in a cluster. However, far-reaching electrification may be hampered by an insufficient grid capacity, the upgrading of which features long lead times (Scholten et al., 2021).
Moreover, the geographic boundary being set at a reference plant modelled after Shell MLO (see Section 5.2.1) may be at odds with drawing policy conclusions at a national level. However, as few data exists about plants other than Shell MLO (which features a large availability of data through the MIDDEN projec, (Wong & van Dril, 2020)) the geographic model boundary could not be easily extended to include other cracker sites. Therefore, one could question the generalizability of the model.
Finally, as was mentioned in the face validity test (Section 5.4.6) including the product side of the industry would have benefited the model.

5.4.8 Conclusions regarding the model's verification & validation

The model behavior can be generally considered valid, though some behavioral elements may be unrealistic. In the reference mode (Section 5.4.1) rapid electrification of compressor turbines is observed. This is in line with the views of industry representatives who expressed expectations that compressor turbines will probably be electrified first due to the large efficiency gain to be achieved with respect to conventional steam-driven turbines (Interviews, 2021).
However, the capacity of the electricity grid is not included in the model so the electricity grid may actually not be able to accommodate such a fast pace of electrification. This limitation of the model was addressed in the face validity test (Section 5.4.6) and the boundary adequacy assessment (Section 5.4.7). This discrepancy reflects the concern of the industry that the profitability of electrification may outpace the grid capacity (see Section 4.2.1).
The reference mode also indicates that electrification may lead to an emission increase in the short term, which is in line with (Koelemeijer et al., 2018). Moreover, the rising production costs per tonne ethylene reflect the concerns of the industry about the future profitability of ethylene production (Interviews, 2021).

The extreme conditions tests (Section 5.4.4) generally produce the expected behavior. With an electricity price of 0, an extremely high gas price, an extremely high ETS price or extremely high investment costs for conventional retrofits, all investments are channeled to electrification, resulting in high electrification rates. In these extreme conditions, electrification occurs even though electricity is not 100% renewable yet, resulting in a sharp increase in emissions in the short term. In case of an extremely high electricity price or extremely high investment costs for electrification, no electrification occurs, as expected. Some emission reduction occurs, though, but this can be attributed to efficiency improvements. Contrary to what was expected, some electrification of boilers occurs when the gas price is set to 0. However, this electrification soon comes to a halt with a rising electricity price.

In the sensitivity analysis (Section 5.4.5), varying specific input parameters from -10% to +10% with respect to their base case also produced the expected results. It turned out that the electricity price projection for 2030 has the largest impact on the CO_2 emissions of the input parameters included, followed by the SDE++ base fee and the projected renewables share in 2030.

The model boundary is generally adequate, though two important concepts are not included: the grid capacity and the product side of the industry. However, it is also concluded that omitting the grid capacity from the model does not impact the conclusions about policy options as including the grid capacity would not alter the ranking of the simulation results; it would temper the electrification rates in all simulation outcomes.

The model structure is also considered valid, though the quality of the model could be strengthened by improving the SDE++ subsidy subcomponent, modelling it more closely after the SDE++ calculations made by PBL (Netherlands Environmental Assessment Agency). Furthermore, it should be mentioned that the effect of costs ratios on investments as included in the model represents a highly aggregated version of reality and a modelling choice motivated by the continuous nature of the model.

6 Exploratory Modelling & Analysis

As introduced in Section 3.2.4 Exploratory Modelling & Analysis (EMA) will be used to perform experiments on the electrification model.
The outcomes of these experiments are then used to analyze how the model's input parameters influence the output variables (Kwakkel, 2018). To answer this question the simulation results are first plotted in order to perform visual analysis. Subsequently, a more advanced vulnerability analysis is conducted in order to determine which parameters are most influential on the simulation results. Two different techniques will be used in this regard: scenario discovery and Extra-Trees feature scoring.
Moreover, a robust policy search is performed. In this step the system dynamics model is subjected to an optimization algorithm which will yield a list of robust policies: policies that maximize system performance across a range of plausible futures.

The EMA workbench, developed by Kwakkel (2017a), is a Python toolkit for performing Exploratory Modelling & Analysis. In this research several EMA workbench modules have been used and adapted for application on the electrification model. The resulting Python scripts can be found in Appendix G.

In Section 6.1 the experiments performed on the electrification model will be described. Then follows Section 6.2 with a visual analysis of the simulation results. In Section 6.3 the vulnerability analysis is conducted, including a characterization of outcomes of interest through scenario discovery (Section 6.3.1) followed by a global sensitivity analysis through Extra-Trees feature scoring (Section 6.3.2). Finally, in Section 6.4 conclusions will be drawn with regard to the analyses performed in this chapter.

6.1 Performing experiments on the electrification model

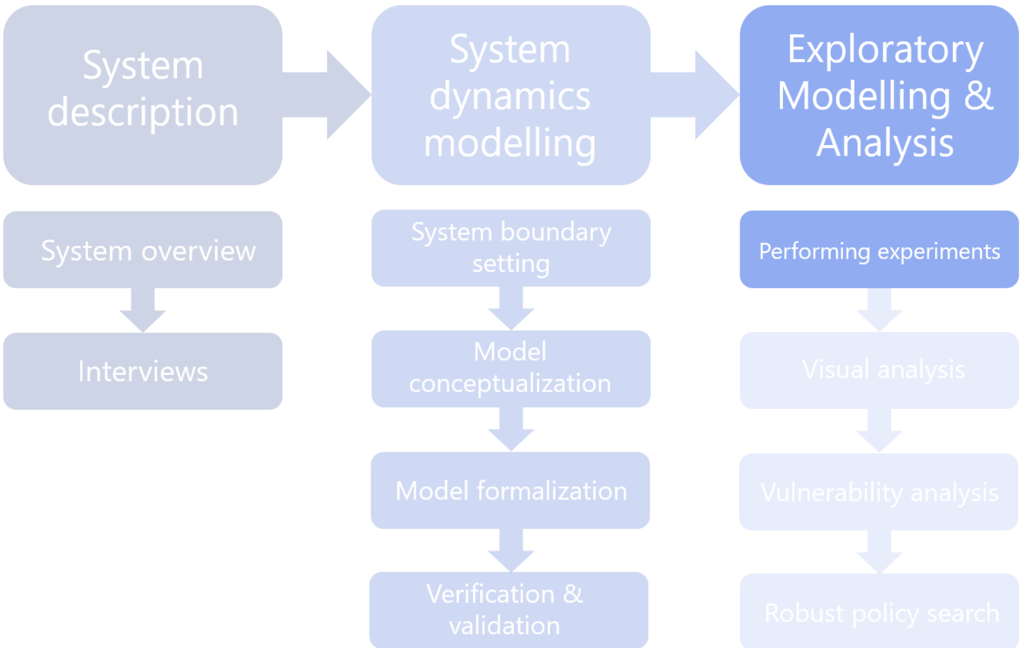

Figure 43: Position of the performing experiments step in the research roadmap.

In this section the system dynamics model developed in Chapter 5 is used for simulation. This is done by performing experiments on the model, illustrated by Figure 44. Each experiment represents a combination between a *scenario* and a *policy*. According to Kwakkel (2018): "a scenario is understood as a point in the uncertainty space, while a policy is a point in the decision space."
The uncertainty space is a multi-dimensional space bounded by the value ranges of the uncertain factors included in the simulation. Imagine there are three uncertain factors k, l and m in an experiment with uncertainty ranges as follows: $1 \leq k \leq 1.5$, $0.01 \leq l \leq 0.03$ and $100 \leq m \leq 200$. Then a *scenario* is any point contained within this three-dimensional space, e.g. (1.2, 0.02, 150) or (1.3, 0.012, 122). With more uncertain factors included in the experiment, the more dimensions the uncertainty space will have.

Similarly, the decision space is a multi-dimensional space bounded by the value ranges of the policy options. As each experiment represents a different combination of two points, one in the uncertainty space and one in the decision space, each experiment will yield a different simulation result.
Together the outcomes of the experiments form a database of simulation results. This database comprises time plots of the key performance indicators of the model: CO_2 emissions, production costs and policy costs.

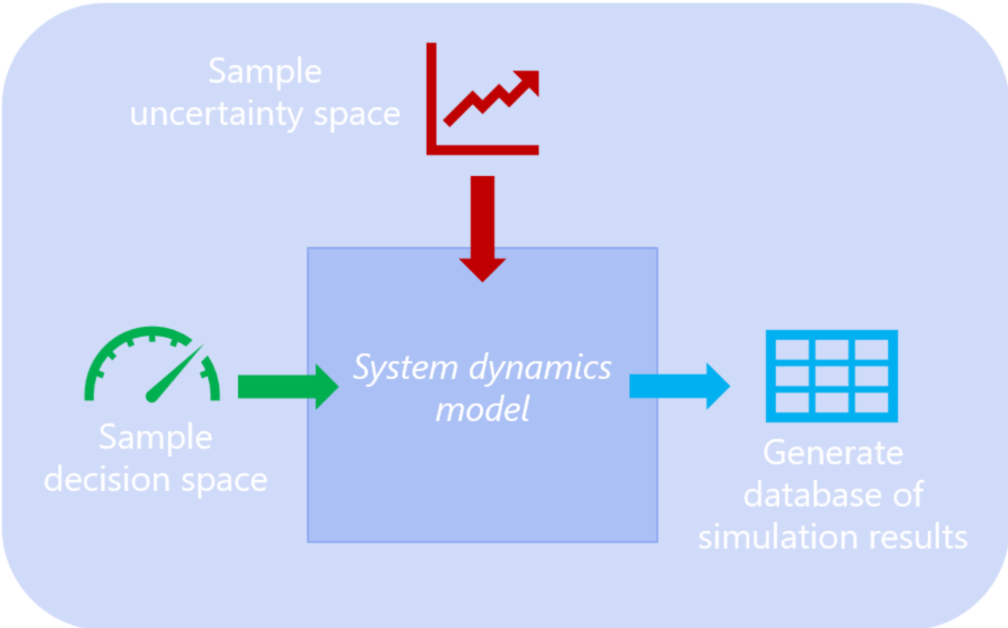

Figure 44: Illustration of the performing of experiments. By sampling the decision space different *policies* are generated. By sampling the uncertainty space *scenarios* are generated. Every combination of a *policy* and a *scenario* is called an *experiment*. In this way the input parameters are varied across the experiments. Each experiment produces an time plot of the model's key performance indicators; this is the simulation result. Multiple experiments are performed which together form a database of simulation results.

In Section 6.1.1 the design of these experiments in outlined. Section 6.1.2 gives an overview of the output variables studied in the visual analysis that follows in Section 6.2.

6.1.1 Experiment design

Each experiment to which the electrification model is subjected is composed of two elements: a *scenario* - or point in the uncertainty space - and a *policy* - or point in the decision space. The uncertainty space is determined by the bandwidths of the uncertain factors included in the simulation. A list of the 24 uncertain factors and their respective bandwidths can be found in Appendix H, Table 5. Similarly, the decision space is determined by the bandwidths of the 11 policy options (see Appendix H, Table 6). The uncertainty bandwidths are based on various scenario studies, e.g. PBL (2020) and Aalbers et al. (2016). The policy bandwidths have been set such that the attainable value are not unrealistically large or small. For each policy option, the decision space has been explored in the “desirable” direction. That is, only increases in the gas tax are considered, while only reductions in the electricity tax have been considered.
It should be noted that in the context of this study the decision space not only includes policy options but also grid tariffs. As grid tariffs are determined by the grid operators they are considered part of the decision space and therefore they are included as policy options in the EMA framework.

To construct the experiment design the algorithm used for performing the experiments (see Appendix G) samples across the uncertainty space and decision space using Latin Hypercube sampling (Kwakkel, 2017a). As such, each experiment combines a point sampled from the uncertainty space and a point sampled from the decision space.
The simulation performed in this study features 300 scenarios and 100 policies, yielding 30,000 experiments and hence, 30,000 simulation results.

6.1.2 Output variables studied

Ideally CO_2 emissions are minimized, while production costs and policy costs are minimized as well. Therefore, we are interested in the simulation results that feature those characteristics and the experiments (i.e. combinations of scenarios and policies) that generate them.
As we are concerned with minimizing the CO_2 concentration in the atmosphere we are interested in *cumulative* emissions. We also look at cumulative production costs and cumulative policy costs because these reflect the total costs of electrification between 2019 and 2050 for the industry and the government, respectively. However, we are also interested in the dynamics behavior of the emissions, the production costs and the policy costs as these may explain the resulting cumulative output variables. Hence, these are also considered in the analyses.
Hence, in the following analyses a total of six out variables are studied that are reflective of the three performance indicators:

1. Cumulative CO_2 emissions in 2050 [megatonne CO_2]
2. Cumulative production costs in 2050 [billion euro]
3. Cumulative policy costs in 2050 [billion euro]
4. Annual CO_2 emissions [kilotonne CO_2/year]
5. Production costs per tonne ethylene [euro/tonne]
6. Annual policy costs [million euro/year]

6.2 Visual analysis of the simulation results

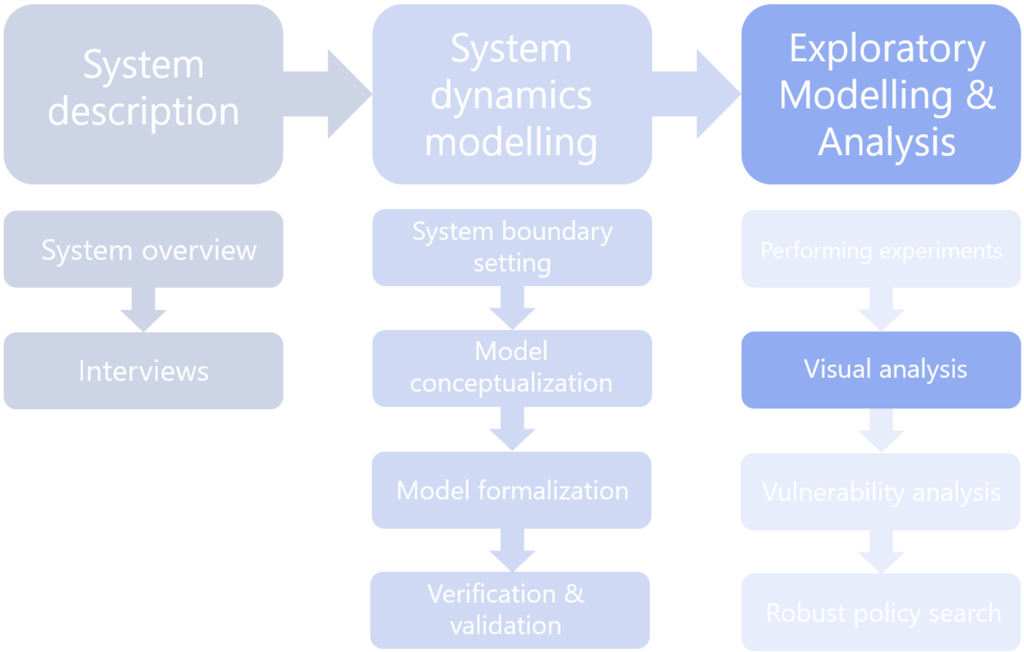

Figure 45: Position of the visual analysis step in the research roadmap.

As the simulation concerns a large number (30,000) of experiments, the simulation results are divided into clusters to aid the visual analysis of the results. Each cluster includes 10% of the simulation results, grouped by the results with the largest cumulative emissions in 2050. Hence, cluster 1 represents the simulation results with the 10% largest cumulative emissions in 2050 (or the results with emissions above the 90^{th} percentile), cluster 2 represents the simulation results with the next 10% largest cumulative emissions in 2050 (or the results with emissions between the the 80^{th} percentile and 90^{th} percentile), etc.

6.2.1 Cumulative CO_2 emissions

The clustering is visualized in Figure 46 which shows the development of the cumulative emissions resulting from naphtha cracking over time for the 30,000 different outcomes. Next to the plot two Kernel density estimation (KDE) plots are displayed, which show the distribution of the outcomes. The left KDE plot shows the distribution for each of the clusters C1-C10, the right KDE plot shows the distribution for the entire outcome space.

The simulation outcomes show a large variety when it comes to the cumulative emissions, ranging from 28.5 megatonne CO_2 to 47.6 megatonne CO_2 in 2050. This difference amounts to the annual emissions of 12.8 million cars, almost 1.5 times the total number of cars in the Netherlands (CLO, 2017; CBS, 2020). Moreover, the maximum of 47.6 megatonne is just 1 megatonne lower than the resulting cumulative emissions were the naphtha cracking industry to continue its emissions at the current pace (1569 kilotonne/year for the reference plant). Hence, in this worst-case scenario very little emission reduction occurs.

Furthermore, it appears that until 2028 the simulation outcomes keep pace with each other as far as the cumulative emissions are concerned. Only from 2028 onwards the outcomes start to diverge and emissions are being curbed due to increasing electrification, at least for the higher clusters.
What is remarkable, is that the KDE plot features a peak at the top of the spectrum and a peak at the bottom of the spectrum. This effect can be attributed to two reasons. First, in a significant number of plausible futures, electrification does not cross the threshold because the expected costs of electric retrofits remain too high. Second, in a considerable number of plausible futures, electrification is implemented on the medium term, but is reversed on the long term due to fast rising electricity prices. This last phenomenon will be further discussed in Section 6.2.5.

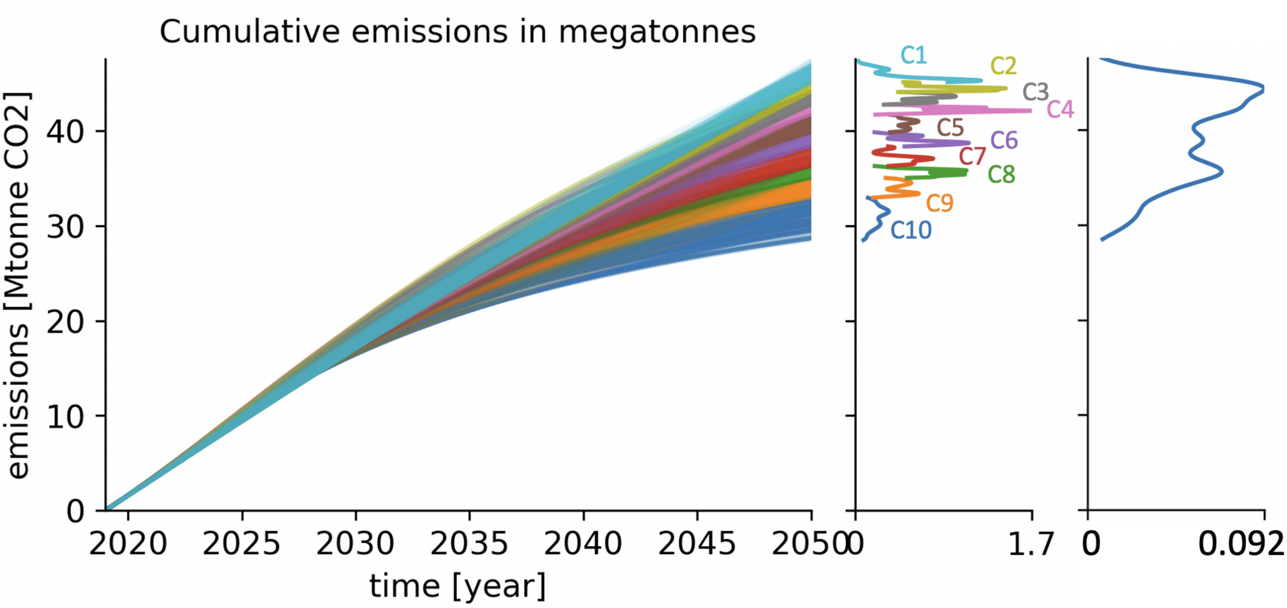

Figure 46: Simulation results for the cumulative CO_2 emissions associated to naphtha cracking for the reference plant, clustered by cumulative emissions in 2050. C1 represents the outcomes with cumulative emissions in 2050 above the 90^{th} percentile, C2 represents the outcomes with cumulative emissions between the 80^{th} percentile and the 90^{th} percentile, etc. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, both for the individual clusters as well as for the entire outcome space.

6.2.2 Cumulative production costs

In Figure 47 the simulation results for the cumulative production costs associated to naphtha cracking for the reference plant are shown, again clustered by the height of the cumulative emissions corresponding to each result. The cumulative production costs in 2050 range from 18.7 to 44.4 billion euros. From the results clusters indicated on the left KDE plot it appears that no strong relation exists between the cumulative production costs and the cumulative emissions. Cluster 1 (which features the highest cumulative emissions in 2050) is concentrated on the bottom of the production costs spectrum but the distributions of the other clusters largely overlap, with cluster 10 (lowest cumulative emissions) concentrated somewhere around the middle of the spectrum.
This indicates that large-scale electrification does not necessarily lead to higher production costs for the naphtha cracking industry. Rather, the impact of electrification on the production costs is highly scenario-dependent.

6.2.3 Cumulative policy costs

Figure 48 shows the simulation results for the cumulative costs of combined policy options associated to the reference plant. In contrast to the cumulative production costs, a correlation between the policy costs and emissions becomes apparent from the clusters indicated next to the left KDE plot. It can be seen that clusters with lower emissions (notably cluster 10) are associated with higher cumulative policy costs. However, clusters 3-9 do show a large overlap.
It can also be observed that the cumulative policy costs are negative in most scenarios, indicating that the electricity, gas and carbon taxes associated with the naphtha cracking industry are larger than the granted SDE++ subsidy in most outcomes.

6.2.4 Correlating cumulative emissions, production costs and policy costs

Figure 49 combines the data visualized in Figures 47 - 48 by means of a scatter plot. This plot allows us to see more clearly the correlations between the key performance indicators mentioned before. In the bottom left window it can clearly be seen that cumulative policy costs are strongly correlated with cumulative emissions: cluster 10 (lowest cumulative emissions) features a spectrum of -500 million to 500 million euros in cumulative policy costs while this bandwidth is shifted to <-1000 million to 0 for cluster 1 (highest cumulative emissions).

Moreover, in the right-most middle window an interesting relationship between the cumulative policy costs and cumulative production costs can be observed: simulation results on the higher end of the cumulative policy

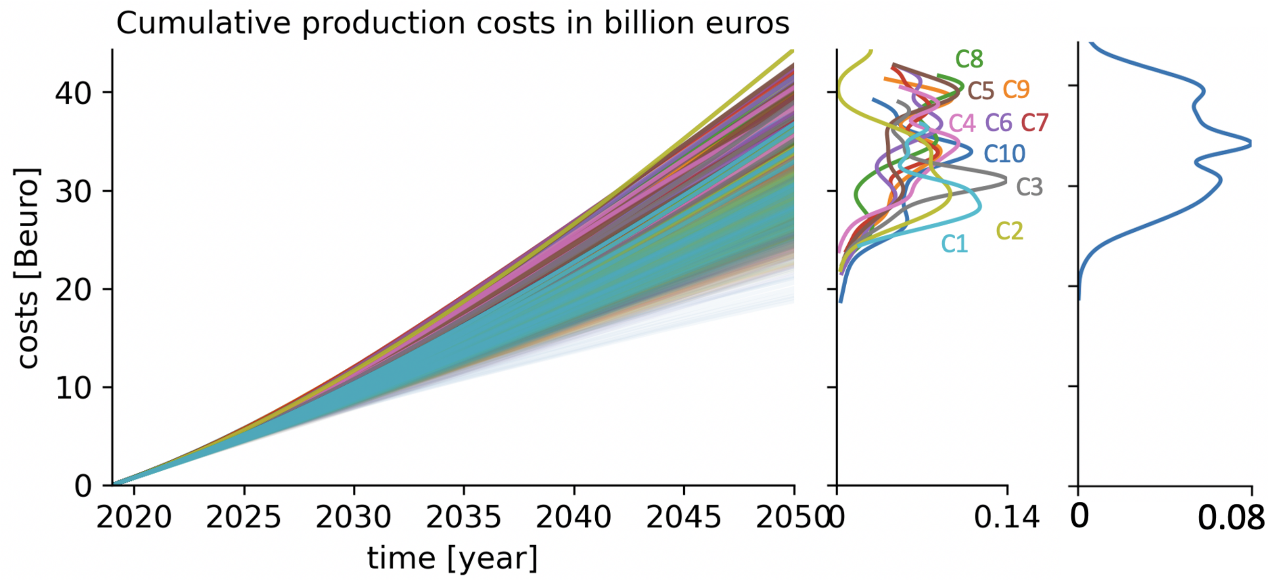

Figure 47: Simulation results for the cumulative production costs associated to naphtha cracking for the reference plant, clustered by cumulative emissions in 2050. C1 represents the outcomes with cumulative emissions in 2050 above the 90^{th} percentile, C2 represents the outcomes with cumulative emissions between the 80^{th} percentile and the 90^{th} percentile, etc. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, both for the individual clusters as well as for the entire outcome space.

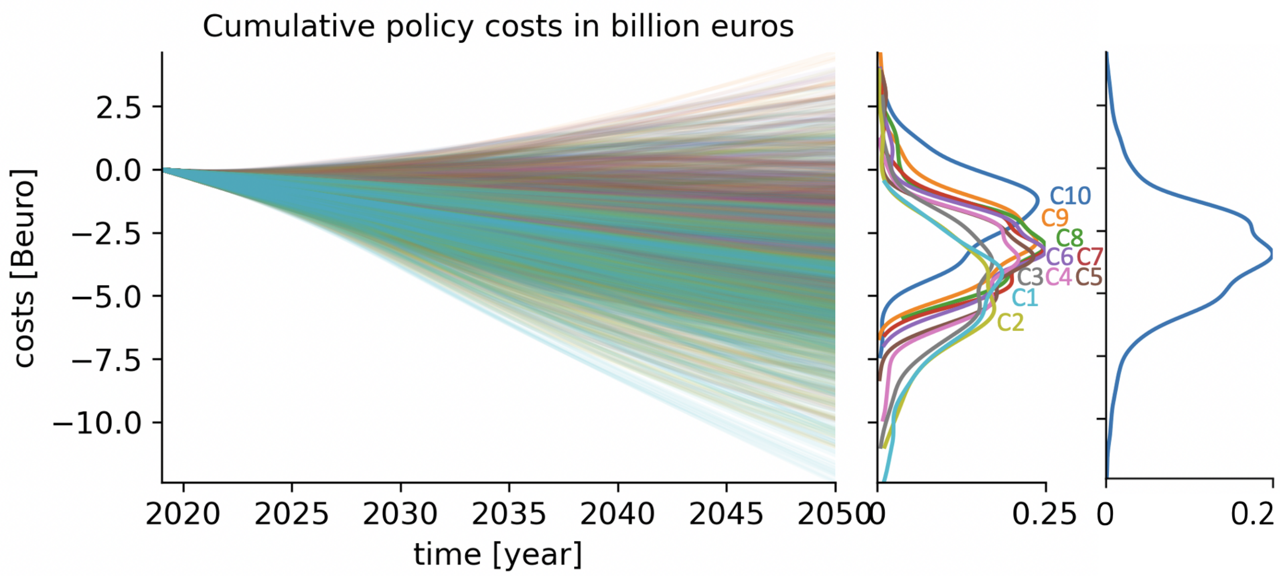

Figure 48: Simulation results for the cumulative costs of combined policy options associated to the reference plant, clustered by cumulative emissions in 2050. C1 represents the outcomes with cumulative emissions in 2050 above the 90^{th} percentile, C2 represents the outcomes with cumulative emissions between the 80^{th} percentile and the 90^{th} percentile, etc. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, both for the individual clusters as well as for the entire outcome space.

costs spectrum tend to feature lower cumulative production costs. These results also feature lower cumulative emissions. However, in the middle of the cumulative policy costs spectrum a large spread of cumulative production costs can be observed, indicating that the impact of the policy costs on the production costs is scenario-dependent. This is also where the majority of the simulation outcomes is concentrated as can be seen in the bottom right window. On the other hand, for cumulative policy costs on the lower end of the spectrum we again see more consistent relationship with the cumulative production costs can be observed.

The scatter plot also confirms the observation that was made based on Figure 47: clusters 1-4 are concentrated on the bottom of the production costs spectrum but the distributions of the other clusters largely overlap. This indicates that the simulation results with the 40% largest cumulative emissions are associated with generally lower cumulative production costs.

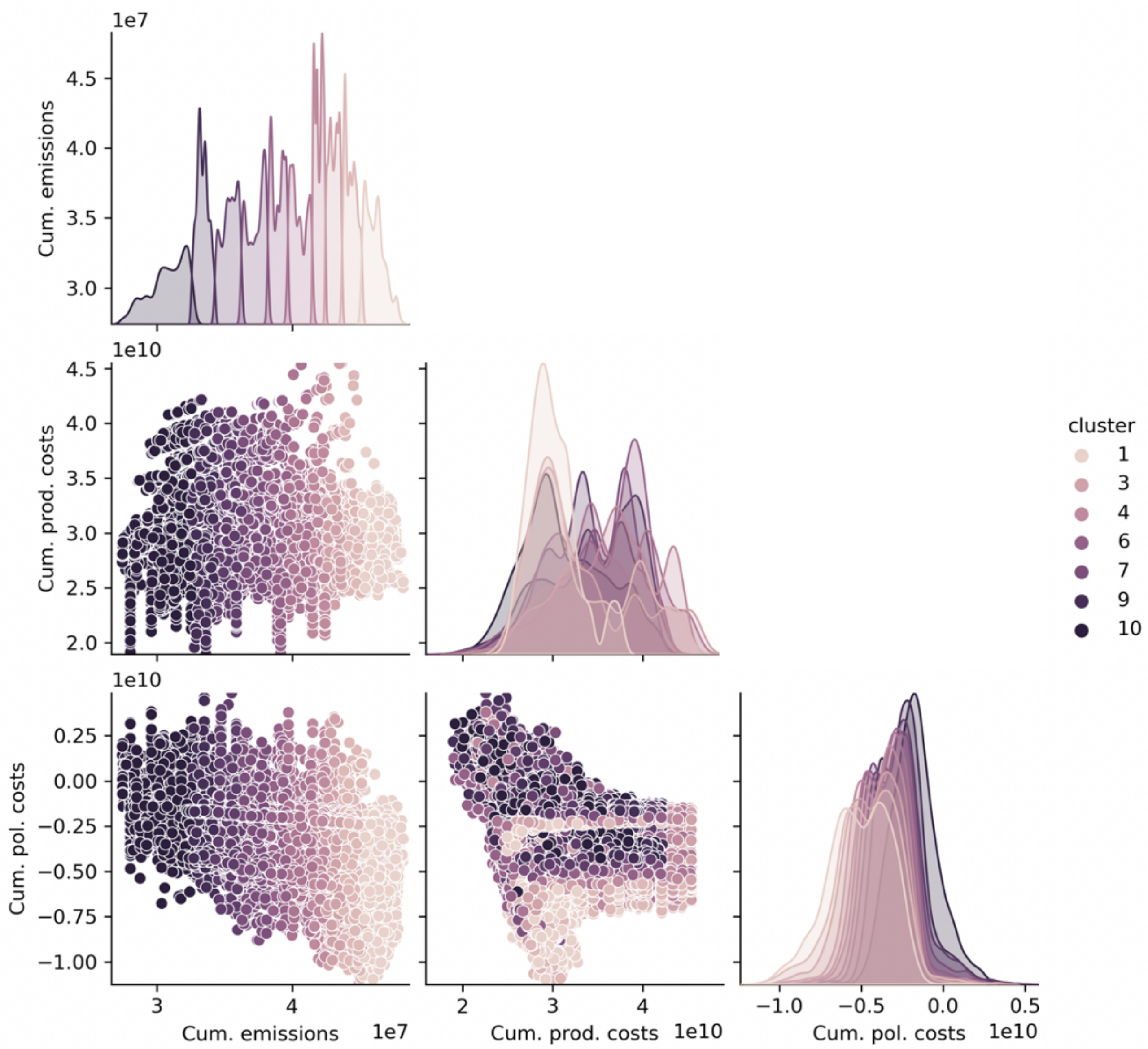

Figure 49: Scatter plot of the simulation results showing cumulative CO_2 emissions, cumulative production costs and cumulative policy costs associated to naphtha cracking for the reference plant in 2050, clustered by cumulative emissions in 2050. C1 represents the outcomes with cumulative emissions in 2050 above the 90^{th} percentile, C2 represents the outcomes with cumulative emissions between the 80^{th} percentile and the 90^{th} percentile, etc. Note: 1e7 denotes 10^7 and 1e10 denotes 10^{10}.

6.2.5 Annual CO_2 emissions

For studying the time-dependent output variables associated to the key performance indicators the outcomes are clustered based on the annual CO_2 emissions. With regard to CO_2 emissions (Figure 50) the simulation results feature emission reductions ranging from 5.21% the worst case (from 1569 to 1488 ktonne CO_2 anually) to 80.9% in the best case (300 ktonne CO_2 in 2050). In line with what was noted in Section 5.4.1 it can be observed that outcomes with lower emissions in the long-term feature an emission increase in the short term. This is in line with e.g. Koelemeijer et al. (2018) who state that ”electrification can lead to extra emissions in the short term”.

For clusters 1 and 2 little, though some, emission reduction occurs. Upon inspection of the behavior of underlying model output variables (Appendix I) it can be seen that this emission reduction occurs not due to electrification but due to efficiency improvements in conventional technologies. Therefore, emissions in these clusters stabilize over time as efficiency limits are reached. In these clusters electrification does not provide a profitable business case for the industry.
In clusters 3-10 electrification does occur in varying degrees. Looking at the development of the costs of electric versus conventional technologies (Appendix I) it can be seen that in most outcomes electric technologies become relatively cheaper in time due to decreasing investment costs and rising carbon and gas prices. Hence, in most outcomes investments in electrification increase over time, causing emissions to decrease. However, it can also be observed that the cost reductions for electric technologies stabilize over time. In some outcomes they even increase again due to a fast-rising electricity market price or a relatively slowly increasing ETS carbon price, that causes the business case for conventional technologies to become attractive again. Hence, in Figure 50 some outcomes feature emissions that "bounce back" after an initial decrease. In Figure 50 this development is reflected by the curves crossing the spectrum between 2035 and 2050.

Like in Figure 46, two peaks can be observed in the KDE plot. As was mentioned before, the top peak represents scenarios where electrification does not cross the threshold as the expected costs for electrification remain too high. Moreover, plausible futures in which electrification "bounce back" contribute to this peak.

Furthermore, in Appendix I it can be observed that strong electrification occurs in compressor turbines, while the electrification of furnaces and boilers show a much larger variation. In almost all experiments the electrification rate is above 80%. Upon inspection, this is due to the favourable costs development of electric compressors. Hence, electrification of compressors seem a no-regret electrification option. For boilers and especially for furnaces, the business cases are not as favourable. This confirms the analyses of the interviews held among industry representatives, who mentioned that electric compressor turbines will likely be the first step in electrification due to the low efficiencies of conventional steam-driven turbines (Interviews, 2021).

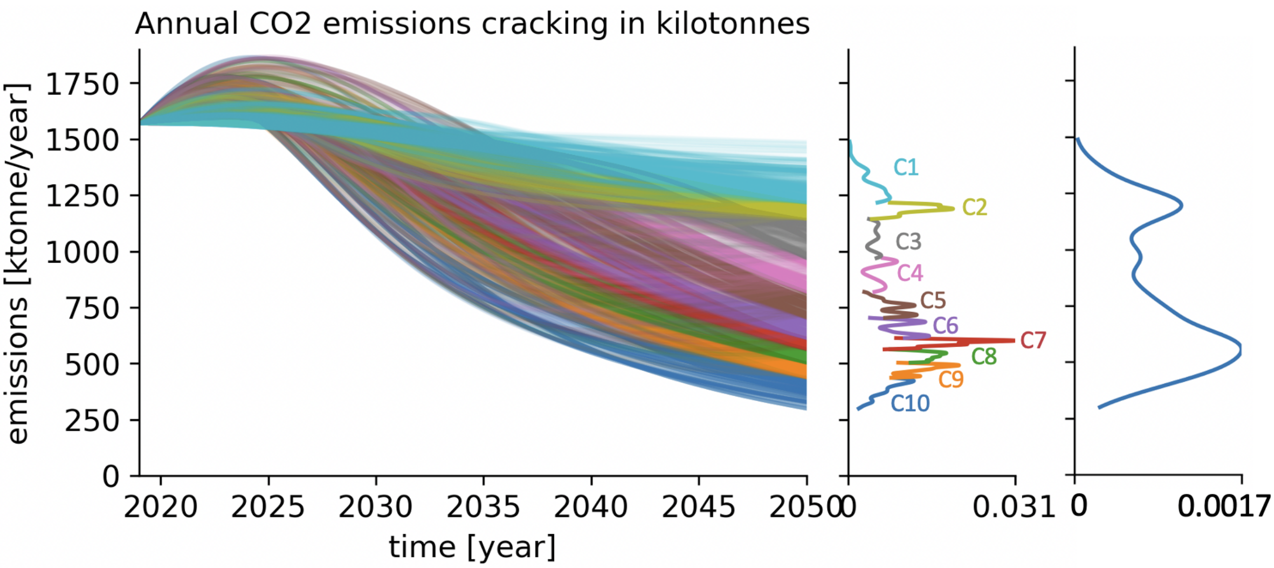

Figure 50: Simulation results for the annual emissions associated to naphtha cracking for the reference plant, clustered by emissions in 2050. C1 represents the outcomes with emissions in 2050 above the 90^{th} percentile, C2 represents the outcomes with emissions between the 80^{th} percentile and the 90^{th} percentile, etc. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, both for the individual clusters as well as for the entire outcome space.

6.2.6 Production costs per tonne ethylene over time

The production costs per tonne ethylene in 2050 show a large spread: from 650 euro/tonne to 2103 euro/tonne, with most outcomes concentrated between 1000 and roughly 1900 euro/tonne. The current market price of ethylene is 1003 euro/tonne (PBL, 2021). Hence, the production costs per tonne ethylene may become too large for ethylene production to remain profitable in the future.

No clear relation between the production costs and the annual emissions in 2050 can be observed. The only exception is the outcomes in cluster 1 (10% highest emissions), which tend to be concentrated on the downside of the production costs spectrum. This is due to the fact that these outcomes feature a low ETS carbon price, which is the single most influential factor with regard to the production costs and also has a significant impact on the CO_2 emissions (see Section 6.3.2). The other clusters are quite spread over the production costs spectrum.

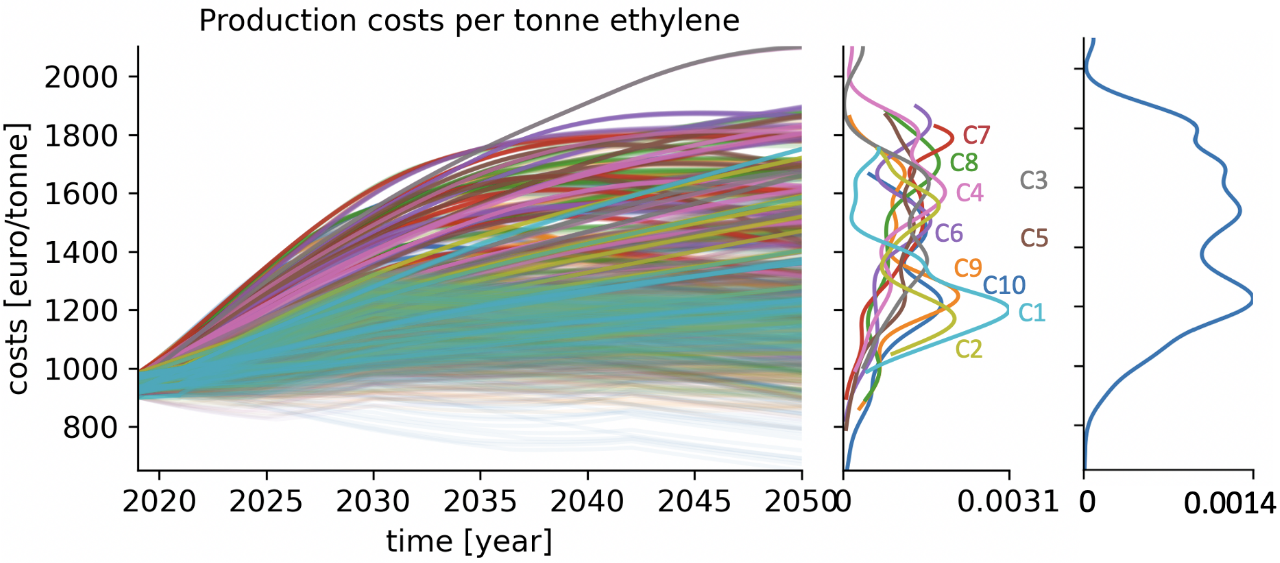

Figure 51: Simulation results for the production costs per tonne ethylene at the reference plant, clustered by emissions in 2050. C1 represents the outcomes with emissions in 2050 above the 90^{th} percentile, C2 represents the outcomes with emissions between the 80^{th} percentile and the 90^{th} percentile, etc. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, both for the individual clusters as well as for the entire outcome space.

6.2.7 Annual policy costs

When looking at the annual policy costs (Figure 52) it can be observed that for the year 2050, most outcomes are concentrated around roughly -50 million euro/year. These outcomes also appear to feature linear curves over time. Upon inspection this behavior can be attributed to the electrification of furnaces. Even in the best case the percentage of electric furnace capacity is 75%. Hence, in most simulation outcomes the gas consumption by furnaces remains significant. As the furnaces account for 76% of the gas consumption at the start of the simulation this generates a high amount of gas taxes paid, dominating the behavior of the policy costs.

The bends in the curve can be attributed to the development of the carbon levy over time. This was elaborated in Section 5.4.1.

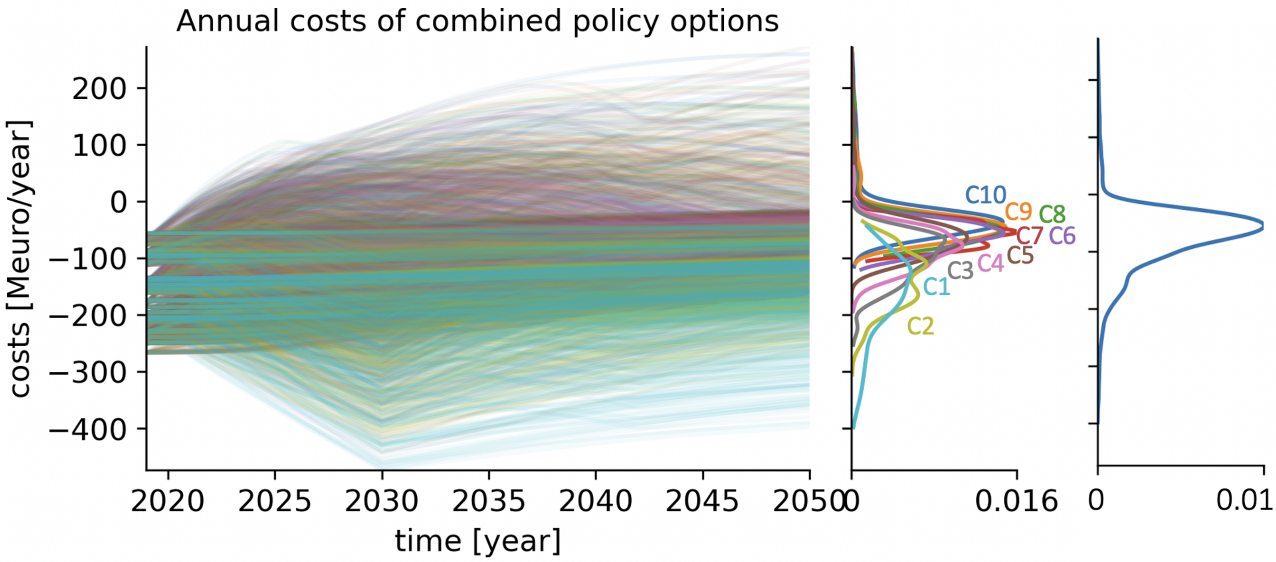

Figure 52: Simulation results for the annual policy costs associated to naphtha cracking for the reference plant, clustered by emissions in 2050. C1 represents the outcomes with emissions in 2050 above the 90^{th} percentile, C2 represents the outcomes with emissions between the 80^{th} percentile and the 90^{th} percentile, etc. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, both for the individual clusters as well as for the entire outcome space.

6.3 Vulnerability analysis

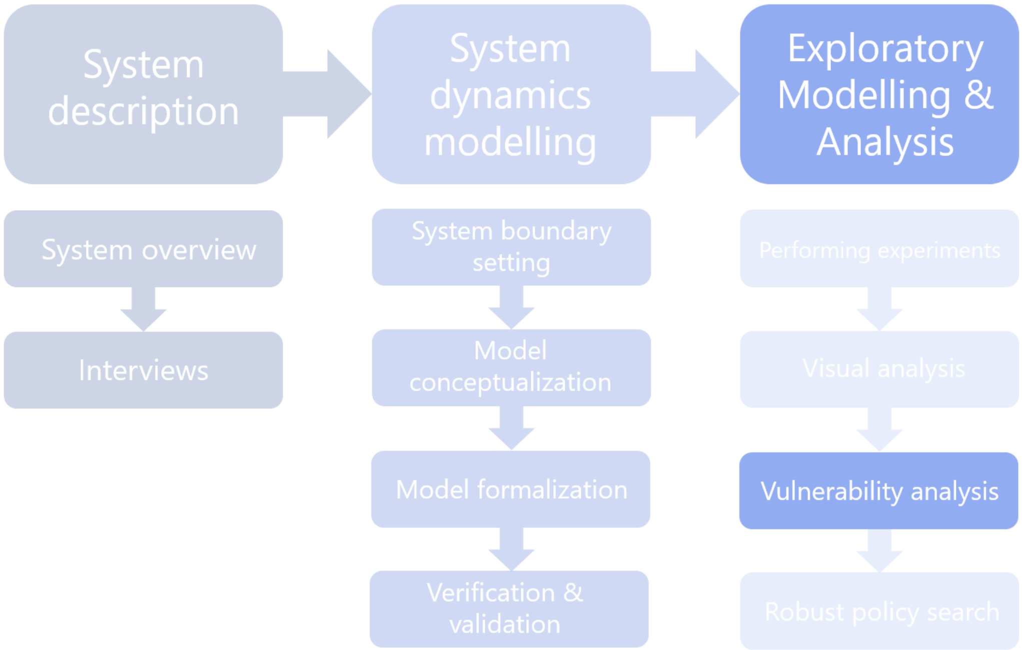

Figure 53: Position of the vulnerability step in the research roadmap.

The goal of vulnerability analysis is to determine how the model inputs (uncertainties and policy options) translate to the model outputs or key performance indicators. As such, vulnerability analysis allows us to determine which model parameters are most influential on the simulation outcomes presented in Section 6.2. Two different techniques will be used as part of the vulnerability analysis: scenario discovery (Section 6.3.1) and Extra-Trees feature scoring (Section 6.3.2).

6.3.1 Characterization of outcomes of interest through scenario discovery

Scenario discovery, which was originally introduced by Bryant & Lempert (2010), is a technique to characterize regions of interest within the outcome space. In the case of this research these are regions with low emissions while featuring low production costs and low policy costs. In terms of policy relevance, these are the most interesting regions.
Through statistical or data-mining algorithms scenario discovery identifies which combinations of input parameters (uncertain factors and policy options in our case) most strongly predict these regions in the output space. In this study, we describe these regions in the input parameters space by multi-dimensional “boxes”, also called hypercubes. A box is a set of constraints on the input parameters which, combined, are considered most predictive of a selected region of interest within the outcome space.

As such, scenario discovery not only identifies the input parameters most influential on the simulation outcomes - which is done through traditional sensitivity analysis - but also reveals which combinations of input parameters and which constraints most strongly predict specific regions of interest within the outcome space (Bryant & Lempert, 2010).

Key concepts in scenario discovery: density and coverage

Two key concepts in scenario discovery are *density* and *coverage*. *Density* is defined as the ratio of outcomes of interest contained in a box to the total number of simulation outcomes in that box. Hence, the higher the density value of a box, the higher its ”purity” in terms of policy-relevant simulation outcomes.
Coverage is defined as the ratio of outcomes of interest contained in a box to the total number of outcomes of interest identified. Hence, the higher the coverage value of a box, the better it captures the identified region of interest within the outcome space.
Ideally, a box features both high density *and* high coverage. However, in practice these are often conflicting objectives. Hence, when selecting a box a trade-off between density and coverage has to be made (Bryant &

Lempert, 2010).

Performing scenario discovery with the EMA workbench

The EMA workbench provides support for performing scenario discovery using the Patient Rule Induction Method (PRIM) algorithm, which was first introduced by Friedman & Fisher (1999). The module generates a set of boxes, each with a different number of restricted dimensions (i.e. constraints on the input parameters).
Imagine we perform experiments on a model that generate simulation results with emissions ranging from 10 to 20 megatonne CO_2. We are interested in exploring the outcome space of 10 to 12 megatonne as these emissions align with our emission reduction targets. The PRIM algorithm then generates a box with just one restricted dimension put on an input parameter k, which can attain a value ranging from $1 \leq k \leq 2$. The box specifies the restricted range of k as being $1.5 \leq k \leq 2$. This indicates that a value of k ranging from 1.5 to 2 is most predictive of a attaining emissions below 12 Mtonne. By contrast, value of k lower than 1.5 makes it very unlikely to attain emissions below 12 Mtonne.

Besides the restricted dimensions for each of the boxes, PRIM shows their respective coverage and density scores as a trade-off curve. Based on a trade-off between coverage and density a suitable box can be selected through trial and error.
Moreover, for every input parameter the qp-value is shown. The higher this value, the higher the likelihood that PRIM constrained this parameter purely by chance. Hence, the qp-value should be as close to zero as possible. (Bryant & Lempert, 2010; Kwakkel, 2018).

Scenario discovery has been performed for the cumulative emissions, the cumulative production costs and cumulative policy costs. For the first two output variables the regions with the 20% lowest values have been studied. For the cumulative emissions this region corresponds to clusters 9 and 10 combined (see Figure 46). For the cumulative policy costs the region with the 40% lowest values has been studied as in Section 6.2.3 it was observed that the cumulative policy costs show a rather peak-shaped distribution.

Results of the scenario discovery analysis for the cumulative emissions

In Figure 54 the selected box for the region in the outcome space with the 20% lowest cumulative emissions is shown. From the box it becomes clear that the share of renewable electricity in 2030 is most strongly constrained: it should be 69% at minimum in order for the emission intensity of electricity to decrease fast enough to let electrification lead to a significant reduction in emissions. The projected electricity market price in 2030 should also be constrained to 61 $euro/kWh$; this limits the growth rate of the electricity price to 1.82 $euro/(kWh \cdot year)$ at most (as the electricity price is linearly forecasted based on its projected value, see Section 5.3.1). Otherwise, the business case for electrification does not become attractive in due time, slowing the development of electrification and thus, the pace of emission reduction.

What is remarkable is that the investment costs associated to electrification are not constrained by the PRIM analysis. This would have logically been expected as the investment costs are indicated by the industry's representatives to form one of the main barriers of electrification. This can be explained by the fact that, with respect to the capital expensens, the size of operational expenses are rather large. Another explanation is the way energy prices are modelled. That is, energy prices are assumed to increase linearly based on their projected value in 2030, which is used as an input parameter for the model. Consequently, an increase in the electricity price or the gas price in this projection year implies that the energy prices increase faster, causing a prolonged effect on the operational expenses. By contrast, the initial investment costs of electric technologies are independent of time. Hence, the sensitivity of the simulation outcomes to changes in the investment costs turns out relatively lower.
Moreover, as a consequence of the present value calculation (see Section 5.3.2), the operational expenses are counted multiple times, while the investment costs are only counted once, making the simulation outcomes relatively more sensitive to an increase in energy prices.

Moreover, the box does not include policy options either, indicating that their impact on emission reduction is low if the conditions of a fast growth of renewable electricity and slow growth of the electricity market price are not fulfilled.
Therefore, it becomes apparent that the availability of renewable electricity is vital to let electrification have the desired effect on emission reduction.

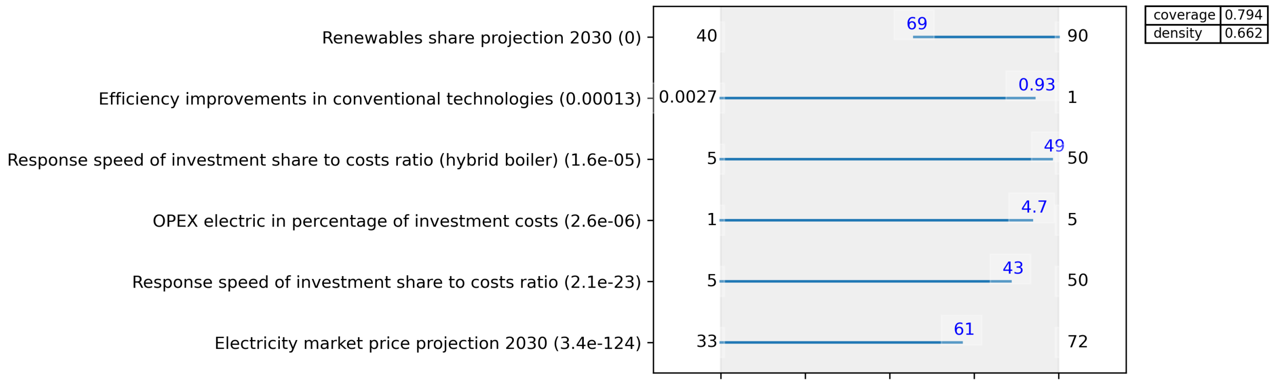

Figure 54: Selected box generated by the PRIM analysis for the cumulative emissions. The box shows the limits for the constrained input parameters that most strongly predict the subset of outcomes with the 20% lowest cumulative emissions. Next to the name of each input parameter the qp-value of the constraint is shown. To the right the coverage and density values for the selected box are displayed.

Results of the scenario discovery analysis for the cumulative production costs

Figure 55 shows the selected box for the region in the outcome space with the 20% lowest cumulative production costs. The only constraint that is significant is the ETS carbon price projection in 2050, which should be 310 $euro/tonne$ at most in order to keep the ETS carbon price increase limited to 9.19 $euro/(tonne \cdot year$. The high impact of the ETS price on the production costs is further discussed in Section 6.3.2.
As the investment costs associated did not appear decisive for the cumulative emissions, neither do they for the cumulative production costs.

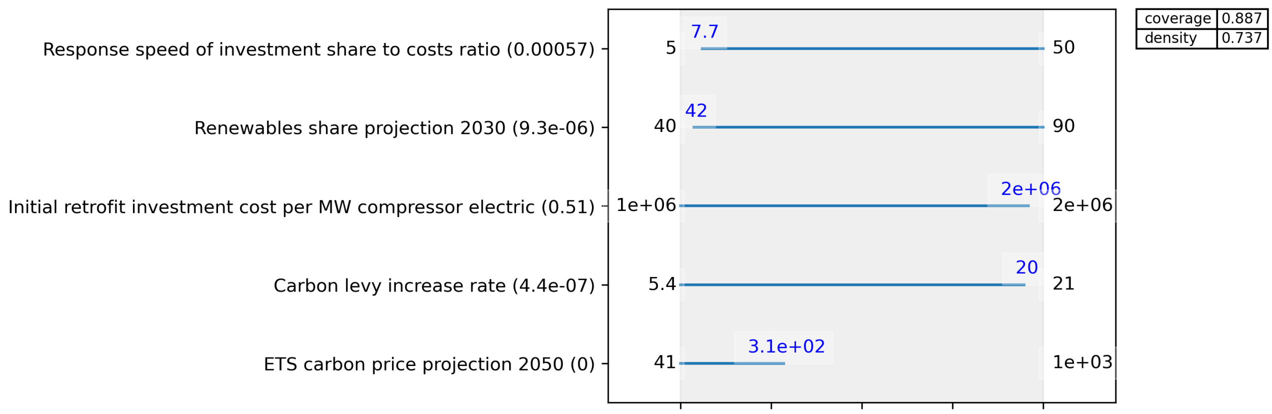

Figure 55: Selected box generated by the PRIM analysis for the cumulative production costs. The box shows the limits for the constrained input parameters that most strongly predict the subset of outcomes with the 20% lowest cumulative production costs. Next to the name of each input parameter the qp-value of the constraint is shown. To the right the coverage and density values for the selected box are displayed.

Results of the scenario discovery analysis for the cumulative policy costs

In Figure 56 the selected box for the subset of outcomes with the 40% lowest cumulative policy costs is displayed. One can observe that for minimizing the cumulative policy costs the ODE gas (*Opslag Duurzame Energie* or Sustainable Energy Premium for gas) should be high while the SDE++ (Stimulation Scheme for Sustainable Energy Production) subsidy base fee should remain limited. For the subset of outcomes with the 40% lowest cumulative policy costs the ODE gas should be at least 0.11 $euro/m^3$, an increase of 4.6 times the current value. The SDE++ base fee should be at most 0.11 $euro/kWh$.

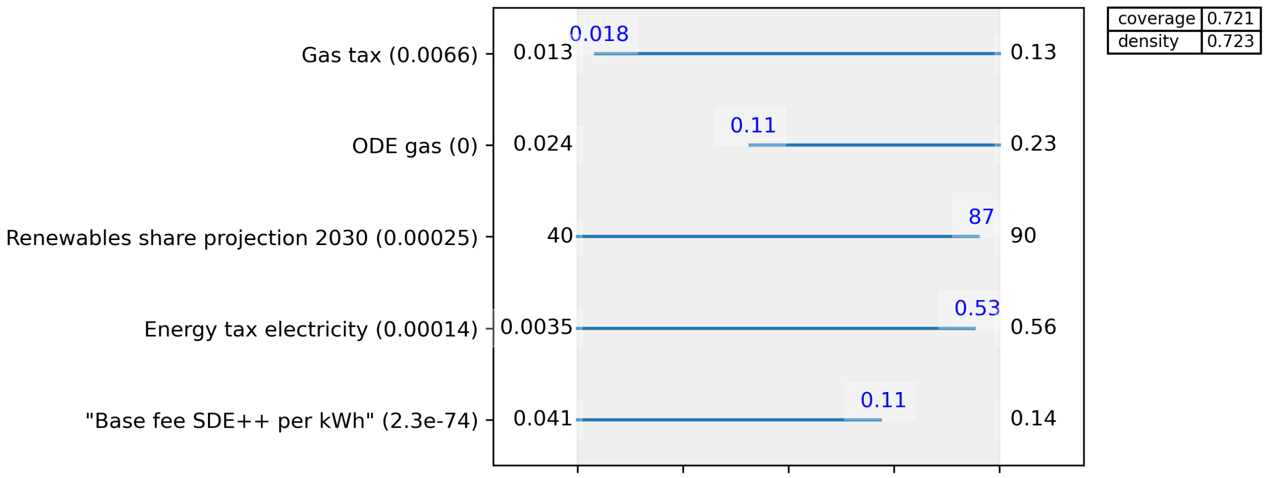

Figure 56: Selected box generated by the PRIM analysis for the cumulative policy costs. The box shows the limits for the constrained input parameters that most strongly predict the subset of outcomes with the 40% lowest cumulative policy costs. Next to the name of each input parameter the qp-value of the constraint is shown. To the right the coverage and density values for the selected box are displayed.

6.3.2 Global sensitivity analysis through Extra-Trees feature scoring

Another technique that has been applied in the context of this vulnerability analysis is Extra-Trees feature scoring, short for extremely randomized trees feature scoring. Feature scoring is a family of machine learning techniques that can be used to reveal the relative influence of individual input parameters on the model outcomes, being a machine learning alternative to global sensitivity analysis as such (Kwakkel, 2018). In this research the Extra-Trees (or extremely randomized trees) developed by Geurts et al. (2006) is used.

In Figures 57 and 58 the Extra-Trees feature scores of the input parameters are shown for the three output variables cumulative emissions, cumulative production costs and cumulative policy costs.

Contrary to the scenario discovery performed (Section 6.3.1), also the Extra-Trees feature scores for the time-dependent output variables annual CO_2 emissions, production costs per tonne ethylene and annual policy costs are assessed. These results are displayed in Figures 59 to 61.

Extra-Trees feature scores for the cumulative emissions

For the cumulative emissions it can be observed in Figures 57 and 58 that the projected share of renewable electricity in 2030 is the most influential input parameter, followed by the projected electricity market price in 2030. This confirms our earlier observation from the scenario discovery analysis (Section 6.3.1). The relatively high influence of the availability of renewable electricity on the cumulative emissions can be explained by the fact that the impact of the projected renewables share on the emissions is twofold: a higher projected renewables share (1) leads to faster electrification as the carbon costs for electricity are lower and (2) influences emissions directly as the emissions resulting from electricity consumption are lower.
The third and fourth most influential parameters are the SDE++ subsidy base fee and the projected ETS carbon price in 2050, respectively. Hence, the SDE++ subsidy is identified as the policy option with the most influence on the cumulative emissions. As both the electricity market price and the SDE++ subsidy influence the operating expenses for electric technologies directly, it can be concluded that limiting the operating expenses for electric technologies by any means possible is crucial in reducing emissions, more so than limiting the investment costs. The reasons for these observations were addressed in Section 6.3.1.

Extra-Trees feature scores for the cumulative production costs

When looking at the Extra-Trees feature scores of the input parameters for the cumulative production costs in Figures 57 and 58, the projected ETS carbon price is obviously the most influential parameters, which could be expected based on the scenario discovery analysis (Section 6.3.1). The high impact of the ETS carbon price on the production costs can be explained by the fact that it affects the industry regardless of the development of electrification. As electricity only becomes fully renewable on the medium to long term, electricity consumption will still cause CO_2 emissions on the shorter term. Hence, even if electrification progresses rapidly and the emission intensity of electricity consumption becomes lower than gas, the industry will face higher carbon costs if the ETS price increases. It can be observed in Figure 60 that the influence of the ETS price reduces over time as electricity becomes cleaner and electrification gains momentum.

Other input parameters are much less influential, which explains the broad constraints observed in Figure 55. However, the relative influence of the availability of renewable electricity and the electricity market price is still significant.
As the availability of renewable electricity determines the emission intensity of electricity and therefore, the carbon costs of electricity, the high influence of the availability of renewable energy on both the cumulative emissions and the cumulative production costs indicates that there exists a considerable number of scenarios where electrification provides a better business case than maintaining conventional operations but electricity consumption still leads to a considerable amount of CO_2 emissions. This also explains why the electricity market price has a higher influence on the cumulative production costs than the gas market price projection.

Extra-Trees feature scores for the cumulative policy costs

Finally, the Extra-Trees feature scores for the cumulative policy costs are assessed (Figures 57 and 58). It can be observed that ODE gas and the SDE++ subsidy base fee are the most influential input parameters, confirming earlier observations in Section 6.3.1. In addition, it can be observed that the projected ETS carbon price in 2050 is nearly as influential as the SDE++ subsidy base fee. This can be explained by the fact that the higher

the ETS carbon price, the lower the effective carbon tax paid by the industry as the effective carbon tax is the difference between the carbon levy and the ETS carbon price (see Appendix D.6).
Moreover, the gas tax also has a significant influence on the policy costs.

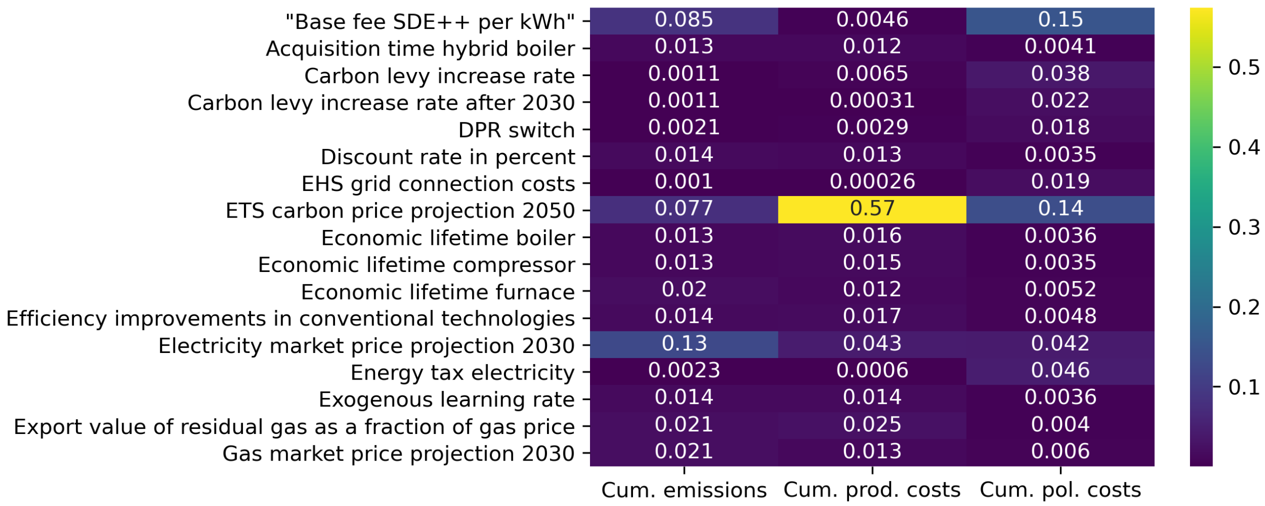

Figure 57: Extra-Trees feature scores of input parameters 1 to 17 for output variables cumulative emissions, cumulative production costs and cumulative policy costs. The higher the score, the higher the influence of the input parameter on one of the output variables.

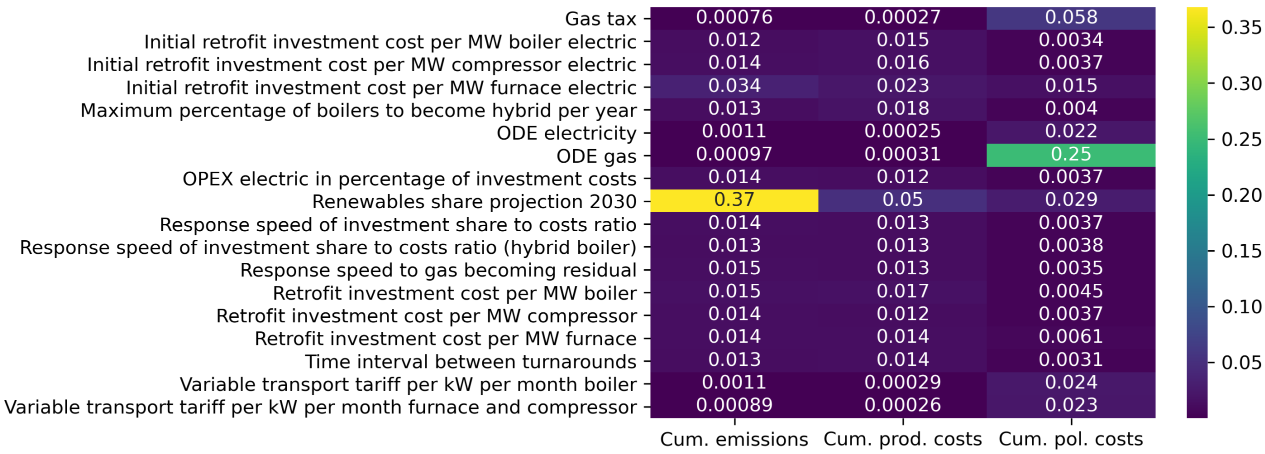

Figure 58: Extra-Trees feature scores of input parameters 18 to 36 for output variables cumulative emissions, cumulative production costs and cumulative policy costs. The higher the score, the higher the influence of the input parameter on one of the output variables.

Extra-Trees feature scores over time: annual emissions

Figure 59 shows the development of the Extra-Trees feature scores over time for the input parameters that are most influential on the annual CO_2 emissions. For the major part of the time span the projected share of renewable electricity in 2030 is the most influential parameter as could be expected from its feature score for the cumulative emissions. However, it can be observed that up until 2025 the SDE++ subsidy base fee is the most influential parameter. Why the availability of renewable electricity overtakes the SDE++ subsidy base fee can be attributed to the relationship between the base fee and the *effective* SDE++ subsidy. The effective SDE++ subsidy is computed by subtracting the avoided gas and carbon costs from the base fee (see Appendix D.1). Hence, as gas and carbon prices increase the effective SDE++ subsidy decreases, reducing the relative influence of the base fee.

It can also be observed that gradually the electricity market price overtakes the projected share of renewable electricity. This effect can be explained by the fact that, even in the worst-case scenario (of a projected 40% share in 2030) the share of renewable electricity increases to 83.6% in 2050, thus substantially reducing the emission intensity of electricity and hence, the carbon costs associated with electricity consumption. Therefore, over time, the electricity market price starts to dominate the costs associated with electricity consumption rather than the availability of renewable electricity. This is also in line with the observations made based on Figure 50 where one can see the emissions "bouncing back" after an initial decrease in some scenarios. In these scenarios, the electricity market price becomes too high at some point, rendering the business case for electrification unattractive again.

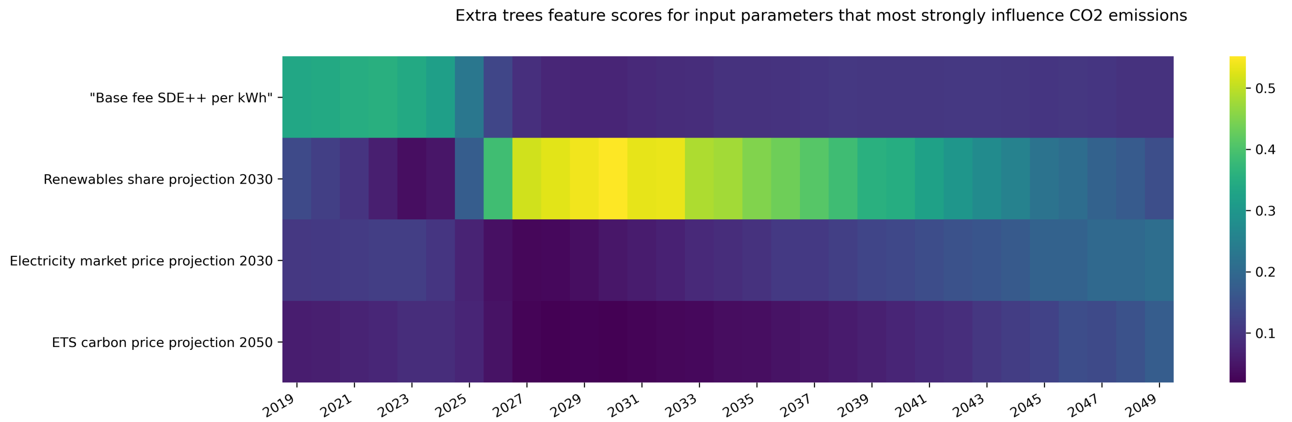

Figure 59: Time-dependent behavior of the Extra-Trees feature scores of the input parameters that most strongly influence the annual CO_2 emissions. The higher the score, the higher the influence of the input parameter on one of the output variables at a particular time instant.

Extra-Trees feature scores over time: production costs per tonne ethylene

Looking at Figure 60 it can be observed that the ETS carbon price is obviously the input parameter with the most influence on the production costs. Over time the electricity market price and the share of renewable electricity gain in influence, indicating the effect of electrification. Though, as the availability of renewable electricity increases and the emission intensity of electricity is reduced, the share of renewables loses influence; this could also be observed in Figure 59.

Extra-Trees feature scores over time: annual policy costs

Drawing on the analyses of Figures 57 and 58 it is not surprising that the ODE gas emerges as the most influential input parameter from Figure 61. However, it can also be observed that over time it loses influence at the expense of the SDE++ subsidy base fee and the ETS carbon price. The increasing influence of the SDE++ subsidy base fee is an indication of increasing electrification in a significant number of outcomes, which results in a higher amount of granted subsidy, hence increasing the policy costs. The ETS carbon price influences the policy costs because it determines the net carbon levy paid by the industry. However, the feature score of ODE gas remains significant (and about equal to the feature score of the SDE++ subsidy base fee), indicating that gas consumption remains substantial in most outcomes. This is plausible because in almost all simulation

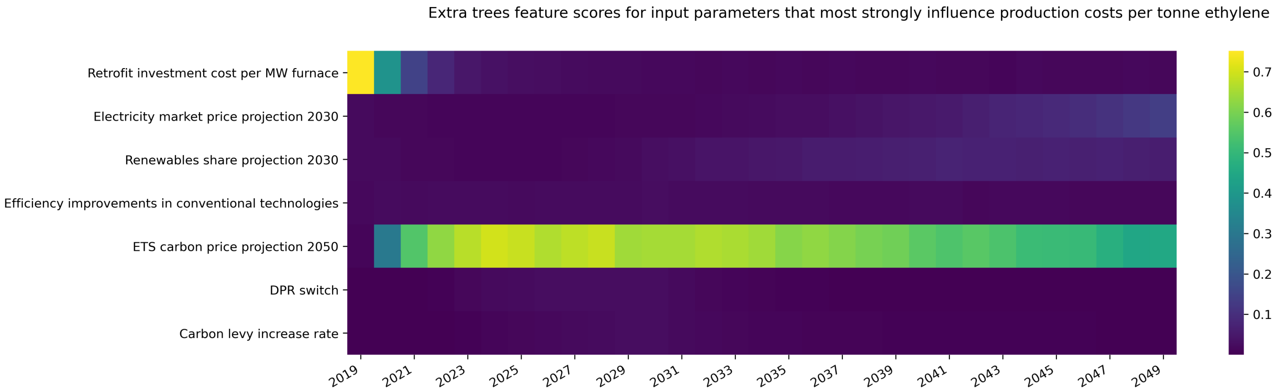

Figure 60: Time-dependent behavior of the Extra-Trees feature scores of the input parameters that most strongly influence the production costs per tonne ethylene. The higher the score, the higher the influence of the input parameter on one of the output variables at a particular time instant.

results the electrification rate of furnaces remains below 70%. Due to the high expected investment costs of electric furnaces electrification of these installations is relatively slow.

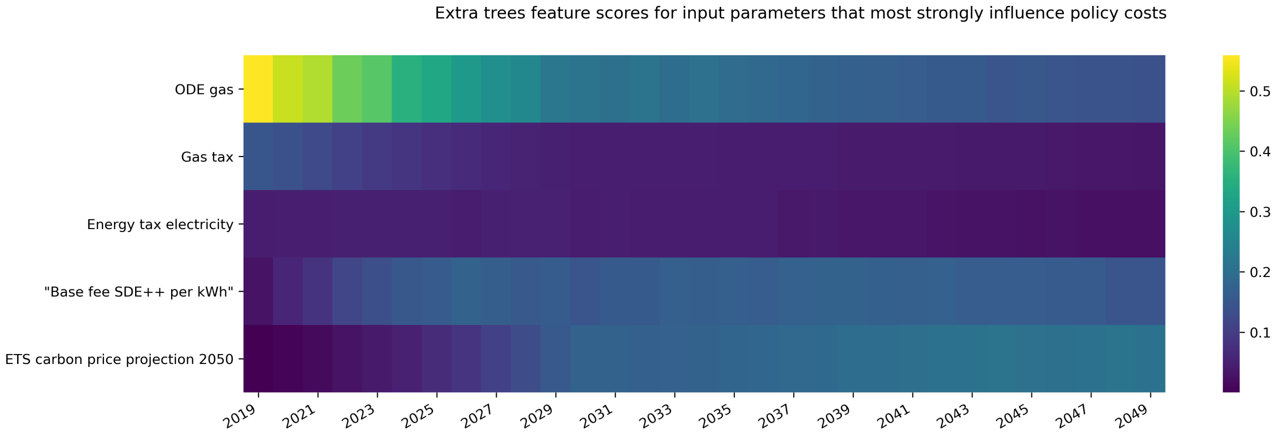

Figure 61: Time-dependent behavior of the Extra-Trees feature scores of the input parameters that most strongly influence the annual policy costs. The higher the score, the higher the influence of the input parameter on one of the output variables at a particular time instant.

6.4 Conclusions of the exploratory analyses

From the visual analysis of the simulation outcomes, the scenario discovery analysis and the Extra-Trees feature scores of the input parameters, the following conclusions can be drawn:

1. The development of electrification and its impact on CO_2 emissions seem highly dependent on the future state of the energy market. This confirms the study by Wiertzema et al. (2020). The availability of renewable electricity is the most influential parameter on the cumulative CO_2 emissions, followed by the electricity market price. Of the policy options considered, the SDE++ subsidy base fee has the highest impact. The importance of a sufficient availability of renewable electricity has also been emphasized by the industry (Interviews, 2021). The analyses also showed that electrification is not a linear process. Electrification may pose an attractive business case on the medium term, but may become unprofitable on the longer term due to rising electricity prices. Hence, policies to accelerate electrification should be focused on long-term objectives and should be adaptive in order to respond to changes in the energy market. These results are line with Johansson et al. (2018), Bataille et al. (2018) and Chen et al. (2019).

2. Electrification of compressors seems a no-regret electrification option. In almost all experiments the electrification rate is above 80%. Due to the poor efficiencies of steam-driven turbines electric compressors provide a viable business case in the near future. For boilers and especially for furnaces achieving a viable business case for electrification is more uncertain.

3. Regarding the cumulative production costs, the ETS carbon price has the highest impact, followed at a distance by the availability of renewable electricity. The high impact of the ETS carbon price on the production costs can be explained by the fact that it affects the industry regardless of the development of electrification. Because electricity consumption will still cause CO_2 emissions in the medium term, even with a high pace of electrification and a relatively lower emission intensity of electricity consumption compared to gas, the industry will face higher carbon costs if the ETS price increases. As electricity becomes cleaner and eletrification progresses, the impact of the ETS price on the production costs is reduced.

4. ODE gas is the most influential parameter on the cumulative policy costs, followed closely by the SDE++ subsidy base fee and the ETS carbon price. To keep the cumulative costs of policy limited below the 40^{th} percentile, the ODE gas should be increased substantially while the SDE++ subsidy base fee should not be too high.

5. The variable grid tariffs do not seem a barrier for electrification as their influence on the cumulative CO_2 emissions is very limited. This is plausible as, when converted to euro/(MW·year), they turn out relatively small compared to electricity costs. However, the variable grid tariffs have considerable impact on the cumulative policy costs, indicating that, if the variable grid tariffs remain low, fewer government expenditures are necessary to stimulate electrification.

6. The ETS carbon price is the only input parameter with a significant influence on all three key performance indicators: CO_2 emissions, production costs and policy costs.

7. Electrification does not necessarily lead to an increase in production costs on the long term. If gas and carbon prices rise fast, electricity consumption becomes relatively more attractive. This illustrates the potential economic advantage that electrification offers to the industry (den Ouden et al., 2018; Wiertzema et al., 2020; Interviews, 2021). However, it should be mentioned that the adjustment costs induced by electrification for integral onsite systems, such as the methane and steam cycles, are not taken into account and hence, the capital expenses for electrification may be depicted as too optimistic.
   Regardless of the potential economic advantage of electrification, the future profitability of ethylene production may be under pressure in general due to rising energy and carbon prices, whether or not far-reaching electrification is implemented. This confirms the concerns of the industry expressed in the interviews (see Section 4.2.1): the revenue may be currently already insufficient for a viable business case for electrification. Developments in circularity, which were not modelled in this study, may put even further pressure of the production costs of ethylene. Over the course of the simulation the ETS carbon price is the parameter with the strongest influence on the production costs. However, the electricity market price gains influence over time, an indication of increasing electrification in a significant number of outcomes.

8. Contrary to what was expected based on Interviews (2021) and literature (e.g. den Ouden et al. (2018)) the investment costs of electric technologies do not appear to be among the most influential parameters. Rather, operational expenses such as energy costs and carbon prices, appear to be bigger drivers of

electrification. This can be explained by the fact that the size of operational expenses is significant. Moreover, for the energy prices, their projected value in 2030 is used as an input parameter for the model and energy prices are assumed to increase linearly based on their projected value. Therefore, an increase in the electricity price or the gas price in this projection year implies that the increase rate of energy prices becomes larger, incurring a prolonged effect on the operational expenses. By contrast, the initial investment costs of electric technologies do not change over time. Hence, the simulation outcomes are less sensitive to a change in the investment costs.
In addition, as a consequence of the present value calculation (see Section 5.3.2) the operational expenses are counted multiple times, while the investment costs are only counted once, making the simulation outcomes relatively more sensitive to an increase in energy prices.

9. The relationship between the policy costs and production costs is less evident and seems highly scenario-dependent. Only for cumulative policy costs at the extremes of the spectrum a more consistent relationship with the cumulative production costs can be observed. High cumulative policy costs tend to results in relatively lower cumulative production costs.

10. Simulation results characterized by far-reaching electrification generally feature higher policy costs. The SDE++ subsidy base fee is the policy option with the highest influence on the cumulative CO_2 emissions. In fact, in the short term (until 2025) it is the most influential input parameter on annual CO_2 emissions. On the other hand, the effect of policy on the resulting emissions is much less significant than the influence of the availability of renewable electricity and the electricity market price.

11. Electrification may lead to increase in emissions in the short term. This has also been noted by (Koelemeijer et al., 2018). In some simulation outcomes electrification poses a better business case than conventional retrofitting without the emission intensity of electricity being lower than the emission intensity of gas. This leads to an increase in emissions in the short term and may lead to relatively higher cumulative emissions in the end as well.

6.5 Robust policy search

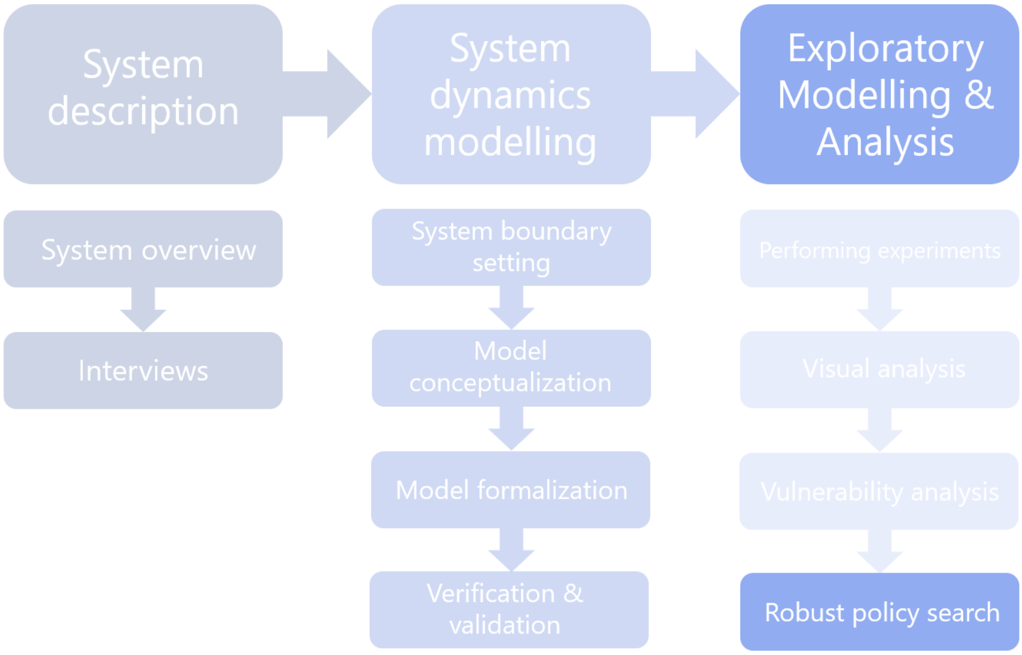

Figure 62: Position of the robust policy search step in the research roadmap.

Now the outcomes of the simulation have been explored and the mapping of the input parameter space onto the outcome space has been investigated, combinations of policy options are sought that are *robust*. According to Giuliani & Castelletti (2016) "a robust decision is a decision that is as much as possible insensitive to a large degree of uncertainty and ensures certain performance across multiple plausible futures." In the case of this study performance is measured based on the three key performance indicators: CO_2 emissions, production costs and policy costs.

In the robust policy search, robust policies are generated through an optimization algorithm and are subsequently used as input for experiments to analyze their impact on the simulation outcomes. These experiments are performed in a way similar to the experiments performed in Section 6.1. However, instead of generating policies randomly by sampling the uncertainty space, the policies are now predefined as being the robust policies. The robust policy search consists of multiple steps, an overview of which is provided below.
In step 1, the system dynamics model is subjected to three different optimizations. As no single definition of robustness exists, three different definitions are used. These optimization yield three databases of robust policies. As the optimization yields a rather large number of policies to be analyzed, a subset of policies is selected in step 2. This subset is selected such that is reflects the variety of policies across the databases. In step 3, this subset of policies is used to perform experiments. Then, based on visual analysis of the simulation results, the best-performing policies for each KPI are selected in step 4. In step 5, the visual analysis zooms in to these best-performing policies, leading to final selection of robust policies. Note that steps 2 and 4 involve some background analyses that are discussed in Appendix K.

6.5.1 Performing the multi-objective robust optimizations

Multi-objective optimization problems are optimization problems in which multiple objectives are to be either minimized or maximized (Deb, 2011). Such optimizations lead to a so-called Pareto-approximate set of solutions (Kasprzyk et al., 2013). However, Pareto-approximate solutions are vulnerable to changes in the problem's input parameters (Sniedovich, 2016). Hence, in problems featuring deep uncertainty it is important to consider the robustness of such Pareto-approximate solutions. Therefore, in the context robust decision-making we are concerned with multi-objective *robust* optimization. In a multi-objective robust optimization problem we seek solutions that perform well across a range of plausible futures instead of a particular plausible future (Lempert, 2002; C. Brown & Asce, 2010; Hine & Hall, 2010; C. Brown et al., 2011). A further theoretical background on multi-objective robust optimization can be found in Appendix J.1.

Step		Output	Discussed in section
1	Performing the multi-objective robust optimizations	3 databases of robust policies (1 for each optimization)	6.5.1
2	Analysis of the outcomes of the robust optimization	Subset of policies	6.5.1 (K.1)
3	Performing experiments with the policies subset	Database of simulation results	6.5.2
4	Visual analysis of the simulation results	Selection of best-performing policies for each KPI	6.5.2 (K.2)
5	Visual analysis of the simulation results for the best-performing policies	Final policy selection	6.5.3

Robustness can be measured in a variety of ways. In fact, many different robustness metrics exists. For a more elaborate discussion see Appendix J.2. The choice of robustness metric greatly influences the solution of a robust decision-making problem. In fact, different robustness metrics can lead to mutually conflicting solutions. Therefore, in the literature on robustness metrics it is often suggested to consider multiple robustness metrics simultaneously and combine the results from each of the metrics (Giuliani & Castelletti, 2016; Kwakkel, Eker, & Pruyt, 2016; McPhail & Maier, 2018). In this research three different robustness metrics are used, which are described in Appendix J.3.

The multi-objective robust optimization can be formulated as follows (using the notation applied by Kwakkel, Eker, & Pruyt (2016)):

$$\text{minimize } F(L) = [f_{CO_2}, f_{prod.costs}, f_{pol.costs}] \tag{38}$$

where f_{CO_2} are the cumulative CO_2 emissions, $f_{prod.costs}$ are the cumulative production costs and $f_{pol.costs}$ are the cumulative policy costs in 2050. L are the policy options and grid tariffs, which obey the same constraints as in the experiments performed in Section 6.1, which are specified in Appendix H, Table 6.
Three distinct optimizations are run, specifying f_{CO_2}, $f_{prod.costs}$ and $f_{pol.costs}$ according to the robustness metrics outlined in Section J.3.

The EMA workbench provides support for multi-objective robust optimization using the MOEA Epsilon Non-dominated Sorted Genetic Algorithm II (ϵ-NSGAII), first introduced by Kollat & Reed (2006), as a default. The EMA workbench does not contain predefined robustness metrics but these can be straightforwardly implemented. Regarding the generation of plausible futures, the same experiment design is employed as in the exploratory analyses conducted in Chapter 6 (see Appendix H, Table 5). Latin Hypercube sampling across the uncertainty space is then used to generate 50 scenarios.

The number of function evaluations $F(L)$ was set to 5000 for robustness optimization 1 and 2000 for robustness optimizations 2 and 3. This is due to the extensive computational time required for robustness optimizations 2 and 3. The long computational time for metrics 2 and 3 can be explained by the fact that they include the mean μ_i as a separate objective, hence effectively incorporating 6 objectives instead of 3 objectives as is the case with robustness metric 1.

Robust optimization 1 yielded 237 policies, robust optimization 2 762 policies and robust optimization 3 348 policies.
Due to the large number of policies they were split up in different clusters and visual analysis was performed on each of these clusters using parallel coordinate plots (for more details see see Appendix K). Through these parallel coordinate plots a selection of policies was made that is deemed representative of the variety of policies across the database. This process yielded a selection of 21 policies which were then used to perform experiments, yielding a database of simulation results.

6.5.2 Visual analysis of the simulation results

The subset of 21 policies selected in Section 6.5.1 were fed back into the simulation model through the performance of experiments. The experimental setup for these experiments is similar to Section 6.1. However, instead of *sampling* the input policies across the decision space, the policies are now *predefined* as the 21 selected poli-

cies.
To generate plausible futures still sampling was applied across the uncertainty space according to the experiment design discussed in Section 6.1, creating 300 scenarios. With the robust policies as input for the experiments, the performance of the cumulative CO_2 emissions, cumulative production costs and cumulative policy costs under the range of plausible futures was then evaluated through visual analysis.

The simulation results were then subjected to a visual analysis which can be found in Appendix K.2. Based on this visual analysis a few best-performing policies were selected for each key peformance indicator. These are the following:

- Cumulative CO_2 emissions: policies 15 and 16
- Cumulative production costs: policies 10, 13, 14 and 15
- Cumulative policy costs: policies 3 and 4

6.5.3 Visual analysis of the simulation results for the best-performing policies

Now the best-performing policies have been selected for each KPI we consider how these policies compare with regard to the three KPIs combined, instead of just one particular KPI. This has been done by means of a scatter plot, shown in Figure 63. In addition, the performance of the policies for the individual KPIs can be found in Figures 64, 65 and 66, respectively.
Upon inspection of Figure 63 it is concluded that policies 3 and 4 lead to undesirable results for the cumulative CO_2 emissions because of an excessive concentration of outcomes on the higher end of the emissions spectrum. These results are not much better, or even worse, than the results for the randomly sampled policy options, looking at Figures 49 and 46. By contrast, policies 10 and 13-16 lead to significantly higher concentrations of outcomes in the lower end of the emissions spectrum, though policy 10 still leads to a distribution leaning towards the higher end of the spectrum.

For the cumulative production costs (also see Figure 65) policies 3 and 4 also turn out to be the most undesirable as they result in outcomes distribution strongly inclined to the top of the spectrum. Policy 16 also produces results which tend to be inclined to the higher end of the spectrum, though this inclination is less strong. By contrast, policies 10, 13, 14 and 15 lead to more even distribution, with relatively higher concentrations of outcomes on the bottom of the spectrum. Moreover, these four policies do not produce significantly different outcome distributions.

For the cumulative policy costs, policies 10, 14 and 15 lead to the highest concentrations of outcomes on the top of the spectrum. Policy 13 also produces an outcome distribution with outcomes mainly concentrated on the top of the spectrum though leaning towards the lower end of the spectrum. Though policies 3 and 4 clearly produce the best results for the cumulative policy costs, policy 16 is the next-best alternative. Its results are more or less concentrated around the middle of the spectrum, with relatively small deviations to either side.

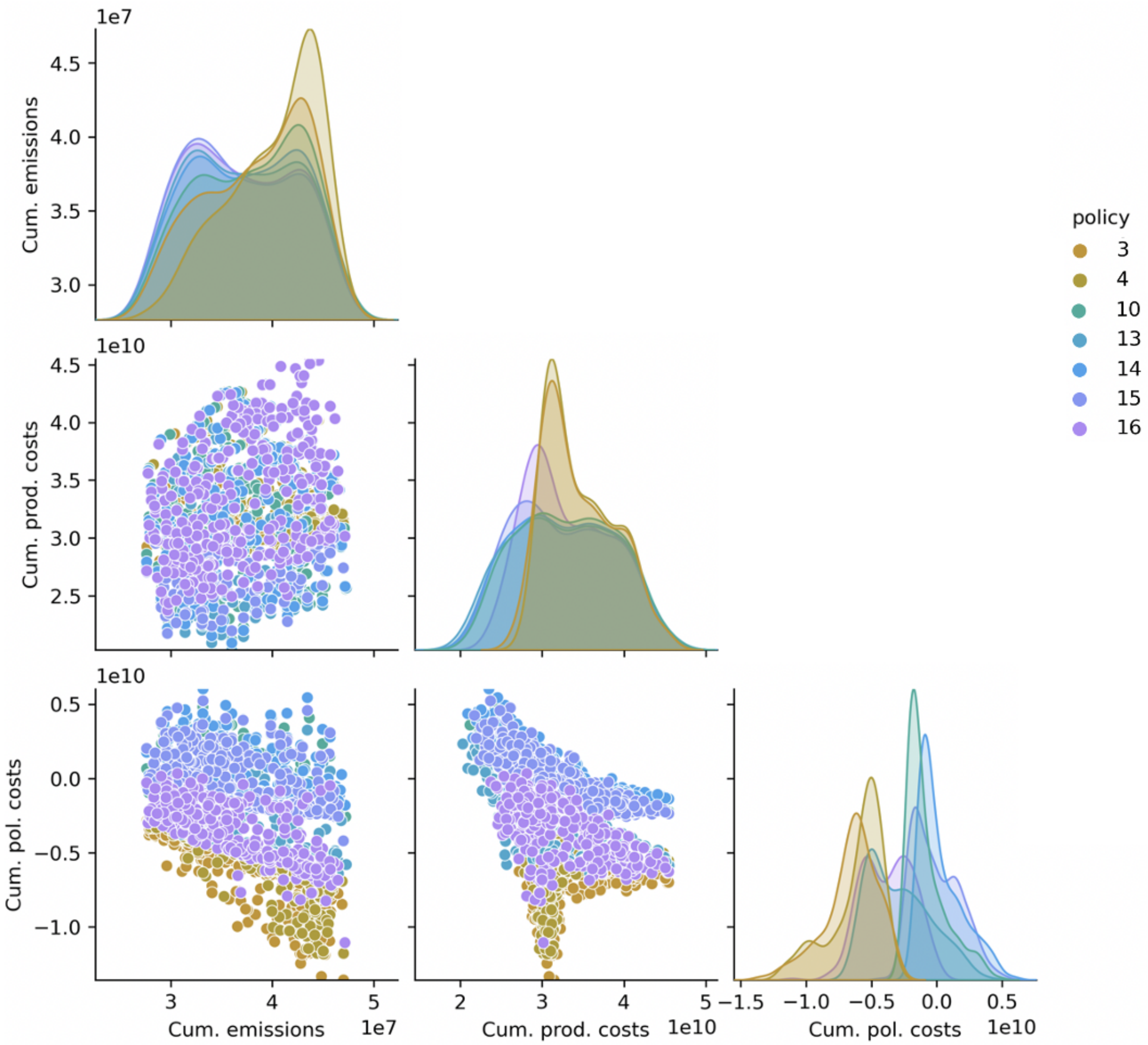

Figure 63: Scatter plot of the simulation results showing cumulative CO_2 emissions, cumulative production costs and cumulative policy costs associated to naphtha cracking for the reference plant in 2050 for the robust policies 3, 4, 10 and 13-16. Note: 1e7 denotes 10^7 and 1e10 denotes 10^{10}.

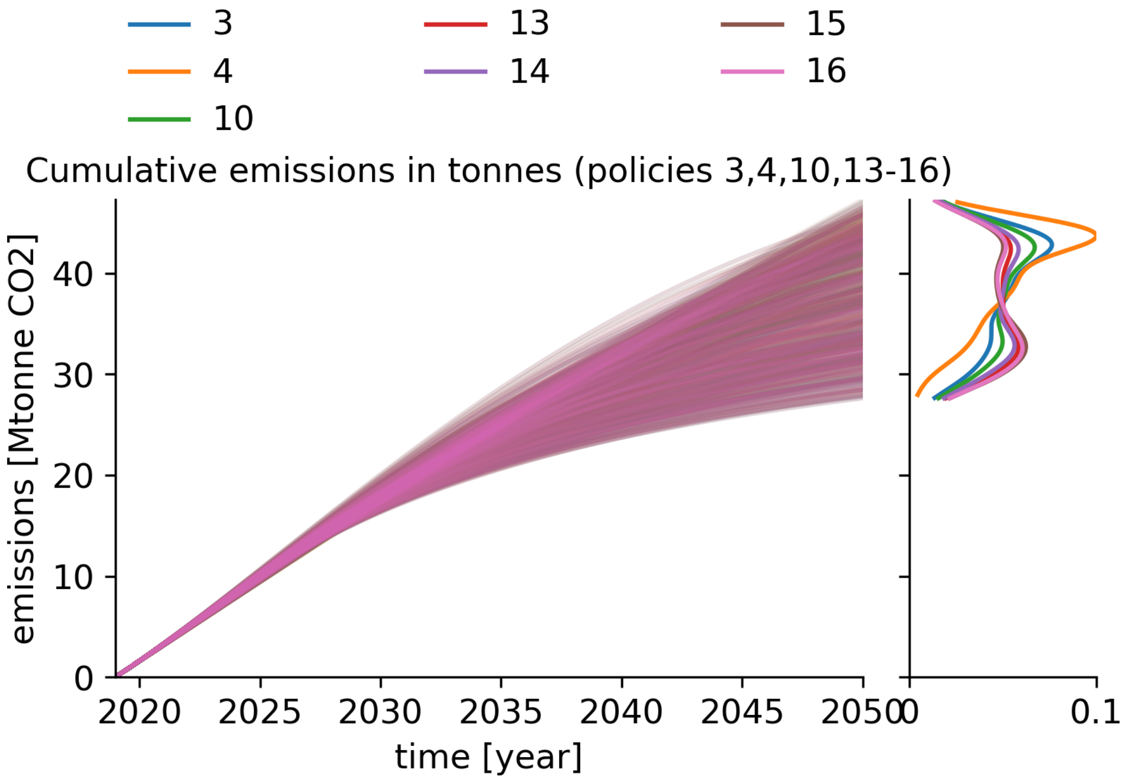

Figure 64: Simulation results for the cumulative CO_2 emissions associated to naphtha cracking for the reference plant, for the best-performing policies (3, 4, 10 and 13-16). To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

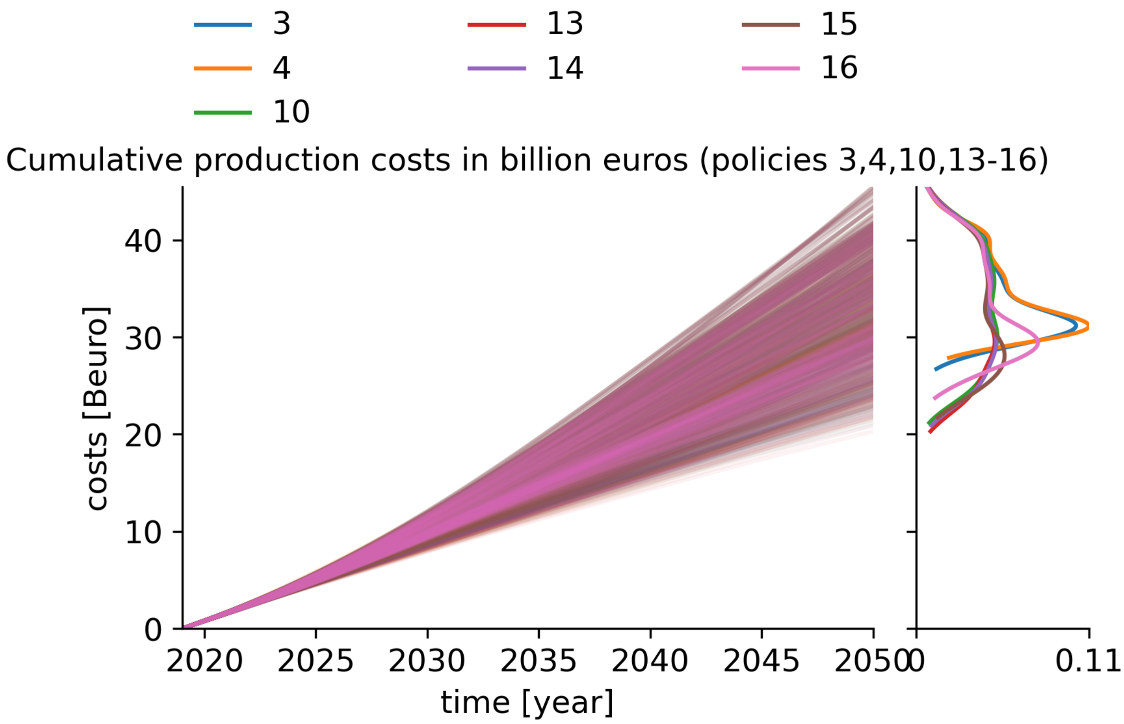

Figure 65: Simulation results for the cumulative production costs associated to naphtha cracking for the reference plant, for the best-performing policies (3, 4, 10 and 13-16). To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

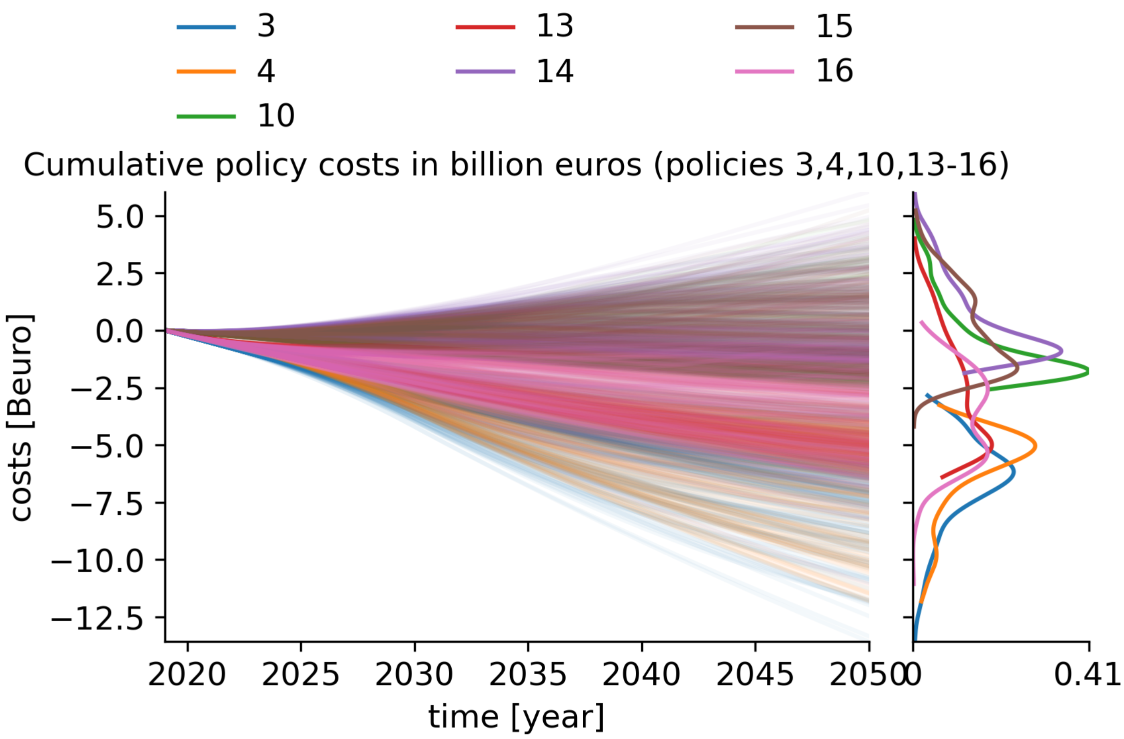

Figure 66: Simulation results for the cumulative policy costs associated to naphtha cracking for the reference plant, for the best-performing policies (3, 4, 10 and 13-16). To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

6.5.4 Resulting robust policies

Based on the visual analysis of Section 6.5.3 it becomes clear that policies 3 and 4 should be ruled out because they lead to the worst outcomes distributions for both the cumulative emissions and the cumulative production costs among the selected policies. Policy 10 can also be ruled out, because its results are on the higher end of the policy costs spectrum and are also less favorable with regard to the cumulative emissions, while its results are on par with policies 13 and 14 for the cumulative production costs.

Consequently, the robust policy search results in four policies, of which the characteristics are outlined in Table 1.
With regard to the policy options the following observations are made with regard to the characteristics of these four policies.

- **Base fee SDE++**. A defining feature of all four policies is the high SDE++ subsidy base fee of more than 0.12 euro/kWh. For comparison: the base fee for industrial electric boilers is set in 2021 at 0.05 euro/kWh (Lensink & Schoots, 2020).

- **Carbon levy**. Except for policy 16, the carbon levy increase rate (until 2030) seems moderate for all policies and turns out even lower than the current value of 10.56 euro/(tonne$_{CO_2}$·year) (NEa, 2020). However, the DPR switch is set to 0 for policies 14, 15 and 16, meaning that the dispensation rights (DPRs) granted to the industry are abolished in these policies. Consequently, no free emission rights are granted to the industry anymore, increasing the effective carbon tax paid by the industry. This is not the case for policy 13, however. On the other hand, the carbon levy increase rate after 2030 is high for policy 13, compared to moderate increases in policies 15 and 16 and only a very slow increase in policy 14.

- **Electricity taxes**. Combined electricity taxes (energy tax and ODE) are lowered in all four policies, ranging from a 27% reduction (policy 13) to a 85% reduction (policy 14).

- **Gas taxes**. Combined gas taxes (regular gas tax and ODE) significantly increase in all four policies. The largest increase can be found in policy 16 which features a 8.5-fold increase. With a 1.85-fold increase policy 14 features the smallest increase in combined gas taxes. For policies 13, 14 and 15 an increase in the gas taxes seems to balance the decrease in the electricity taxes: the more the gas taxes are increased, the less the decrease in the electricity taxes need to be. On the other hand, policy 16 features both a large increase in the gas taxes and a large decrease in the electricity taxes.

- **Grid tariffs and connection costs**. The EHV grid connection costs, which range from $1.5 \cdot 10^6$ million euros to $3.0 \cdot 10^6$ million euros (ACM, 2020), have to remain on the lower side of the spectrum. The transport tariff for the HV grid needs (1.23 euro/(kW·month in the reference case) to be significantly reduced in all four policies. The transport tariff for the MV grid (currently at 2.00 euro/(kW·month) need not be reduced as strongly, except for policy 15.

6.5.5 Conclusions from the robust policy search

From the robust policy search the following conclusions are drawn:

1. To a certain degree, policy is able to influence the development of electrification and to steer towards emission reductions. This can be deduced visual analysis of the simulation results for the robust policies which show higher concentrations of outcomes on the bottom of the emissions spectrum for certain policies. However, it is also observed that even if far-reaching policy adjustments are implemented there remains considerable uncertainty about attaining a significant reduction in emissions as the spread of the simulation outcomes over the emissions spectrum remains rather large. This observation confirms the results of the exploratory analyses and also what has been found by Wiertzema et al. (2020) that certain electrification strategies perform well in certain energy market scenarios but display poor performance in others.

2. The policies resulting from the robust policy search introduce profound changes to the current policy instruments. Pushing one button does not seem sufficient. Instead, multiple changes have to be introduced simultaneously. This is in agreement with e.g. Bataille (2020) and Johansson et al. (2018) who state that current government programs to support decarbonization in energy-intensive industries are unlikely to incur transformative change. Moreover, they agree that carbon pricing alone is not sufficient to bring

Table 1: Policy options and grid tariffs that characterize the four selected robust policies. At the bottom of the table it is also indicated whether a policy results in either the best or the worst performance for a particular KPI, relative to the other policies.

	Unit	Policy 13	Policy 14	Policy 15	Policy 16
Base fee SDE++	euro/kWh	0.134	0.128	0.140	0.140
Carbon levy increase rate	euro/ (tonne$_{CO_2}$·year)	7.98	5.39	10.1	17.5
Carbon levy increase rate after 2030	euro/ (tonne$_{CO_2}$·year)	17.6	0.674	3.70	5.89
EHV grid connection costs	Meuro	1.79	1.91	1.68	1.67
Energy tax electricity	euro/MWh	0.522	0.127	0.404	0.0472
Gas tax	euro/m^3	0.0621	0.0147	0.0222	0.128
ODE electricity	euro/MWh	0.180	0.0151	0.0016	0.248
ODE gas	euro/m^3	0.222	0.0520	0.0929	0.177
Variable transport tariff (HV grid)	euro/ (kW·month)	0.708	0.447	0.149	0.0554
Variable transport tariff (MV grid)	euro/ (kW·month)	1.76	1.41	0.218	1.81
DPR switch	-	1	0	0	0
Best for		Cumulative production costs	Cumulative production costs	Cumulative emissions	Cumulative policy costs
Worst for		None	Cumulative emissions, Cumulative policy costs	None	Cumulative production costs

about the technological innovations needed to achieve far-reaching emission reductions. Furthermore, these robust policies reflect the policy packages suggested by Johansson et al. (2018), combining positive incentives such as subsidies with negative incentives like carbon pricing.

- Base fee SDE++: is substantial in all four robust policies.
- Carbon levy. The dispensation rights (DPRs) are abolished in three out of four robust policies. On the other hand, the increase in the carbon levy remains moderate in these policies. In the one robust policy where the DPRs are not abolished, the carbon levy increase rate should be raised substantially after 2030.
- Electricity taxes. The combined electricity taxes are substantially lowered in all four policies.
- Gas taxes. The combined gas taxes are substantially increased in all four policies. However, for three policies a trade-off between increasing the gas taxes and lowering the electricity taxes seems possible: if the gas taxes are increased more drastically, the electricity taxes can remain closer to their current levels and vice versa. Lowering the electricity taxes and increasing the gas taxes is in agreement with den Ouden et al. (2018) who state that energy taxes need to be altered such that electricity is rendered an attractive alternative to gas.
- Grid tariffs and connection costs. The EHV grid connection costs should remain limited and the transport tariff for the HV grid should be significantly reduced. On the other hand, the transport tariff for the MV grid need not be reduced as strongly. Following the implications of the exploratory analyses, these changes in the grid tariffs are mainly required to keep the policy costs in check. These adjustments to the grid tariffs and connection costs are in line with the suggestions made by den Ouden et al. (2018) who suggested adapting the electricity tariff structures for high capacity connections and reevaluating grid connection costs.

3. All robust policies feature a high SDE++ subsidy base fee. It could be questioned whether this amount of subsidy fits within the current SDE++ system. Hence, these results may imply that a new subsidy instrument is needed, such as an investment subsidy akin to the EU Innovation Fund. This was already suggested by the Ministry of Economic Affairs and Climate (Interview Min. EA&C, 2021).

4. Since it was observed in Section 6.3.2 that the gas taxes are not the main drivers for electrification, as opposed to the SDE++ base fee, it seems that increasing the gas taxes are mainly required to keep the policy costs in check rather than acting as an accelerator for electrification.

5. Robustness metric 1 (maximin) does not seem very useful in the context of this study. Minimizing the worst-case (maximin) seems to negatively affect the performance in other plausible futures, at least in the case of the cumulative emissions and cumulative production costs. This confirms the observation made by Kwakkel, Eker, & Pruyt (2016) who furthermore state that the maximin metric should be used only in specific cases.

6. Robustness metric 2 (undesirable deviations) produces some useful results. Minimizing the undesirable deviations from the median seems to be detrimental to the overall performance; for the cumulative emissions and cumulative production costs optimization using this metric leads to clustering of outcomes at the higher ends of their respective spectra. There also seems to be a strong trade-off between the mean and the undesirable deviations for these two KPIs. However, robust policies that produce low mean emissions and low mean production costs (such as the selected policies 13, 14 and 15) produce good results.

7. The results of robustness metric 3 (percentile-based peakedness), which was reported by Kwakkel, Eker, & Pruyt (2016) to be one of the metrics producing the best results, are on par with the results of robustness metric 2. Especially the results featuring low kurtosis regarding the cumulative emissions (which also happen to feature low mean cumulative emissions, low mean cumulative production costs and low kurtosis of the production costs) produce the best results.

7 Conclusions

In this final chapter conclusions will be drawn on the results presented in this study. First, in Section 7.1 an overview of the research findings will be given. Second, in Section 7.2 an the main research question will be answered. This will be followed by some considerations regarding contribution of this research in Section 7.3. The selected research approach and methods will be reflected on in Section 7.4. Limitations will be discussed in Section 7.5. Afterwards, recommendations for policymakers will be given in Section 7.6 and recommendations for further research in Section 7.7.

7.1 Overview of research findings

Electrification is identified as a key strategy in the decarbonization of energy-intensive industries such as the naphtha cracking industry (Johansson et al., 2018; Chen et al., 2019; Wiertzema et al., 2020; Bataille, 2020) because of its high potential contribution to curbing CO_2 and other industrial emissions (van Kranenburg et al., 2016) and its foreseen economic advantages in light of the fast-decreasing costs of renewable electricity (den Ouden et al., 2018; Wiertzema et al., 2020).
However, various uncertainties complicate the business case for electrification (den Ouden et al., 2018). Among other factors, uncertainties regarding the future energy market play a large role (den Ouden et al., 2018; Griffin et al., 2018; Wiertzema et al., 2020). These challenges call for targeted, long-term policy to accelerate electrification (Chen et al., 2019) which is also adaptive so it can respond to the dynamic energy energy market (Johansson et al., 2018; Bataille et al., 2018).
To aid the making of such policy a need is identified to apply an exploratory modelling approach (Moallemi & Malekpour, 2018) for evaluating the long-term effects of policy interventions (Johansson et al., 2018), which captures not only technological but also societal and political aspects (Li & Strachan, 2019). Hence, the main research question is formulated as follows: *What robust policy options can the Dutch government employ to reduce emissions in the naphtha cracking industry through electrification?*
In this regard, the following key performance indicators are defined: CO_2 emissions, production costs and policy costs (the total sum of subsidies granted to the industry subtracted by the total amount of taxes levied).

To answer this research question, an exploratory modelling approach grounded in the Robust Decision-Making (RDM) framework (Lempert et al., 2013) is outlined. RDM is deemed apt for this research as it provides a framework for testing policy options under an ensemble of plausible futures (Walker et al., 2013a; Kwakkel, Haasnoot, & Walker, 2016; Lempert, 2019). The RDM framework has been adapted to fit this research and comprises three phases: (1) system description, (2) system dynamics (SD) modelling and (3) Exploratory Modelling & Analysis (EMA).

In the system description phase, an initial understanding of the socio-technical system of electrification in the naphtha cracking industry is developed. Interviews with representatives from the industry (Interviews, 2021) reveal that electrification is indeed considered a potentially important decarbonization option for the naphtha cracking industry. However, the interviewees emphasize that the availability of renewable electricity is a critical prerequisite. Moreover, there is uncertainty among the industry concerning the capacity of the electricity grid, which has to be upgraded to accommodate electrification. Next to external developments, certain characteristics of the naphtha cracking industry also make electrification challenging. One is the high degree of integration between systems onsite. As a consequence, electrification of certain parts of the process require adjustments in other systems and cycles. The interviewees think current government policy is inadequate to support the industry in attaining its Climate Agreement goals as it does not sufficiently match the uncertainties faced by the industry concerning investments in electrification.
A representative from the Ministry of Economic Affairs and Climate (Interview Min. EA&C, 2021) recognizes the challenges faced by the industry. The interviewee comments that the ministry strives to support energy-intensive industries in their decarbonization in order to avoid carbon leakage. The interviewee acknowledges that current policy does not provide the industry with sufficient financial incentive to invest in electrification and suggests developing a novel subsidy instrument to foster investments.

Based on the system description, a system dynamics (SD) model is developed that represents the development of electrification in the naphtha cracking industry. The model takes investment decisions within the industry as a starting point. The model only considers retrofits: the upgrading of existing installations by installing new parts. This is because the industry is unlikely to invest in entirely new capacity (Interviews, 2021). Based on the development of external factors such as energy prices, carbon prices, the availability of renewable electricity and efficiency improvements, and policy options such as energy taxes and the SDE++ subsidy, the model computes the aggregate cost of electrification versus the aggregate cost of retrofits using conventional technologies for three types of installations: furnaces, compressors and boilers. The ratio between these costs then determines which portion of the industry's investments is channeled towards electrification. According to the distribution of investments the development of electric and conventional capacities is modelled over time, along with its effects on CO_2 emissions, production costs and policy costs.

The system dynamics model is subjected to Exploratory Modelling & Analysis (EMA), which consists of several steps. First, experiments are performed on the model. Each experiment comprises a different combination of input parameters, i.e., values of external factors and policy options. With the experiments defined, the model is used for simulation, generating a database of simulation results. This database contains the time series for the system's key performance indicators: (cumulative) CO_2 emissions, production costs and policy costs.
The database of simulation results is then subjected to two different analyses: (1) visual analysis and (2) vulnerability analysis. During the visual analysis, the simulation results are plotted in order to study their behavior visually. Vulnerability analysis is a more advanced analysis tool that elicits how the input parameters map onto the system's key performance indicators. Two different methods are used in this regard: scenario discovery and Extra-Trees feature scoring.
From these analyses it becomes apparent that the development of electrification in the naphtha cracking industry is highly dependent on the future state of the energy and carbon markets. The availability of renewable electricity is the single most influential parameter on cumulative CO_2 emissions. Moreover, the development of electrification varies across the different installations considered; compressor turbines stand out as they display an electrification rate of over 80% in almost all scenarios. It also appears that, regardless of the degree of electrification, the production costs of ethylene may be under pressure due to rising energy prices. Furthermore, simulation outcomes with far-reaching electrification feature relatively higher government expenditures.

Apart from the visual analysis and vulnerability analysis, a robust policy search is performed. Robust policies are defined as policies that are relatively insensitive to deep uncertainty and display a certain performance under an ensemble of plausible futures (Giuliani & Castelletti, 2016). As part of the robust policy search the system dynamics model is subjected to a multi-objective robust optimization algorithm which seeks to minimize cumulative CO_2 emissions while also minimizing cumulative production costs and policy costs. This algorithm yields a database of policies, out of which a final selection of four policies is made through consecutive steps.
From the robust policy search it is concluded that policy is able to influence the development of electrification and steer towards emission reduction to a certain degree. However, it is also observed that even with rather radical policy adjustments there remains considerable uncertainty about attaining a significant reduction in emissions. The resulting robust policies introduce profound changes to the current policy instruments and require changes in multiple aspects: a higher SDE++ base fee, a fiscal shift favouring electricity over gas and an increase in the carbon levy, either by abolishing dispensation rights or by substantially raising the carbon levy increase rate post-2030. As all the robust policies feature a rather large SDE++ subsidy base fee it could be questioned whether this amount of subsidy fits within the current SDE++ system. Hence, the results justify the possible introduction of a novel subsidy instrument.

7.2 Answer to the main research question

In Section 2.4 the main research question was formulated as follows:

What robust policy options can the Dutch government employ to reduce CO_2 emissions in the naphtha cracking industry through electrification?

From the system description, it is found that electrification its development is highly sensitive to external factors. Fundamental uncertainties, most importantly the availability of renewable electricity and the capacity of the electricity infrastructure, make the industry hesitant to invest in electrification. Moreover, the high technical complexity of naphtha cracking plants pose considerable difficulties to the implementation of electrification: the high degree of system integration onsite imply that electrification in certain parts of the plant require adjustments in the plant configuration as a whole. From the industry's point of view, current government policy does not echo these challenges yet demands that the industry obeys the goals set in the Climate Agreement (Interviews, 2021). A representative from the Ministry of Economic Affairs and Climate recognizes the challenges voiced by the industry and acknowledges that current policy is insufficient to foster investments in electrification.
These complexities were captured by a system dynamics model that takes investment decisions in the industry

as a starting point. The model only considers retrofits: the upgrading of existing installations by installing new parts. External factors such as energy prices and the ETS carbon price and policy interventions such as taxes determine how the costs for electrification develop relative to the costs for conventional retrofits. Based on expectations of the relative profitability of electrification, existing capacities are electrified, in turn affecting CO_2 emissions, production costs and policy costs over time.

The visual analysis and vulnerability analysis confirm that the naphtha cracking industry system is highly sensitive to external factors. Market developments, i.e. the electricity market price and the ETS carbon price, turn out to be among the main drivers, or inhibitors, of emission reduction in the naphtha cracking industry and more influential than most policy interventions. Moreover, the availability of renewable electricity turns out to be the single most influential factor regarding emissions.
It is also shown that considerable electrification on the medium term is no guarantee for far-reaching electrification on the long term. The energy market is constantly in motion, more so now than before, and rising electricity prices may pose a limit to electrification, causing it to bounce back. In this light, policies to accelerate electrification should be designed such that it is able to respond to change.
Electrification does not necessarily lead to an increase in production costs on the long term. Nonetheless, the future profitability of ethylene production may be under pressure, regardless of the degree of electrification in the industry.

The robust policy search reveals that, although policy has significant impact on the system, even when implementing far-reaching policy interventions there remains considerable uncertainty about attaining a significant reduction in emissions. Profound changes in the current policy instruments are suggested to achieve a significant degree of electrification in the naphtha cracking industry with sufficient certainty. Simultaneous changes are suggested in all policy options considered. First, the analysis suggests an SDE++ subsidy base fee of over 0.12 euro/kWh for the considered technologies. Such a base fee is substantial considering that the current base fee for industrial electric boilers amounts to 0.05 euro/kWh (Marsidi et al., 2021). This reflects the observations of both industry and government representatives that there currently exist too few financial incentives to steer the industry towards electrification (Interviews, 2021; Interview Min. EA&C, 2021).
Second, an increase in the carbon levy should be considered, either by phasing out the dispensation rights (DPRs) currently granted to the industry or by substantially increasing the growth rate of the carbon levy post-2030 to above 17 euro/(tonne$_{CO_2}$ ·year). These results also align with the perspectives of the industry: the industry representatives interviewed argued for a higher carbon levy as the EU ETS carbon price remains too low (Interviews, 2021).
Third, it seems necessary that a fiscal shift is implemented that discourages gas consumption and favors electricity consumption. However, according to the analysis, the extent of this fiscal shift varies among the robust policies and the degree of change to the gas taxes can be traded off against the degree of change to the electricity taxes. However, the analysis points out that increasing the gas taxes are mainly required to keep the policy costs in check rather than acting as an accelerator for electrification.
Finally, the analysis suggests adapting the grid tariff structure such that the connection costs for the Extra High Voltage (EHV) grid are minimized while substantially reducing the variable grid tariffs for the HV grid. The variable grid tariffs for the MV grid require less significant adaptations.

In the design of policy to reduce emissions in the naphtha cracking industry through electrification, fundamental uncertainties should be analyzed and accounted for. Policies that are characterized as robust feature considerable adjustments in almost all current policy instruments in parallel: a higher SDE++ base fee, a fiscal shift favouring electricity over gas and an increase in the carbon levy, either by abolishing dispensation rights or by substantially raising the carbon levy increase rate post-2030. Moreover, as the dynamics of the energy market turn out to be the driving force behind electrification, policy should be designed in an adaptive fashion. Adaptive policy-making involves the construction of a sequence of policy options, which contains both policy options that are implemented upon enacting the policy and contingency plans that are activated based on certain indicators (Walker et al., 2001). In this manner, adaptive policy is able respond to changes in the energy market. Finally, policy-makers should be aware of the fact that emission reduction in the naphtha cracking industry hinges on the availability of renewable electricity. Therefore, policy change to accelerate electrification should go hand in hand with more decisive action regarding the acquisition of capacities for the generation of renewable electricity.

7.3 Contribution of this research

Although policy interventions to accelerate electrification have been suggested in literature (e.g. Johansson et al. (2018), den Ouden et al. (2018) and Bataille (2020)) no previous research has focused on evaluating the impact of policy interventions in the chemical industry using a model-based approach, let alone exploratory modelling. However, as Moallemi & Malekpour (2018) outline, energy transitions are characterized by the combination of deep uncertainty and a multi-actor decision environment. Hence, applying exploratory modelling to such problems could support decision-making as it enables considering an ensemble of plausible futures. Therefore, exploratory modelling can explicitly address uncertainty, the importance of which is underlined by Workman et al. (2020) and Thiele (2020).

This research is a first attempt at studying the impact of policy interventions at a particular energy-intensive industry under deep uncertainty. It studies the impact of a variety plausible futures on the business cases for electrification versus conventional retrofits and the consequences thereof for the development of electrification and CO_2 emissions. By considering innovation in electric technologies and energy efficiency improvements, technological aspects of the transition are also taken into consideration. The study shows that electrification in the naphtha cracking industry hinges on the development of the energy market; even with radical changes in current policy, a lack of renewable electricity or an excessively high electricity price may still inhibit deep decarbonization. In light of this result, policy to accelerate should be targeted at long-term objectives, be adaptive and be able to respond to the dynamics of the energy market. This is line with Johansson et al. (2018), Bataille et al. (2018) and Chen et al. (2019).

The study confirms the uncertainties faced by the industry and the barriers they pose to electrification and decarbonization. The results also show that the profitability of ethylene production may be under pressure due to increasing energy prices, a concern that has been voiced by the industry (Interviews, 2021).
The study also shows that profound changes are required in current policy instruments to give electrification a high probability of succeeding given the range of plausible futures. Pushing one button is not enough; changes in multiple instruments are required simultaneously. This finding is in agreement with Johansson et al. (2018) and Bataille et al. (2018). Due to the high subsidy required in all of the suggested robust policies it could be questioned whether the SDE++ system is adequate. A novel subsidy instrument may well be necessary, which was also hinted at by the Ministry of Economic Affairs & Climate (Interview Min. EA&C, 2021).

7.4 Reflection on the research approach

Because electrification in the naptha cracking industry is characterized by market uncertainties and a multi-actor decision-environment it can be denoted as a wicked problem (Incropera, 2016). Therefore, studying this problem calls for an exploratory modelling approach (Moallemi & Malekpour, 2018). Since we are specifically interested in testing policy interventions under an ensemble of plausible futures the Robust Decision-Making (RDM) framework has been used. RDM does not specify a standard modelling methods; in principle, multiple methods can be used within the RDM framework. In this research, system dynamics (SD) modelling is used. In Section 3.2.3 the advantages of using SD were outlined. These can be summarized as follows:

1. SD is able to model the feedback loops that characterize the socio-technical system at hand.
2. SD is suited to model transitions such as electrification because of its ability to describe the evolution of system over an extended period of time.
3. SD is able to incorporate actor decision through information feedbacks.
4. SD can be used to evaluate the impact of policy interventions in quantitative terms.
5. SD fits well within the RDM framework because it can be combined with Exploratory Modelling & Analysis (EMA).

Upon reflection of the selected research approach and methods it can be concluded that an exploratory modelling approach grounded in the RDM framework is indeed an apt approach. The system description presented in Chapter 4.1 confirms the uncertainties faced by the industry and the complex nature of the decision environment in which government, grid operators and industry all depend on one another. In the interviews, the industry also voiced its need for targeted, long-term policy. In this light, the search for robust policy options is highly relevant.
SD in combination with EMA appears a powerful tool to interpret the uncertainties that characterize the

socio-technical system and elicit the driving factors behind electrification while weighing the impact of policy interventions against the background of an ensemble of plausible futures.

However, the chosen research approach also has several shortcomings.
First, it proved difficult to quantify the relationships for some components of the social-technical system. Many assumptions had to be made regarding the behavior of the industry and the way investment decisions are made in reality. The interviews held among the industry could only help structuring these relationships only to a limited degree. A more collaborative and participative modelling approach would certainly have benefited the quality of the model as this would have allowed a more extensive validation of the model.

Second, the relevance of the feedback loops identified in Section 5.2.5 could be questioned as Sections 6.2 and 6.3 did not reveal whether these loops are determinant for the system's behavior. In the case of two out of four loops (the grid connection costs loop and the residual gas loop) the external factors affecting these loops appeared not to be very influential on the system's behavior.

Third, a tension exists between the continuous nature of SD and the discrete nature of real-world actor decisions. While in reality investment decisions are taken at discrete moments in time, they are modelled to adapt continuously to market developments. Moreover, capacity acquisitions occur in discrete amounts within discrete time windows, as installations or parts of installations are retrofitted in their entirety within certain time windows determined by the turnarounds. In the model, however, capacity acquisitions occur unit by unit at each time instant.

Fourth, a tension exists between the high aggregation level of SD modelling and the research scope. By limited the scope to three types of installations possible interactions originating from the integration of systems onsite are ignored. Furthermore, limiting the scope to electrification also implies interactions between different transitions in the industry are not taken into account: i.e., circularity and hydrogen-fuelled cracking. Such interactions do affect the business case for electrification as became apparent from the interviews held among the industry (Interviews, 2021).

7.5 Limitation of this research

In the following, limitations of the research approach are discussed. Some limitations are related to the analyses performed (see Section 7.5.1), others to the usage of system dynamics as a modelling method; (Section 7.5.2). The limitations related to the modelling assumptions made are discussed in Section 7.5.3).

7.5.1 Limitations of the analyses

As part of Exploratory Modelling & Analysis several different analyses were performed: scenario discovery, global sensitivity analysis through Extra-Trees feature scoring and robust policy search using multi-objective robust optimization. These kinds of analyses have several limitations, which are discussed below.

1. Quality of the uncertainty and decision spaces. Though in the analyses the uncertainty and decision spaces are thoroughly explored through sampling, the setting of those spaces is still quite arbitrary. Therefore, there remains uncertainty about whether the selected uncertainty and decision spaces are an accurate representation of what is plausible. Setting the decision space in consultation with policymakers would definitely have benefited the quality of the decision space.

2. In the experiment design of the exploratory analyses no distinction is made between the inherent uncertainties related to the plausible future states of the world and the uncertainties concerning the structure of the system, e.g. economic lifetimes of installations and investment costs of conventional technologies. These latter factors are denoted as uncertain because not sufficient information about the system exists to include them as fixed parameters in the model. Hence, including these factors as uncertainties makes the uncertainty space larger than the uncertainty space is in reality to the industry and policymakers.

3. Only relative system performance has been studied. Because no explicit goals have been formulated regarding the KPIs (emissions, production costs and policy costs) only relative system performance has been studied. Formulating concrete goals in consultation with the industry and government representatives regarding the KPIs would have solidified the selection of robust policies. This would have required more extensive stakeholder collaboration and involving stakeholders in the modelling process.

Specifically with regard to the robust policy search the following limitations should be mentioned.

1. The multi-objective robust optimization is not conclusive. Due to the large computational time required for the optimizations, the number of function evaluations had to be limited. As a result, the optimizations have not fully converged. Therefore, there is no certainty that the Pareto-approximate set is sufficiently close to the theoretical Pareto-optimal front.

2. The number of solutions yielded by the multi-objective robust optimizations is rather large. Feeding all of this solutions back into the simulation model would have generated to big of a database of simulation outcomes. Therefore, a selection of 21 policies was made based on visual analysis. This visual analysis is not rock-solid; the possibility that there exist policies that are deemed more favorable cannot be excluded.

3. Three robustness metrics were considered in the multi-objective robust optimization. The results of robustness metric 1 have been proven not to be very useful. Moreover, not all results of robustness metrics 2 and 3 lead to desirable results. Hence, including more robustness metrics would have benefited the robust policy search by ensuring a greater diversity of robust solutions.

7.5.2 Limitations of system dynamics as a modelling method

The continuous nature of the SD modelling method poses a limitation in the sense that discrete events, decisions and processes cannot be modelled accurately. For example, scheduled turnarounds are discrete events in time. Investments are discrete and such are the retrofits of the installations considered.
In the model, however, the turnarounds are approximated by higher-order time delay equal to the turnaround time. Capacity acquisitions, which consist of a discrete number of MWs, are rather added continuously, that is, MW by MW instead of in discrete MW steps like in reality. Moreover, investments are modelled as a continuous process. Investments in either conventional or electric retrofits continuously adapt to changes in the costs ratio of conventional versus electric costs, while in reality investments are the result of decisions at discrete moments in time.
This last aspect also implies that industrial decision-makers are rational actors who have perfect knowledge of the developments in costs at any moment in time. In fact, uncertainties about future developments have an impact on their decisions. Moreover, they are likely not solely driven by the costs of electrification. They may pursue (or postpone) electrification out of a broader strategic interest or intrinsic motivation for sustainability, or pressured by external factors such as shareholders' attitudes.

7.5.3 Limitations of the model implementation

There exist also several limitations related to the way the model has been implemented.

1. The scope of the model is limited to three types of installations at the naphtha cracking plant. It is questionable whether the development of electrification for these three installations can be considered separately from the other installations onsite as these processes are all highly interconnected. Moreover, there exists a high degree of interconnectivity between chemical production sites and other industrial sites, which are often physically concentrated in clusters (den Ouden et al., 2018; Interviews, 2021).

2. Electrification is just one of the decarbonization pathways in the industry, along with increased industrial symbiosis, energy efficiency improvements, feedstock decarbonization, CCUS, geothermal energy and bionenergy. Though energy efficiency improvements have been modelled, it could be questioned whether it is useful to design policy based on these two decarbonization options only. Possible interactions between these decarbonization pathways should still be considered in policy design. Moreover, though industry representatives discarded the option of hydrogen cracking as being "inefficient" (Interviews, 2021), it is still a possible route for the decarbonization of naphtha crackers (Chang, 2021) and should remain on the table for continued research.

3. The installations included in the model and the available technologies for retrofitting these installations are considered at a rather high level. For example, no distinction is made between different types of furnaces and compressors, which could feature different per MW costs. For example, Shell has recently replaced sixteen small furnaces by eight bigger furnaces (Shell, 2020). Moreover, often multiple retrofit options exist. For example, one could replace an entire furnace or just part of it, e.g. the heat supply system (Interviews, 2021).

4. Regarding investments, only the costs for the separate installations are considered. Costs incurred by electrification, such as adjustment costs for the steam and methane cycles, have not been taken into account. Hence, the business case for electrification may appear more favorable than in reality.

5. The increasing intermittency of the electricity supply due to a rising share of renewable electricity, which poses a concern for the industry as cracking requires a baseload provision of energy, has not been taken into account. Hence, the potential barrier this poses for electrification has not been included in the model.

6. As emphasized by the industry the retrofitting of installations central to the process feature significant operational challenges. As the duration of the interruption of the process should be minimized maintenance and replacement operations have to be performed in a 6-7 week time window, which occurs every 6-7 years. The implications with regard to project planning and financial consequences of the interruption of the process have not been taken into account (Interviews, 2021).

7. Project lead times have been modelled rather optimistically. According to Scholten et al. (2021) electrification requires upgrades in the grid capacity and the grid connection and considerable time for planning and engineering, project licensing, subsidy trajectories, financing, construction and connection, each of which may face delays if another element is not completed yet. For hybrid boilers for example, Scholten et al. (2021) reports lead times of 7 to 13.5 years. Such lead times would introduce significant time delays in the model and hence, the modelled progress of electrification.

8. The sufficiency of the grid capacity has not been modelled as this is highly site-specific. For the electrification of furnaces and compressors the industry has indicated that the cracker sites will require a connection to the EHV grid (Interviews, 2021). These connection costs have been taken into account. However, for this connection to be established there should be sufficient capacity on the local grid.

9. Prices have been assumed to increase linearly at a constant rate, while in reality prices fluctuate. Also, there exists high uncertainty about the development of prices in the long term. Therefore, it is questionable whether the trend towards projected prices in 2030 can be extended towards 2050. Hence, the development of the business cases for electric and conventional retrofitting, respectively, may not have been modelled accurately.

10. In the model it has been assumed that certain key technologies (such as electric cracking and electric boilers for HHP steam) will become available on the short term. However, it is uncertain whether these technologies will indeed reach a commercial breakthrough on the short term, affecting the prospect of profound decarbonization.

11. The market for high-value chemicals (most importantly ethylene and propylene) has not been modelled in detail. It has been assumed that prices for high-value chemicals and therefore the revenue for the cracking industry remains constant over time. In fact, this market is dynamic and subject to developments in circularity, posing an additional uncertainty for decision-makers in the industry (Interviews, 2021).

12. Revenues have not been modelled. In the costs comparison of retrofits, only the operational expenses and capital expenses have been taken into account. Revenues originating from the sale of high-value chemicals have not been modelled; it is assumed the production volumes of the high-value chemicals (ethylene, propylene etc.) remain the same after electrification. However, as a matter of fact, electrification of furnaces may affect the production output and the share of each chemical in the total production volume. Therefore, revenues either increase or decrease, research is still being done into these effects (Interviews, 2021).

13. Energy taxes have been modelled as being constant over time. In reality, taxes will not change abruptly but are likely feature a gradual shift.

14. No interactions or coupling effects between external factors and policy options have been considered. For example, in reality a coupling between the prices of naphtha and gas might be expected. Also, the electricity market price is not independent of the availability of renewable electricity. Moreover, the SDE++ subsidy is linked to the availability of renewable electricity.

15. The policies included in the model are not adaptive: they do not respond to changes in the system. In reality, however, the government is likely to adjust its policy based on the progress of electrification. In fact, the need for adaptive policy has been emphasized by Johansson et al. (2018) and Bataille (2020).

7.6 Recommendations for policymakers

Based on the results the following recommendations to policymakers are made:

1. Policies to accelerate electrification should go hand in hand with a decisive development in renewable electricity sources. Without a sufficient availability of renewable electricity, electrification may actually lead to an increase in emissions in the short term. The availability of renewable electricity is the single most influential factor regarding emission reduction.

2. Include electric compressor turbines in the SDE++. Electrification of compressor turbines seems to be a no-regret electrification option which also reduces the required boiler capacity. However, no category for this technology is included in the SDE++ yet. This suggestion is in line with a recent TNO study (Sebastiaan Hers and Ton van Dril and Adriaan van der Welle, 2021) that also suggests expanding the SDE++ to include electric compressor turbines.

3. As the required increase in the SDE++ base fee foreseen by the suggested robust policies may not be accommodated by the current SDE++ system, consider implementing a novel subsidy instrument, such as an investment subsidy, in collaboration with the industry.

4. Consider phasing out the dispensation rights (DPRs) that are part of the current carbon levy system. If the DPRs are not phased out, the carbon levy should increase significantly faster after 2030 to accelerate electrification.

5. To stimulate electrification a more extensive fiscal shift is required favoring electricity consumption and discouraging gas consumption. Hence, electricity taxes need to decrease while gas taxes need to increase.

6. As the future energy market is highly dynamic, make sure policies to accelerate electrification are adaptive and are able to respond to changes in the market.

7.7 Recommendations for further research

With regard to further research the following recommendations are made:

1. Extend the system dynamics model by including more installations onsite and consider integration of systems both onsite and between sites in production clusters. In this way, the implications of electrification for industrial ecosystems, including the financial consequences they involve, can be studied. An example are the adjustments that are required in the methane and steam cycles as a result of electrification at naphtha cracker sites.

2. Develop a model which allows the specification of adaptive policy options. In this way recommendations can be given about the design of adaptive policy.

3. In further research involving exploratory modelling to study decarbonization of (energy-intensive) industries it is advised to make the exploratory modelling approach participatory. In this way uncertainty and decision spaces can be set together with stakeholders, for example. Moreover, it may improve the quality of the model.

4. Diversify the electrification options for each installation and include additional decarbonization options in future models, such as hydrogen cracking, Carbon Capture, Utilization & Storage (CCUS) and feedstock decarbonization. In this way, multiple decarbonization pathways can be explored and electrification can be considered in relation to these pathways.

5. Include national costs as a key performance indicator rather than production costs and policy costs separately. National costs, a common concepts in policy studies done by PBL, represent the balance of costs and benefits of certain policy for society as a whole. Moreover, the concept of national costs is broader than just monetary costs and often also incorporates air quality and environmental damage (Koelemeijer & Strengers, 2020). Hence, using the concept of national costs gives insight in which policy options are most beneficial for society and as such, offers a more integral approach than just considering production costs and policy costs.

6. Include the product side of the industry in future models. As electrification may impact the composition production output (Interviews, 2021) it is relevant to consider how revenue changes as a consequence of electrification. Moreover, developments in the high-value chemical markets, such as circularity, may impact the development of electrification as well (Interviews, 2021).

7. Consider the adjustment costs that electrification induces for integral systems onsite, such as the methane cycle and the steam cycle. In this way, the business case for electrification can be estimated more accurately.
8. Include potential delays induced by grid capacity upgrades in future models. The lead times of grid capacity upgrades may pose a significantly delay to electrification; it would be worthwhile to explore these effects with regard to emission reduction.
9. Repeat the multi-objective robust optimization of policies while including more robustness metrics. In this manner, a better comparison of the performance of robustness metrics can be made and a greater diversity of robust solutions is ensured. Moreover, increase the number of function evaluations to reach greater certainty that the Pareto-approximate set has sufficiently approached the theoretical Pareto-optimal front.

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A Further background on electrification strategies, application areas and technologies

The deployment of electrification features several alternatives; different strategies, application areas and technologies can be distinguished. An overview of strategies and application areas is provided in Figure 67.
We can distinguish between *baseload electrification* and *flexible electrification* (den Ouden et al., 2018). Baseload electrification means that installations rely on the supply of (renewable) electricity on a full-time basis. Though this electrification strategy has a higher CO_2 reduction potential, it is geared less to the expected larger fluctuations in the future electricity supply. During drops in the supply of renewable energy, other sources of electricity will be needed in order to sustain the operation of installations (den Ouden et al., 2018).

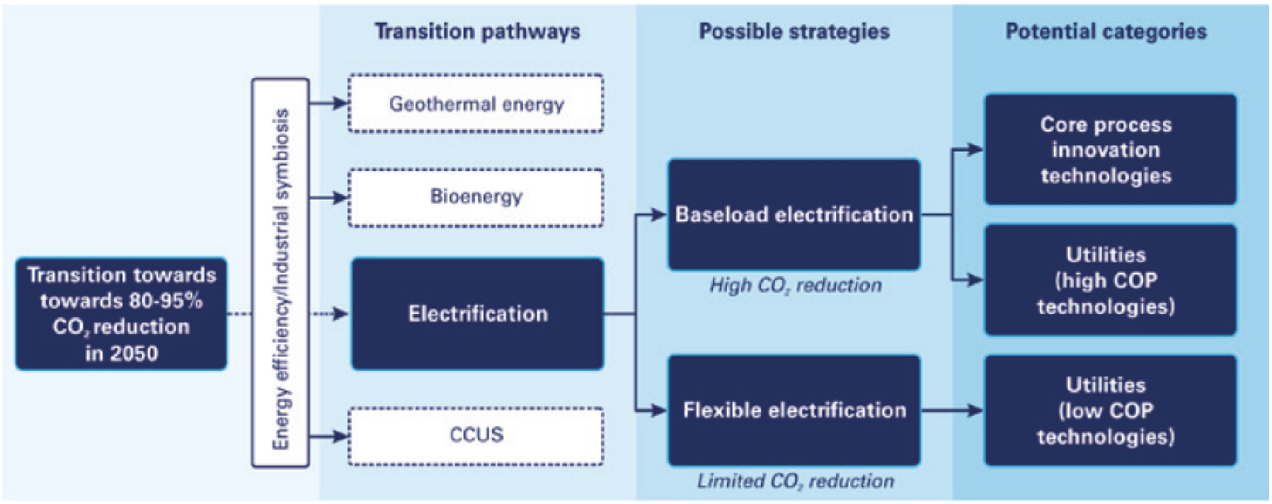

Figure 67: Overview of electrification strategies and their application areas inside the chemical industry. Source: den Ouden et al. (2018).

Flexible electrification, on the other hand, means that installations operate on (renewable) electricity on a part-time basis. In this case, installations use renewable electricity when there is sufficient supply and thus, electricity prices are low. Instead, during lower availability, installations will switch to other sources of electricity or will curtail production. This flexible operation is called *load shifting* (van Kranenburg et al., 2016). With flexible electrification, chemical plants are able to respond to fluctuations in the supply of renewable energy and at the same time, gain profits in times of low electricity prices. This specifically enhances the attractiveness of technologies with a low operational margins, such as electrolysers for the production of hydrogen. These technologies are denoted by "low COP", Coefficient of Performance, in Figure 67, though this concept is usually applied describe the efficiency of heat pumps (Industrial Heat Pumps, n.d.). Technologies with a low COP have high operating costs and hence, low operational margins. Such technologies prompt for flexible electrification since it allows for exploitation of the expected larger fluctuations in electricity prices to increase operational margins. In this manner, the economic attractiveness of technologies with a low COP and operational margins, can be increased (van Kranenburg et al., 2016; den Ouden et al., 2018).

Baseload electrification can be applied in core processes, requiring a turnaround in the process. This is also called direct electrification, as described earlier in Section 2.1.3. It can also be applied in utilities, i.e. facilitating systems not core to the process. Indirect electrification is a designation for this type of electrification. As opposed to flexible electrification, baseload electrification is logically applied in utilities with a high COP since the adoption of such technologies is not incentivized by fluctuating electricity prices (den Ouden et al., 2018).

For the chemical industry various electrification technology types are of interest. A schematic overview is provided in Figure 68. Below follows a description of each technology type and their potential and limitations.

Power-to-Heat (P2H) involves the use of electricity to produce heat, either directly or by upgrading waste heat to useable temperature levels. By recycling heat in this manner, P2H can yield an important contribution to circularity. Combined with energy efficiency gains this grants P2H considerable advantages. Among the

electrification technologies, P2H is the furthest developed, having a high technology readiness level. Certain applications are already commercially available. Therefore, P2H is expected to reach a large-scale breakthrough in the short term. However, the application of P2H is currently limited to low temperatures (¡200°C) while 65% of the final energy use for heat is for temperatures above 200°C.
Certain P2H technologies (Mechanical Vapour Recompression, or MVR) are only suitable for baseload electrification while others accommodate flexible electrification (electric boilers) or both (electromagnetic radiation and heatpumps) (van Kranenburg et al., 2016; den Ouden et al., 2018).

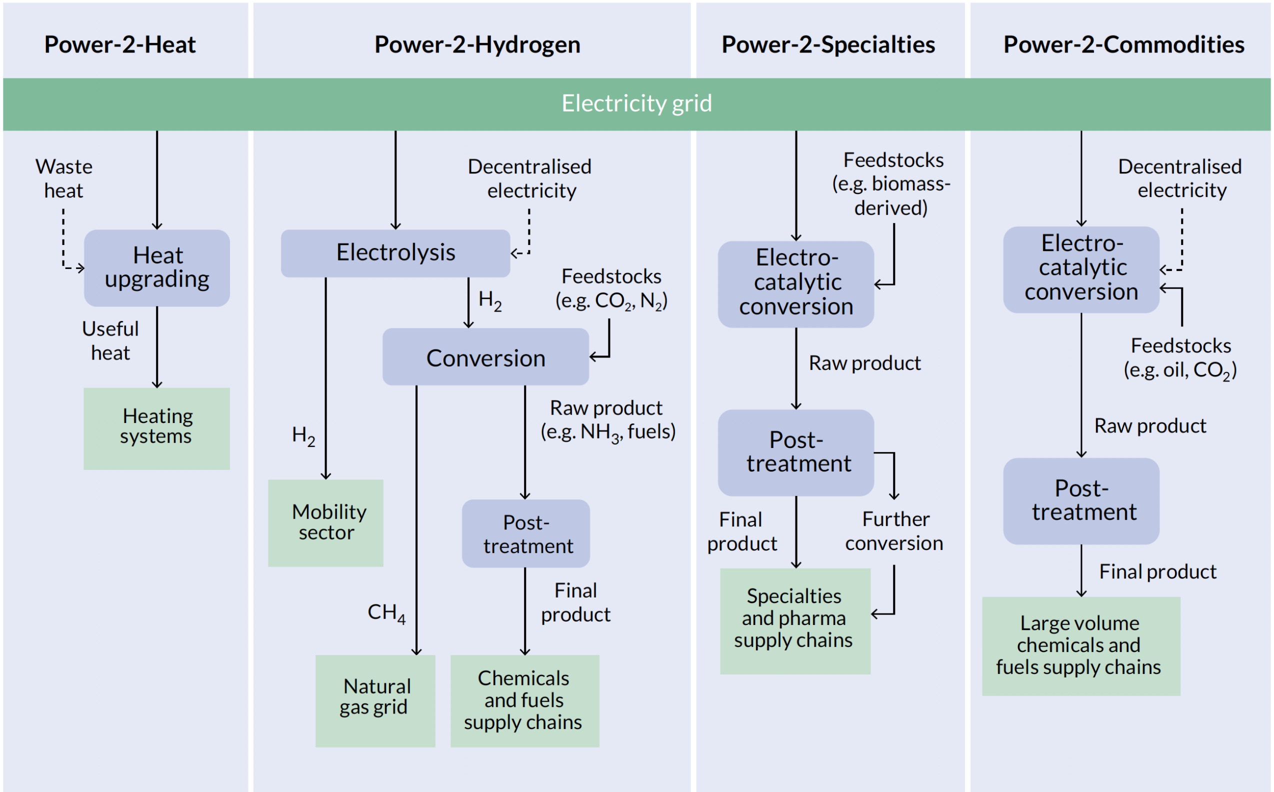

Figure 68: Schematic overview of main electrification technologies of interest to the chemical industry. Source: van Kranenburg et al. (2016).

Power-to-Hydrogen (P2H2) involves the use of electricity to carry out electrolysis of water to produce hydrogen, which can be used for different purposes: as feedstock for chemical processes, as energy storage capacity or as fuel. Hydrogen can also be converted to produce green natural gas (methane or CH_4) by chemically synthesizing it with CO_2. This process is often denoted as a separate technology type called Power-to-Gas (P2G). P2H2 has a high potential but is not yet commercially viable for large-scale application due to the high operating costs of electrolysers. It is therefore only expected to play a role on the long term (10-30 years). On the other hand, through flexible electrification electrolysers can exploit low electricity prices in order to increase operational margins (van Kranenburg et al., 2016; den Ouden et al., 2018).

Power-to-Specialties (P2S) involves the use of electricity to carry out electrochemical synthesis to produce high-value fine and specialty chemical intermediates and products. Electrochemical synthesis produces chemical with higher purity and offers opportunities for the production of new chemicals that are too costly to produce with conventional technologies. Hence, P2S fosters innovation and can increase the competitiveness of the chemical industry. P2S also reduces feedstock demand and waste. However, because specialties are produced in such small volumes, P2S will not lead to a major reduction CO_2 emissions. Though P2S is already applied in some companies, widespread adoption only expected within 5-10 years (van Kranenburg et al., 2016; den Ouden et al., 2018).

Power-to-Commodities (P2Com) is the direct electrochemical synthesis to produce large-volume commodity chemicals using either conventional or sustainable feedstocks such as CO_2. P2C is often taken together with P2S as Power-to-Chemicals (P2Chem). However, since the profit margins for P2Com are lower than for P2S, the adoption of P2Com is driven by different incentives. For instance, reducing greenhouse gas emissions is a main driver for P2Com, which can reduce CO_2 emissions substantially. Another driver is the supply of CO_2 which is expected to increase due to the large-scale deployment of CCUS.

Moreover, P2Com is a promising technology for the chemical industry because it allows for the decentralized production of chemicals that currently need to be transported from central production locations, which sometimes also involves costs for safety measures. It has already been successfully applied at multiple sites in the production of chlorine, a hazardous chemical. The highly automated chlor-alkali electrolysis process avoids high labour costs and reduces transport and handling costs. Moreover, P2Com is especially suitable for flexible electrification.

However, P2Com is expected only to be deployed in the long term (20 years) (van Kranenburg et al., 2016; den Ouden et al., 2018).

B Interview reports (confidential)

This appendix is confidential and only available to academic supervisors. For any further questions, please contact the author.

C Overview of components and subcomponents of the Vensim model

In this appendix an overview of the system dynamics model implemented in Vensim is given. The green-colored parameters represent policy options while the red-colored parameters denote uncertain factors. Grey parameters are so-called "shadow variables" that originate from other model subcomponents.

C.1 Costs component

In the *Costs* component of the model the expected operational expenses (OPEX) for electric and conventional retrofits, respectively, are calculated based on expected energy prices, carbon costs, taxes and subsidies.

C.1.1 Gas costs subcomponent

This subcomponent involves the calculation of the OPEX for conventional retrofits. The structure shown in Figure 69 computes the expectations of the gas price. These expectations are input for the structure in Figure 70, where the OPEX is calculated.

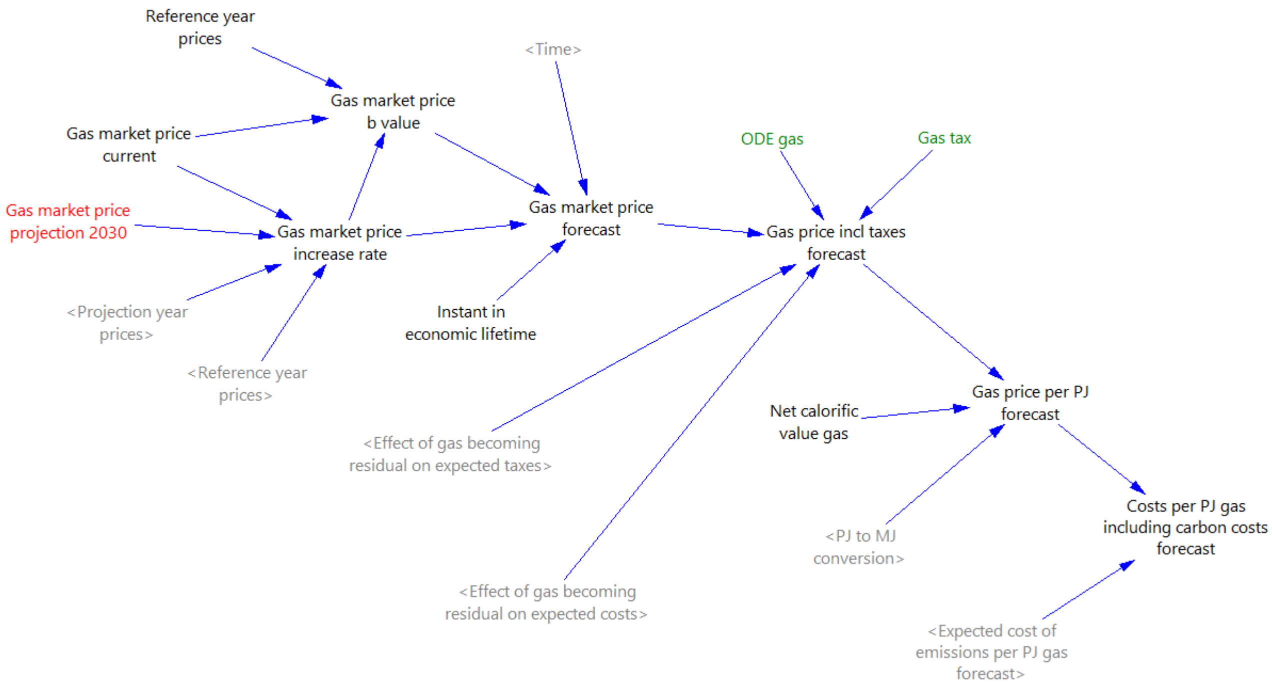

Figure 69: Computation of the gas costs per PJ.

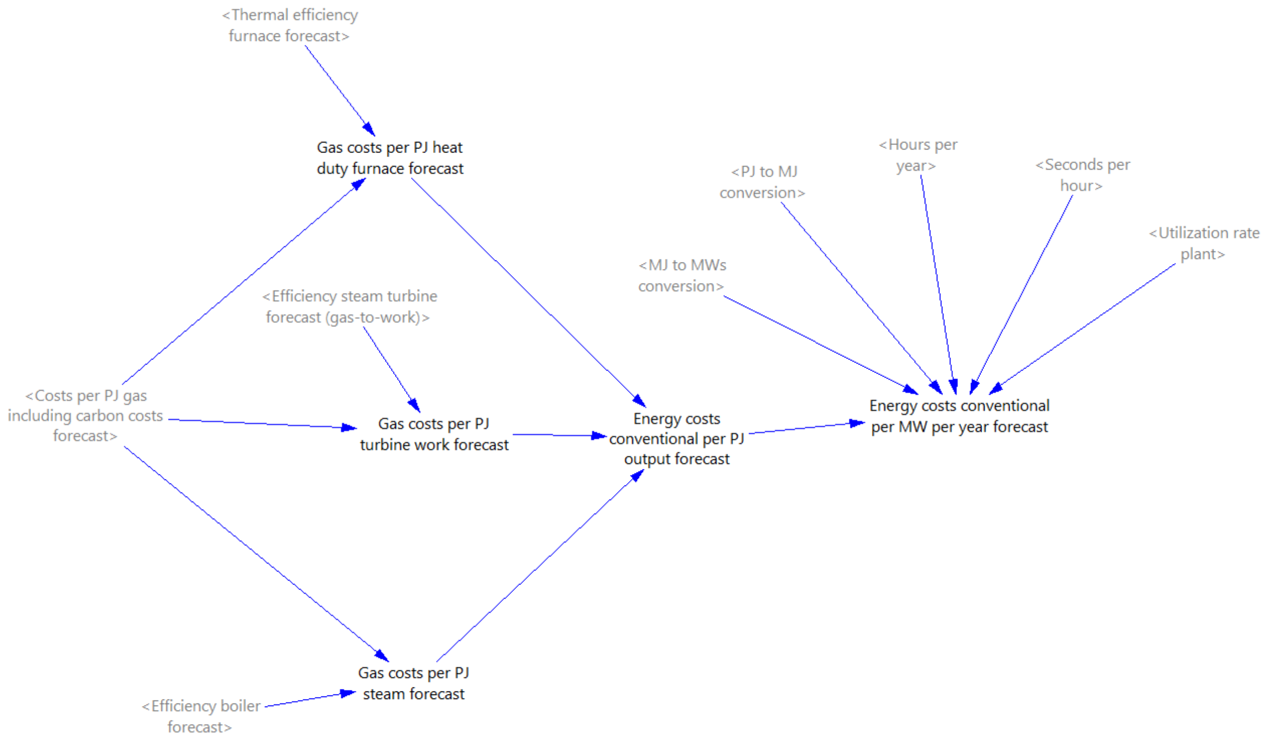

Figure 70: Computation of the energy costs for conventional technologies.

C.1.2 Electricity costs subcomponent

This subcomponent involves the calculation of the OPEX for electric retrofits. The structure shown in Figure 71 computes the expectations of the electricity price. These expectations are input for the structure in Figure 72, where the OPEX is calculated.

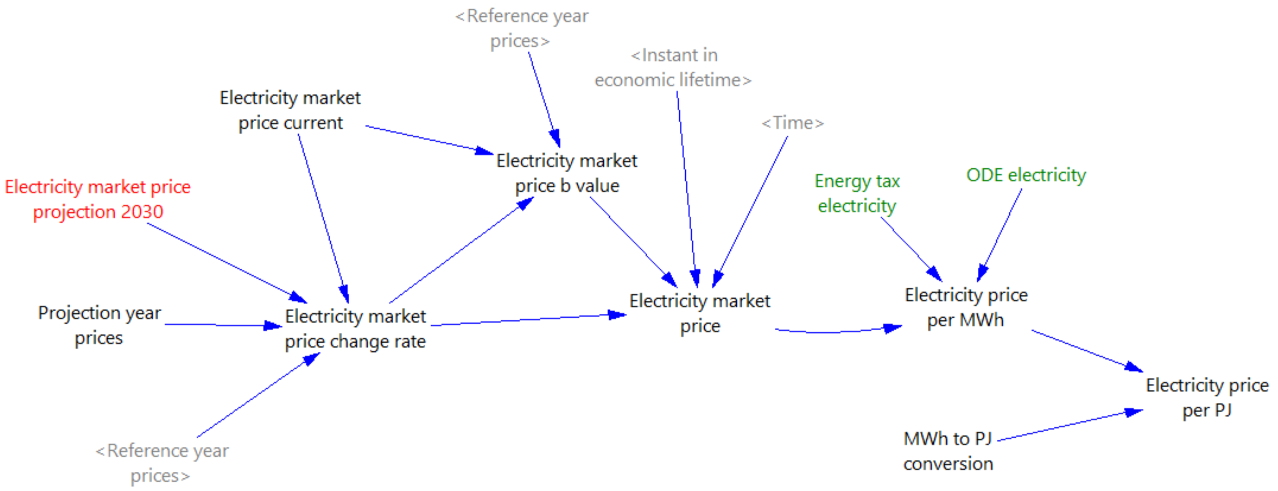

Figure 71: Computation of the electricity price per PJ.

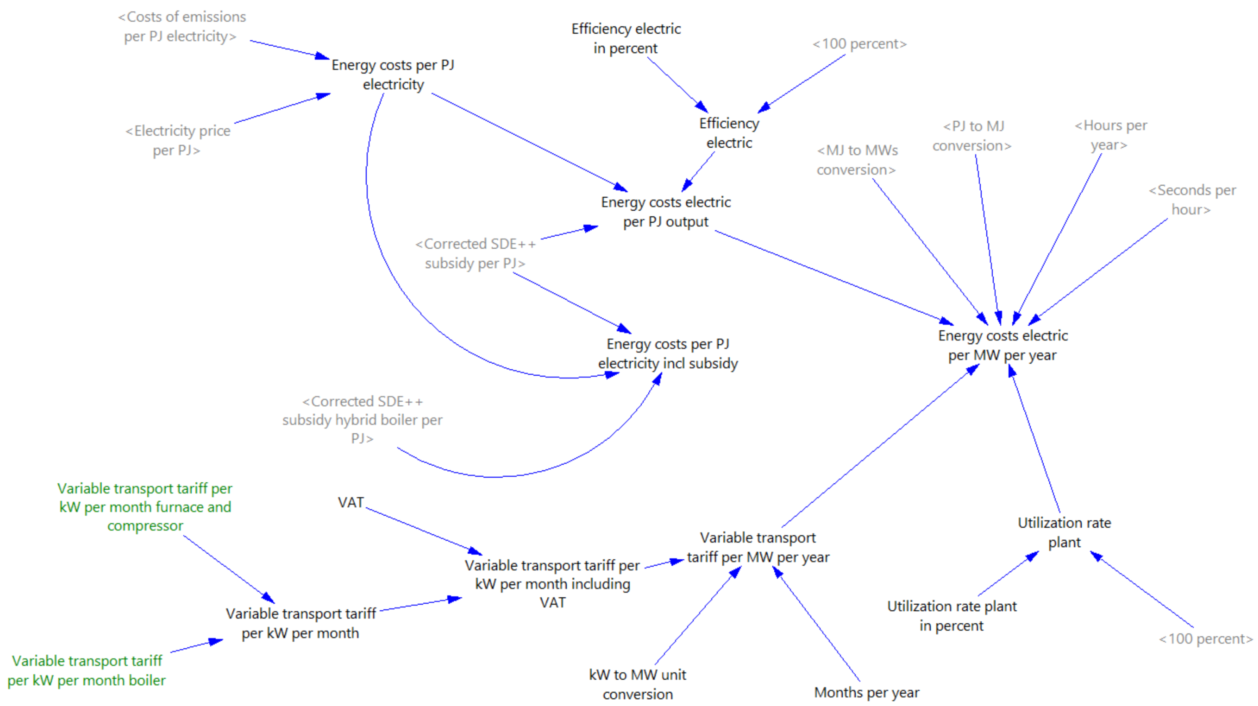

Figure 72: Computation of the energy costs for electric technologies.

C.1.3 Hybrid boiler costs costs subcomponent

This subcomponent involves the calculation of the OPEX for boilers operating in hybrid configuration. Electric boilers in hybrid configuration only operate during the load hours where there is sufficient renewable electricity These load hours are calculated by the structure shown in Figure 73. The OPEX is then computed by the structure shown in Figure 74.

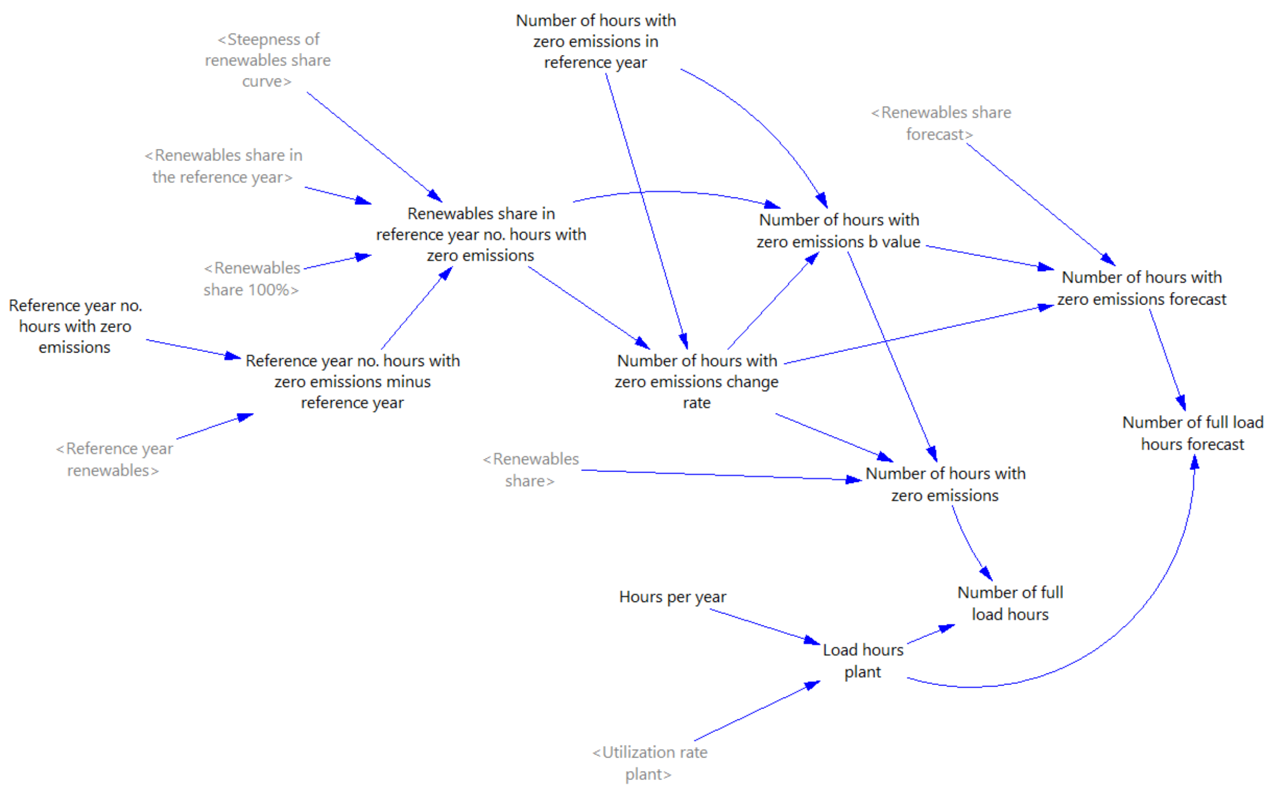

Figure 73: Computation of the load hours of the hybrid electric boilers.

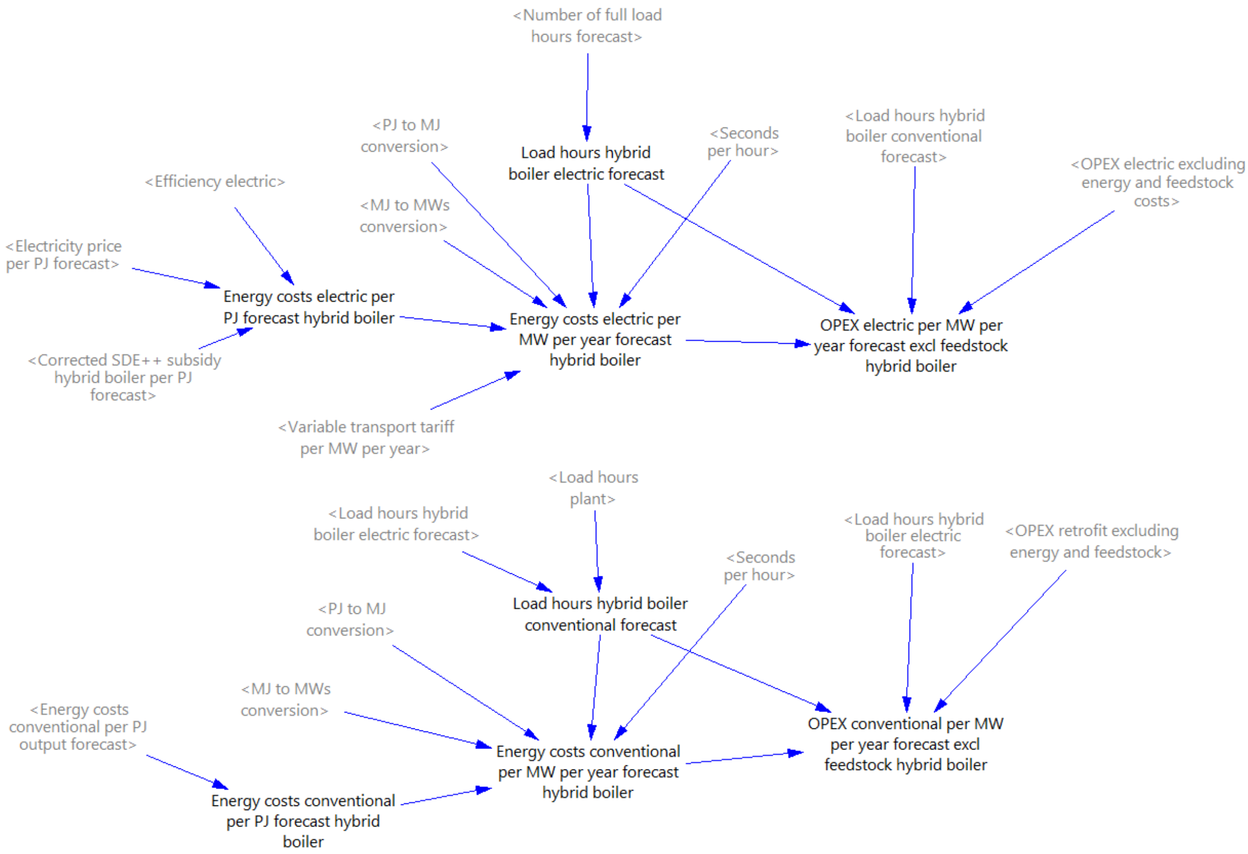

Figure 74: Computation of the energy costs of boiler hybridization.

C.1.4 Carbon costs subcomponent

Carbon costs are input for the OPEX calculations of electric and conventional retrofits and hybrid boilers. Figure 75 shows the calculation of the carbon levy. Using the carbon levy and ETS price as inputs, carbon costs are computed by the structure shown in Figure 76.

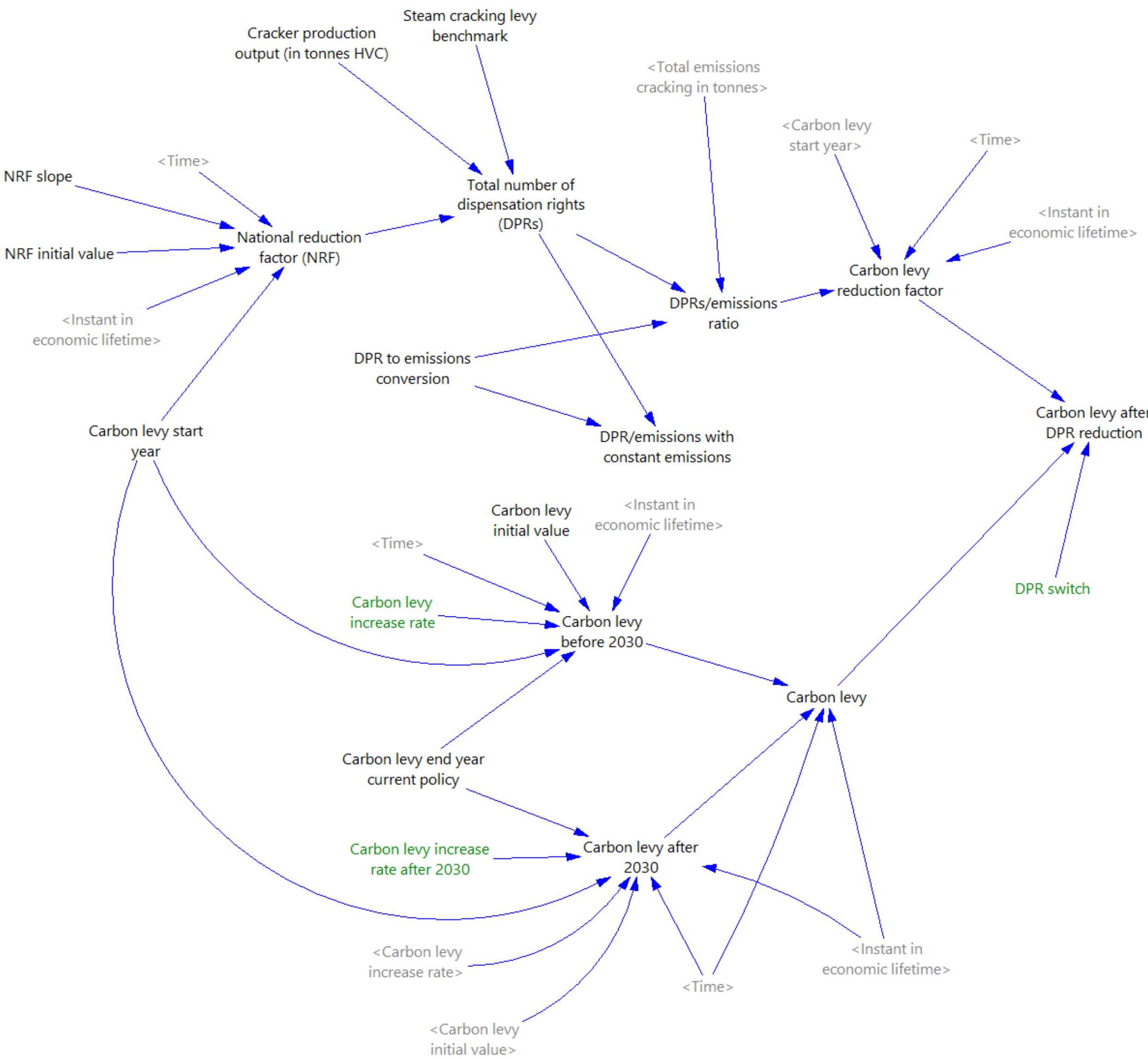

Figure 75: Computation of the carbon levy.

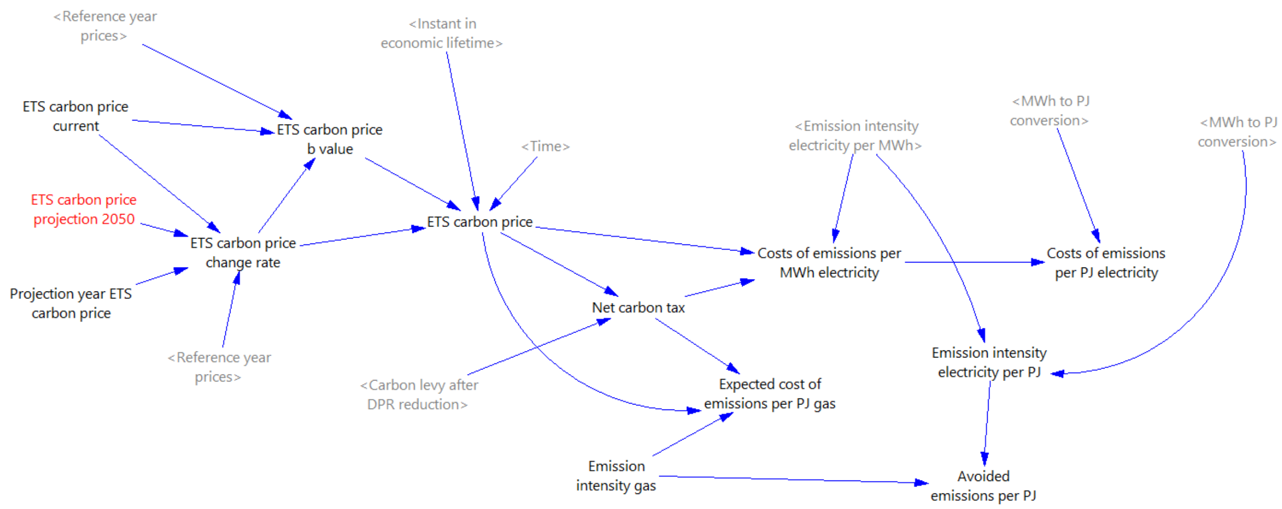

Figure 76: Computation of carbon costs.

C.1.5 SDE++ subsidy subcomponent

The SDE++ subsidy is accounted for in the calculation of the OPEX of electric retrofits (Section C.1.2). Its computation is shown in Figure 77.

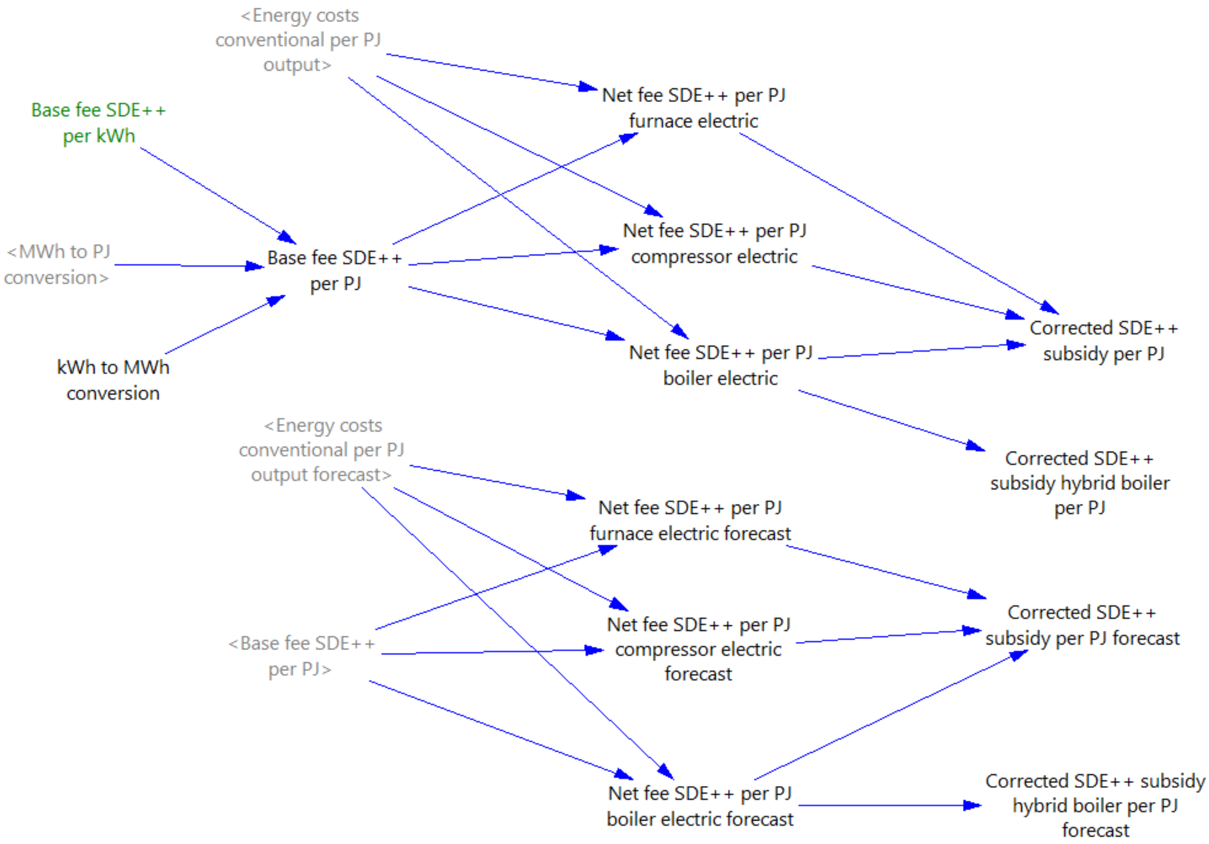

Figure 77: Computation of the SDE++ subsidy.

C.1.6 Efficiencies of conventional technologies subcomponent

The model considers efficiency improvements in conventional technologies. The computation of efficiency improvements is shown in Figures 78 and 79.

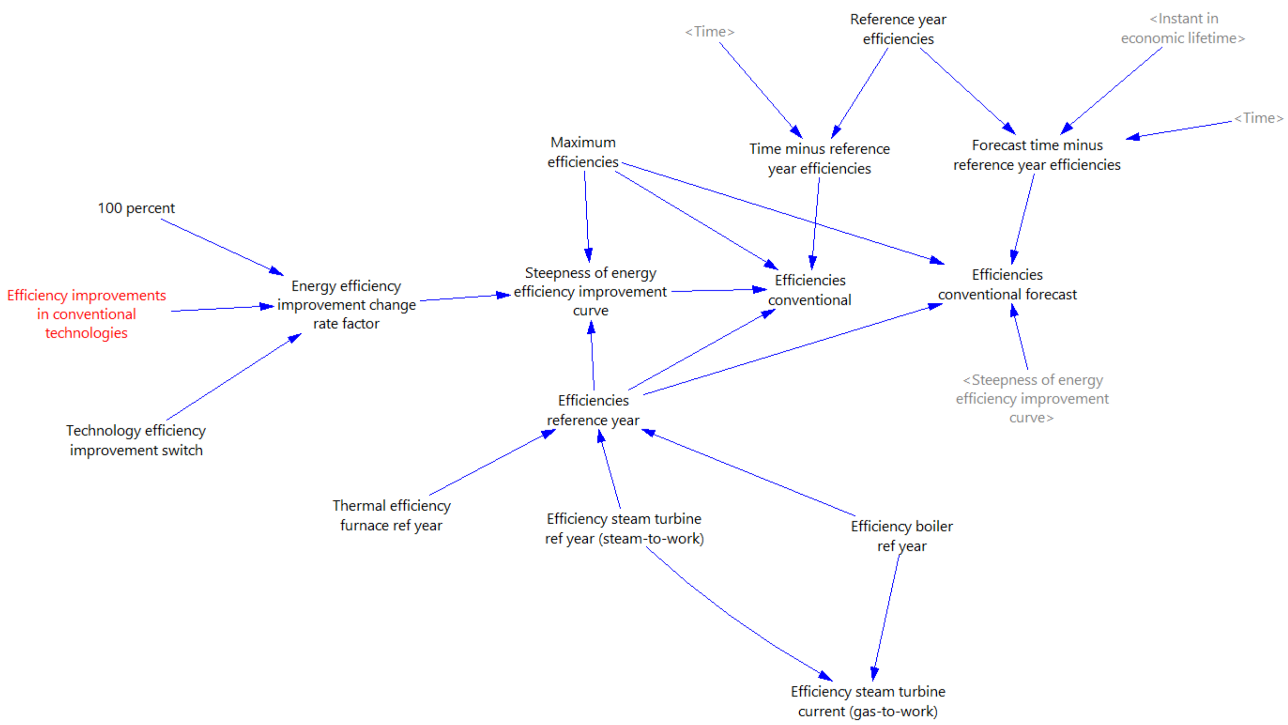

Figure 78: Computation of the efficiencies of conventional technologies, part 1.

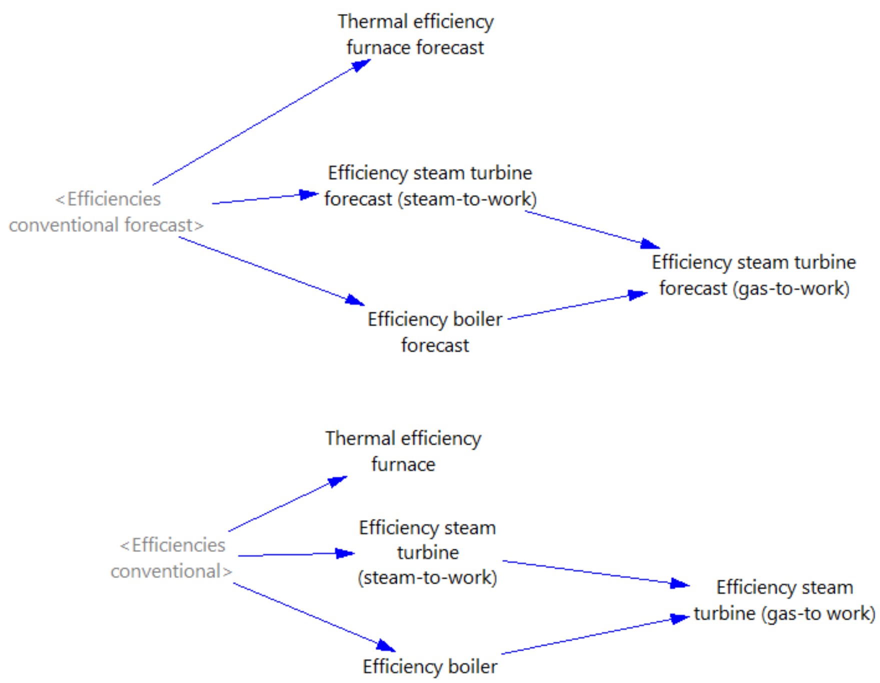

Figure 79: Computation of the efficiencies of conventional technologies, part 2.

C.1.7 Emission intensity electricity subcomponent

The emission intensity of electricity depends on the availability of renewable electricity. These variables are modelled according to the structure shown in Figure 80.

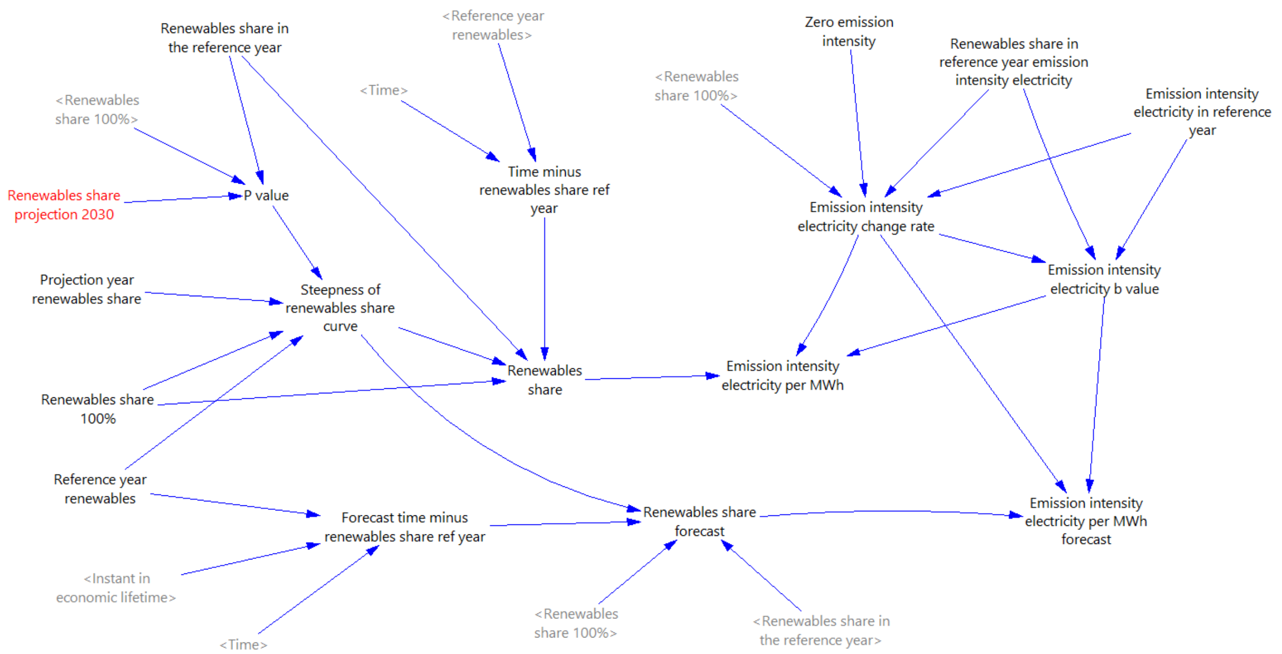

Figure 80: Computation of the emission intensity of electricity.

C.1.8 Value loss of surplus gas subcomponent

In the model, it is assumed that surplus gas will have a lower market value than natural gas. Its value is expressed as a fraction of the value of natural gas. This fraction is computed by the structure shown in Figure 81.

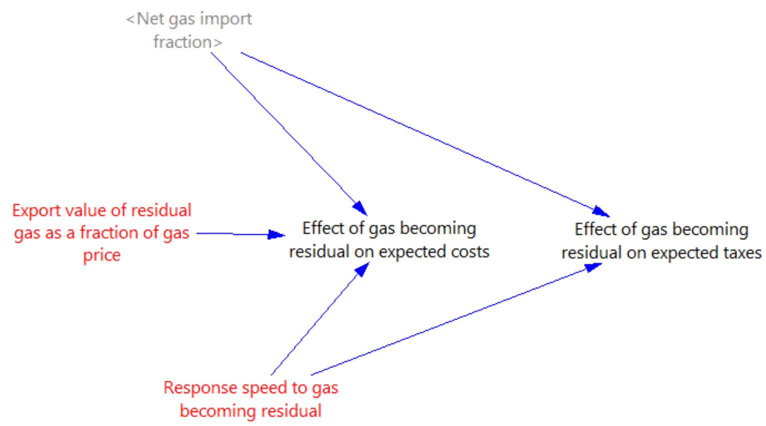

Figure 81: Computation of the value loss due to export of surplus gas.

C.2 Investments component

In the *Investments* component, the cost expectations are translated to investment shares, which determine which part of each investment sum are channeled towards electrification and which is channeled towards conventional retrofitting.

C.2.1 Investments electric subcomponent

Due to technological learning, the investment costs of electric retrofits decrease over time. These calculations are shown in Figure 82.

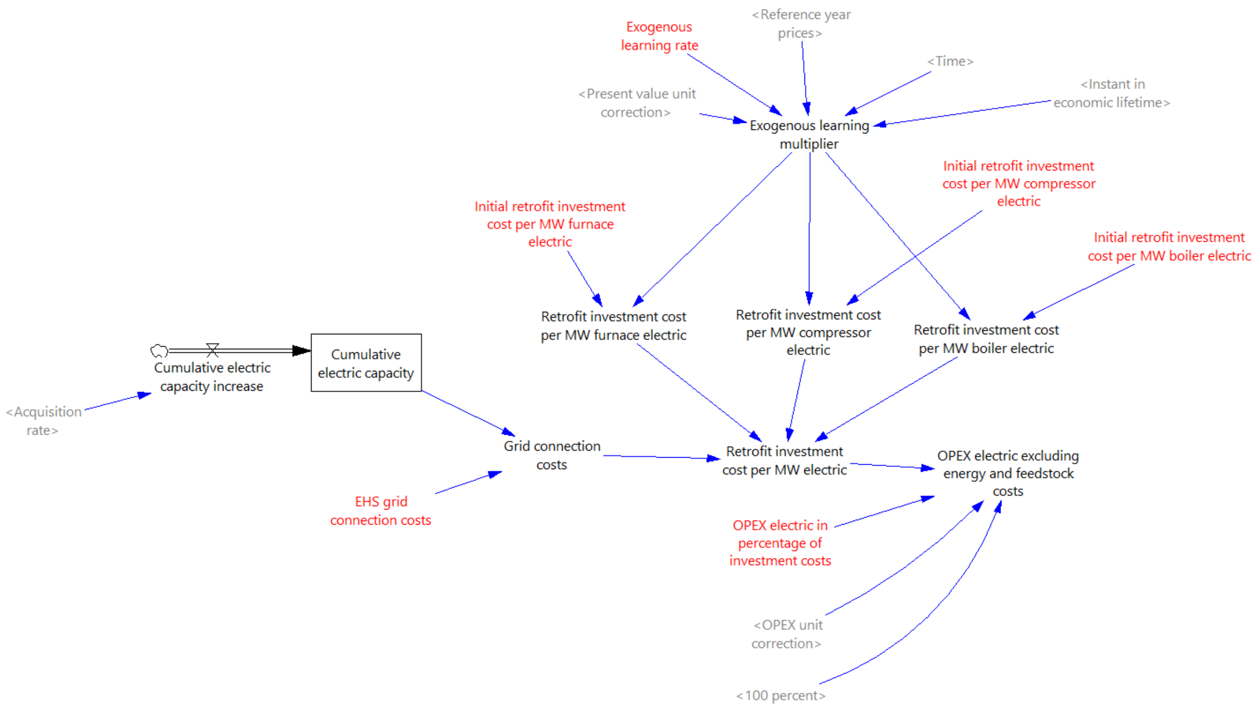

Figure 82: Computation of the investment costs for electric retrofits.

C.2.2 Present value electric retrofit costs subcomponent

Based on the OPEX (Figures 71, 72) and investment costs (Figure 82), the present value of electric retrofits is calculated (see Figure 83).

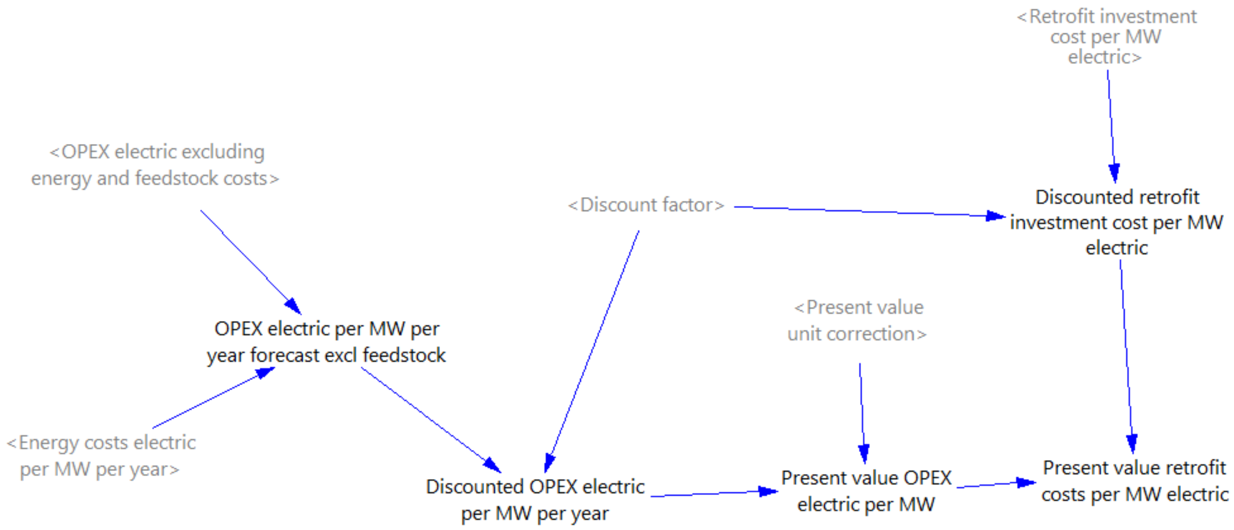

Figure 83: Computation of the present value of the costs for electric retrofits.

C.2.3 Present value conventional retrofit costs subcomponent

Based on the OPEX (Figures 69, 70) and investment costs, the present value of electric retrofits is calculated (see Figure 84).

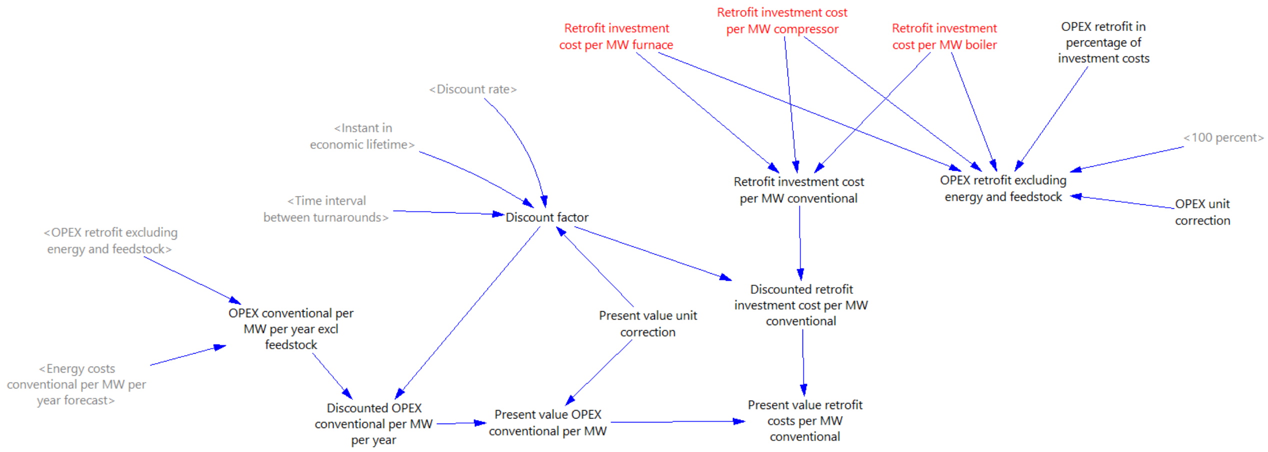

Figure 84: Computation of the present value of the costs for conventional retrofits.

C.2.4 Investment share conventional/electric subcomponent

Based on the ratio of present values for conventional and electric retrofits, respectively, the investment share is calculated (Figure 85).

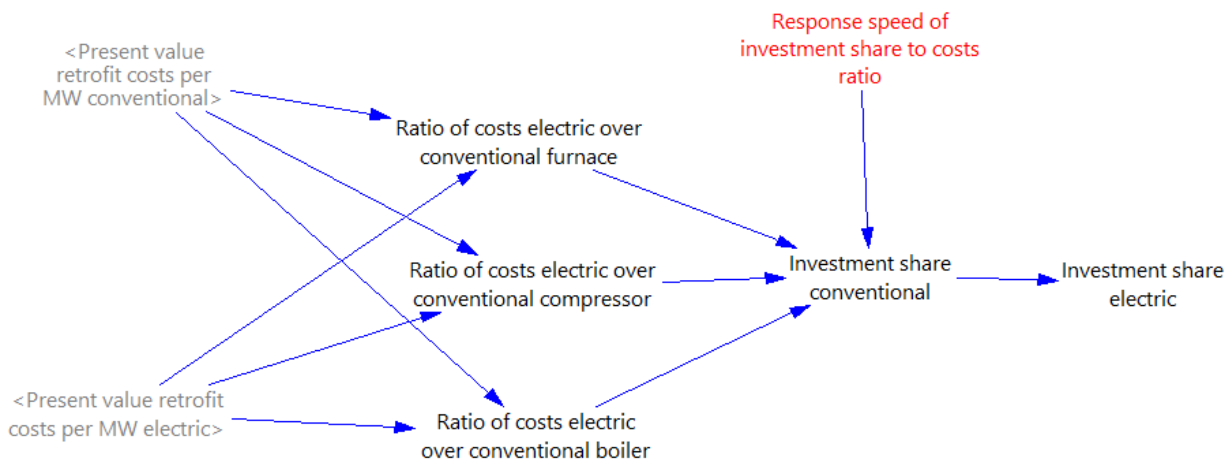

Figure 85: Computation of the investment costs for electric retrofits.

C.2.5 Investment share hybrid boiler subcomponent

Based on the ratio of the present value of the OPEX of gas boilers and the present value of hybrid boilers, the investment share for hybrid boilers is computed (Figure 86).

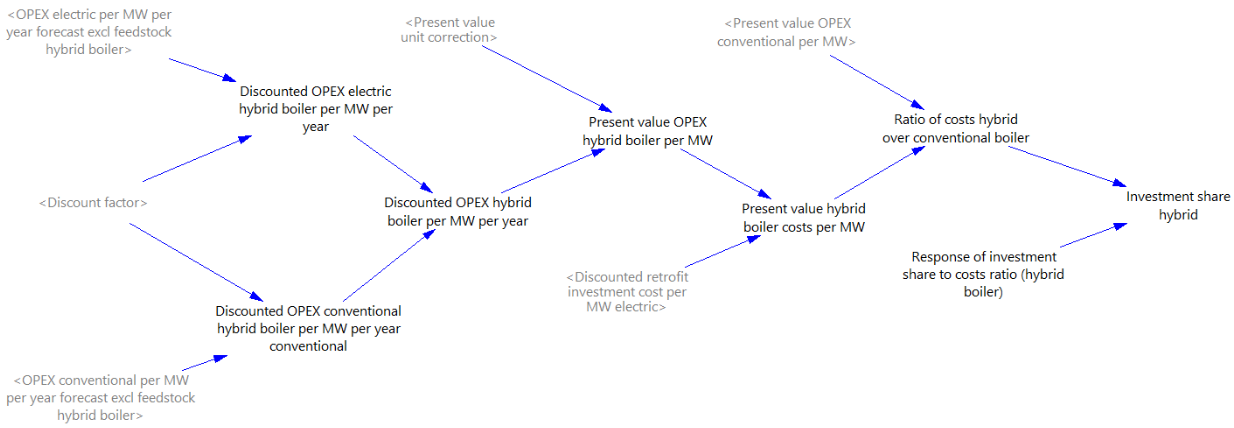

Figure 86: Computation of the investment costs for hybrid boilers.

C.3 Capacities component

The *Capacities* component, investments are translated to capacity acquisitions for each technology. Based on these acquisitions, the model can simulate the development of capacities over time. This affects gas and electricity consumption, which in turn determines the CO_2 emissions of the plant, the production costs and the policy costs: the model output variables. In the following, the computation of capacity acquisition in the model is detailed, followed by the model output variables.

C.3.1 Capacity acquisition subcomponent

This subcomponent models the development of capacities over time by means of a stock-flow structure shown in Figure87.

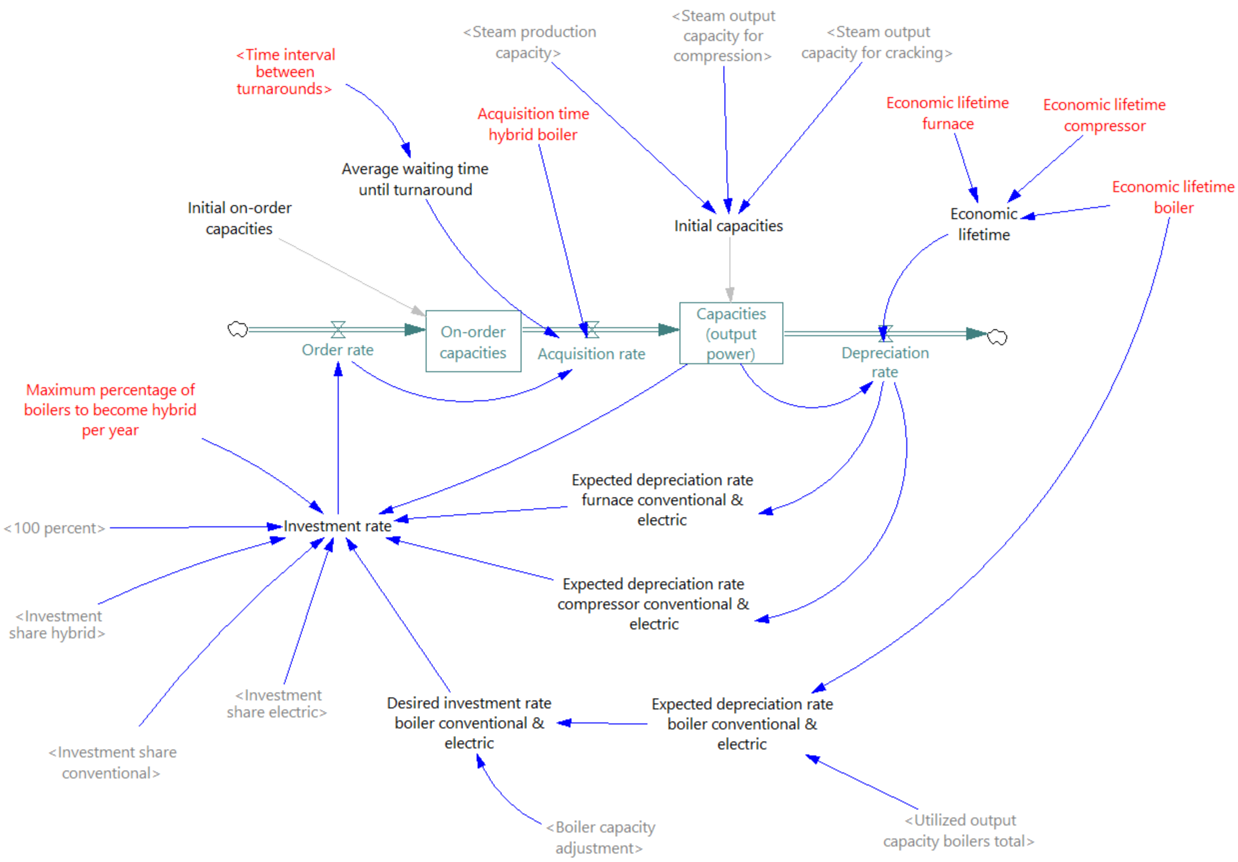

Figure 87: Capacity acquisition and depreciation stock-flow structure.

C.3.2 Boiler capacity adjustment subcomponent

Because an increasing electrification of compressor turbines imply that the steam demand is reduced, this effect needs to be adjusted for in the boiler capacity. With a decreasing steam demand, the boiler capacity is reduced.

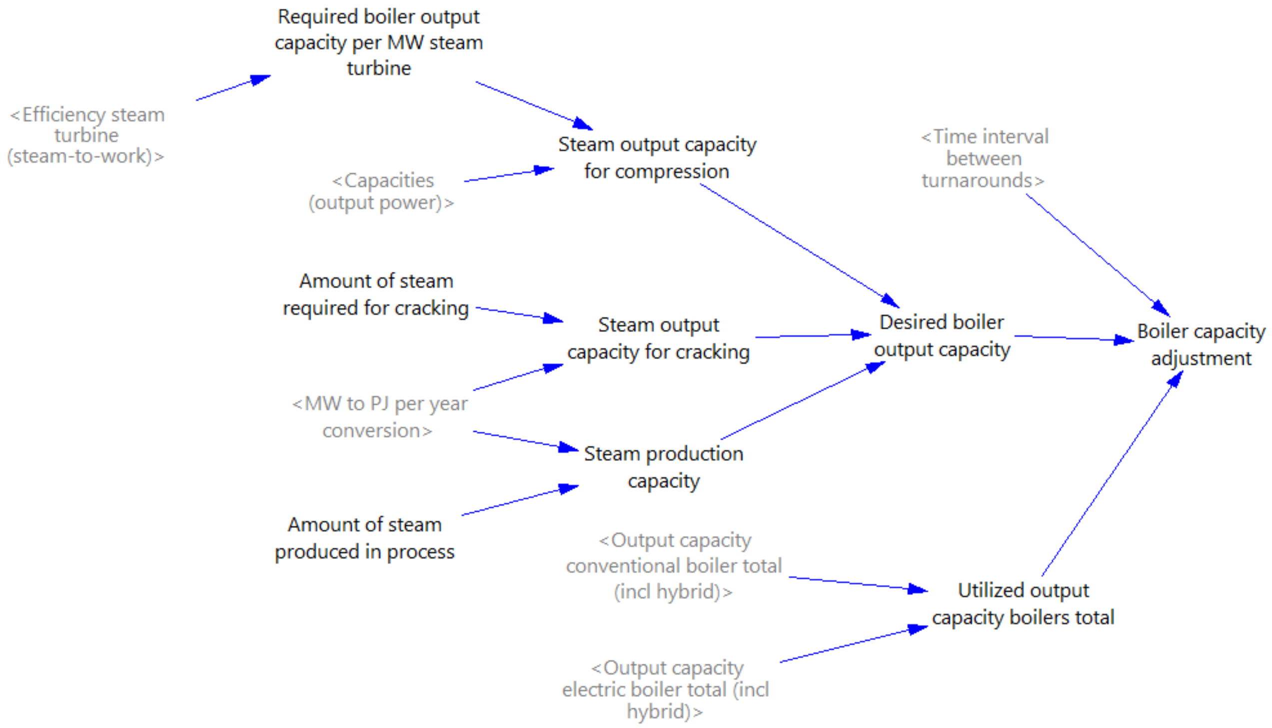

Figure 88: Computation of the boiler capacity adjustment.

C.3.3 Gas consumption subcomponent

Conventional capacities consume gas. However, newer capacities feature improved efficiencies with regard to existing capacities. Hence, the gas consumption is modelled using a co-flow structure (Sterman, 2000) which also computes the aggregate efficiency of the installed conventional capacities.

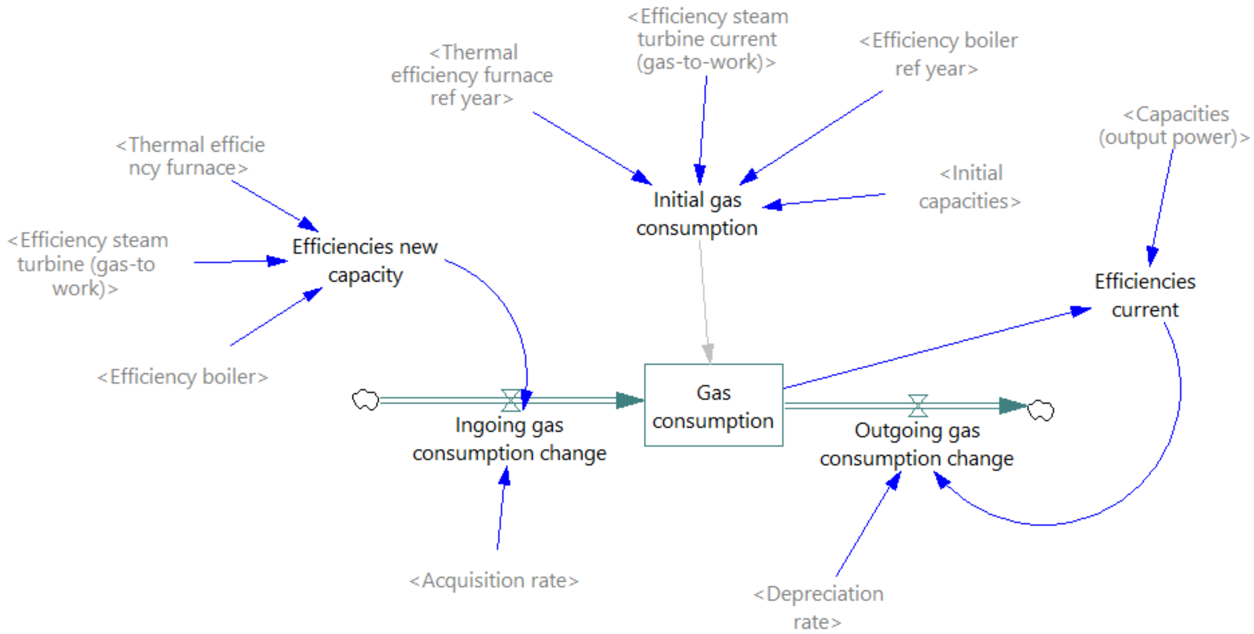

Figure 89: Gas consumption stock-flow structure.

C.3.4 CO_2 emissions subcomponent

Based on electricity consumption and gas consumption and the emission intensities of gas and electricity, CO_2 emissions are calculated. However, first the effective boiler capacity is calculated in Figure 90. As hybrid boilers do not operate full-time, the effective capacity of the installed boilers is lower than the installed capacity. Based on the load hours that hybrid boilers operate, the effective capacity is computed (Figure 90). Then, electricity and gas consumption are computed (Figure 91), which lead to the calculation of emissions (Figure 92).

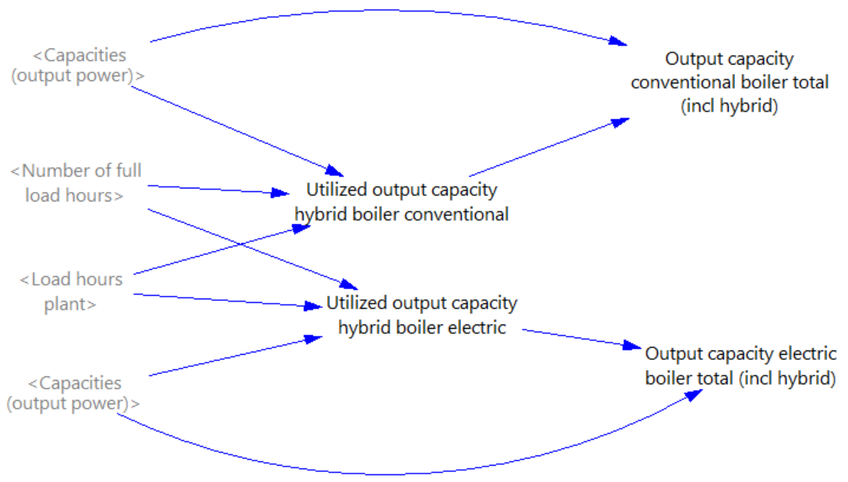

Figure 90: Computation of the effective capacity of hybrid configurations of gas and electric boilers.

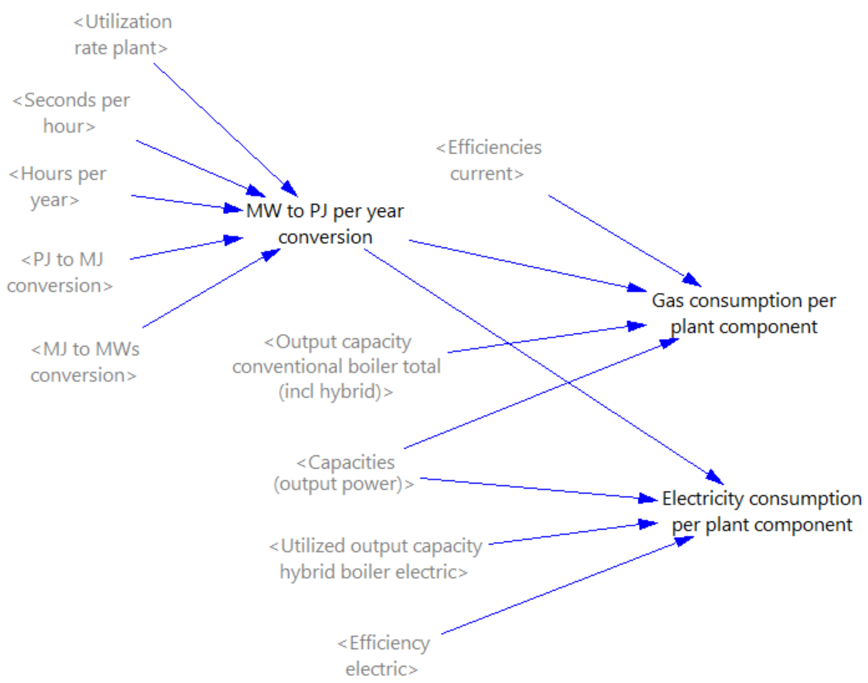

Figure 91: Computation of gas and electricity consumption per plant component.

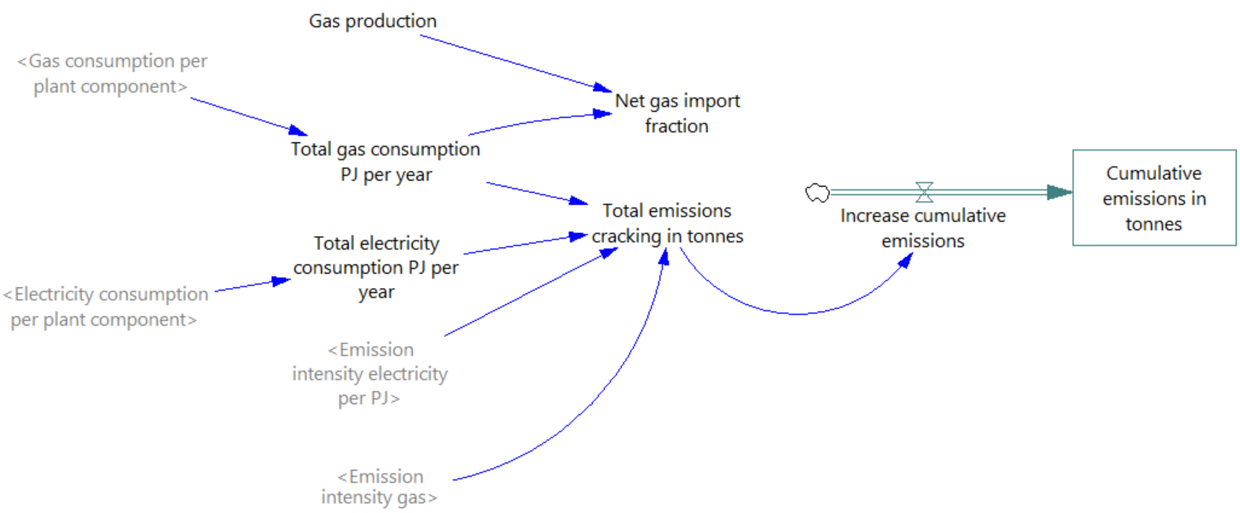

Figure 92: Computation of total emissions and cumulative emissions stock-flow structure

C.3.5 Production costs subcomponent

The production costs take into account OPEX and CAPEX. The total OPEX of the reference plant is computed by the structures shown in Figures 93 and 94. OPEX and CAPEX are added in the structure shown in Figure 95, leading to production costs (Figure 96).

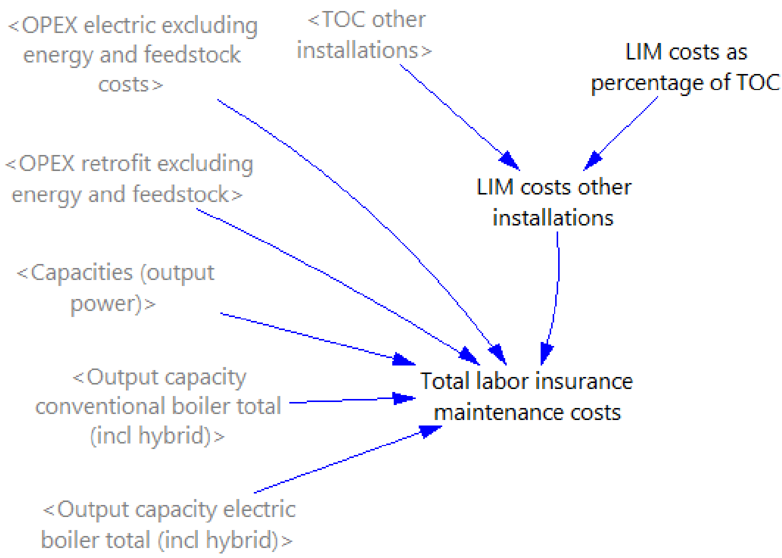

Figure 93: Computation of total labor, insurance and maintenance (LIM) costs.

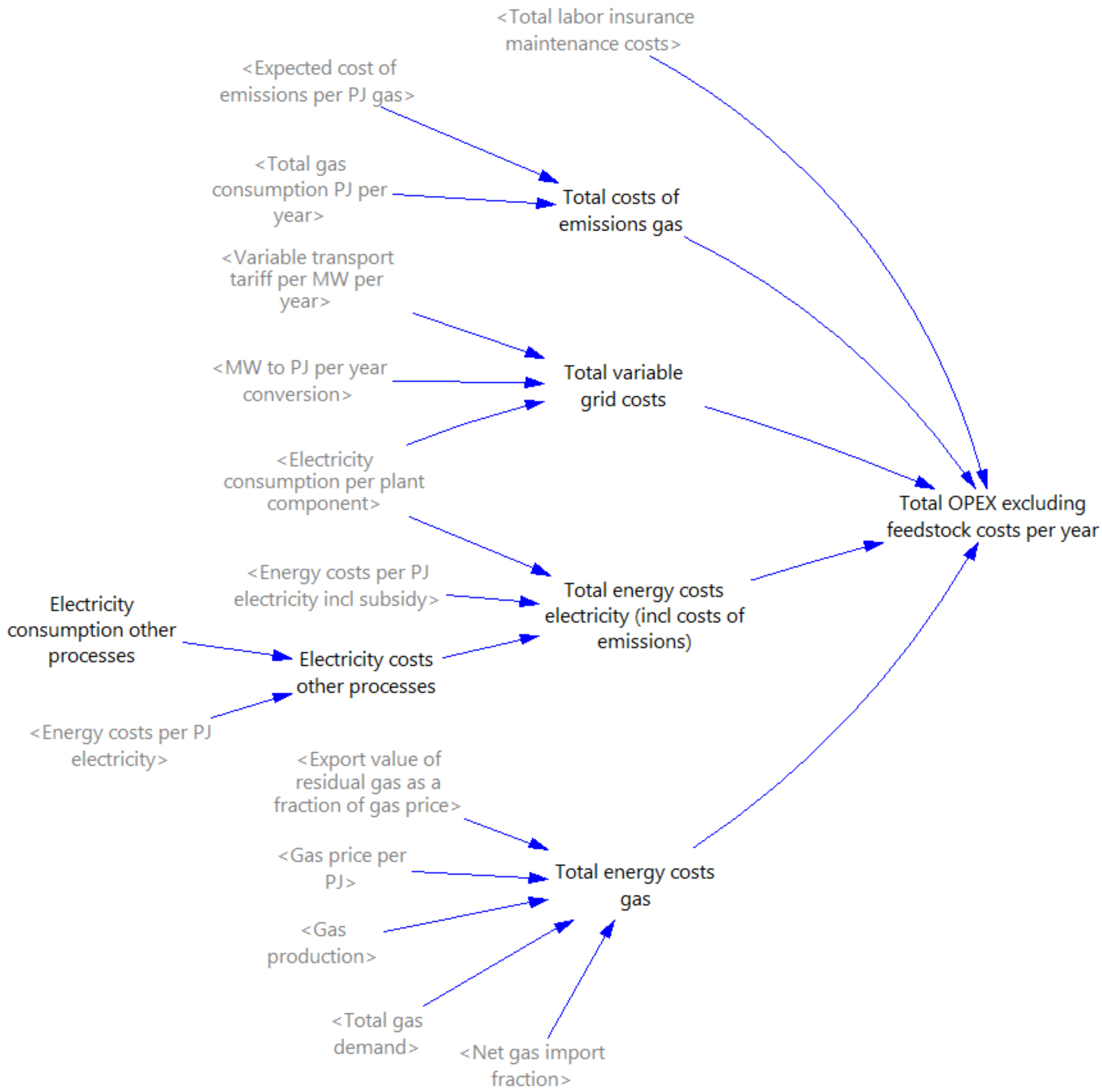

Figure 94: Computation of total OPEX.

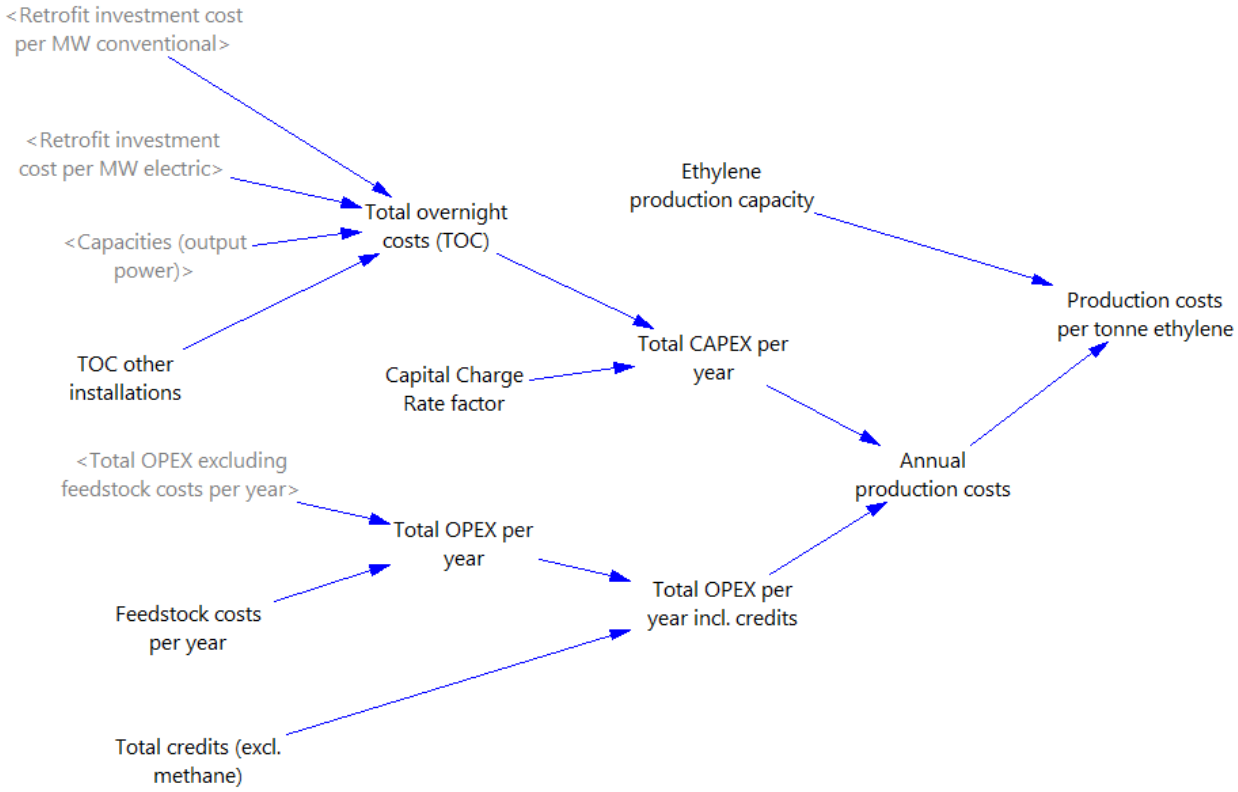

Figure 95: Computation of the production costs per tonne ethylene.

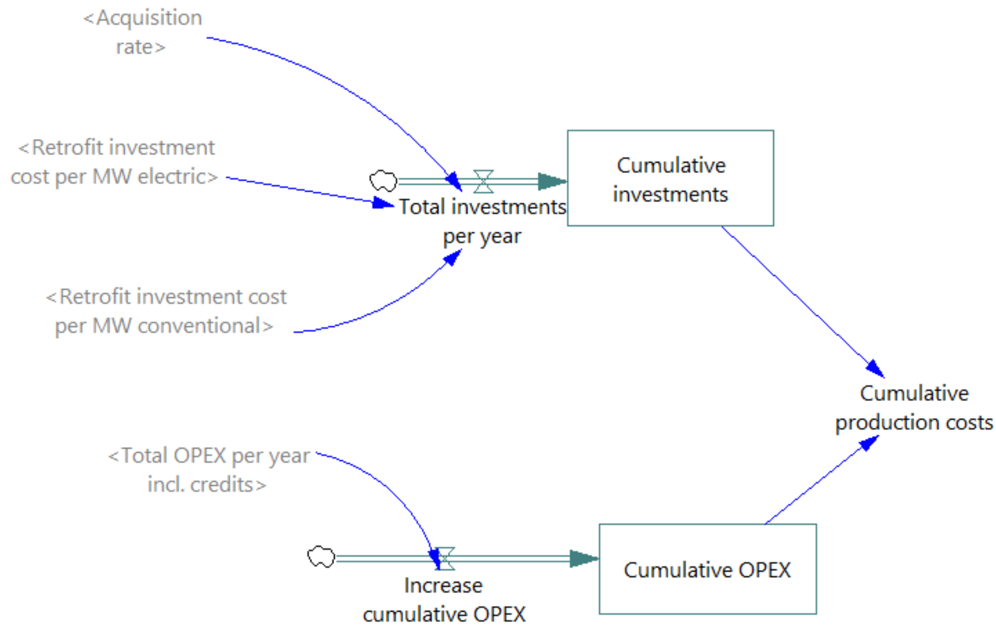

Figure 96: Stock-flow structures of cumulative investments and cumulative OPEX, which together form the cumulative production costs.

C.3.6 Policy costs subcomponent

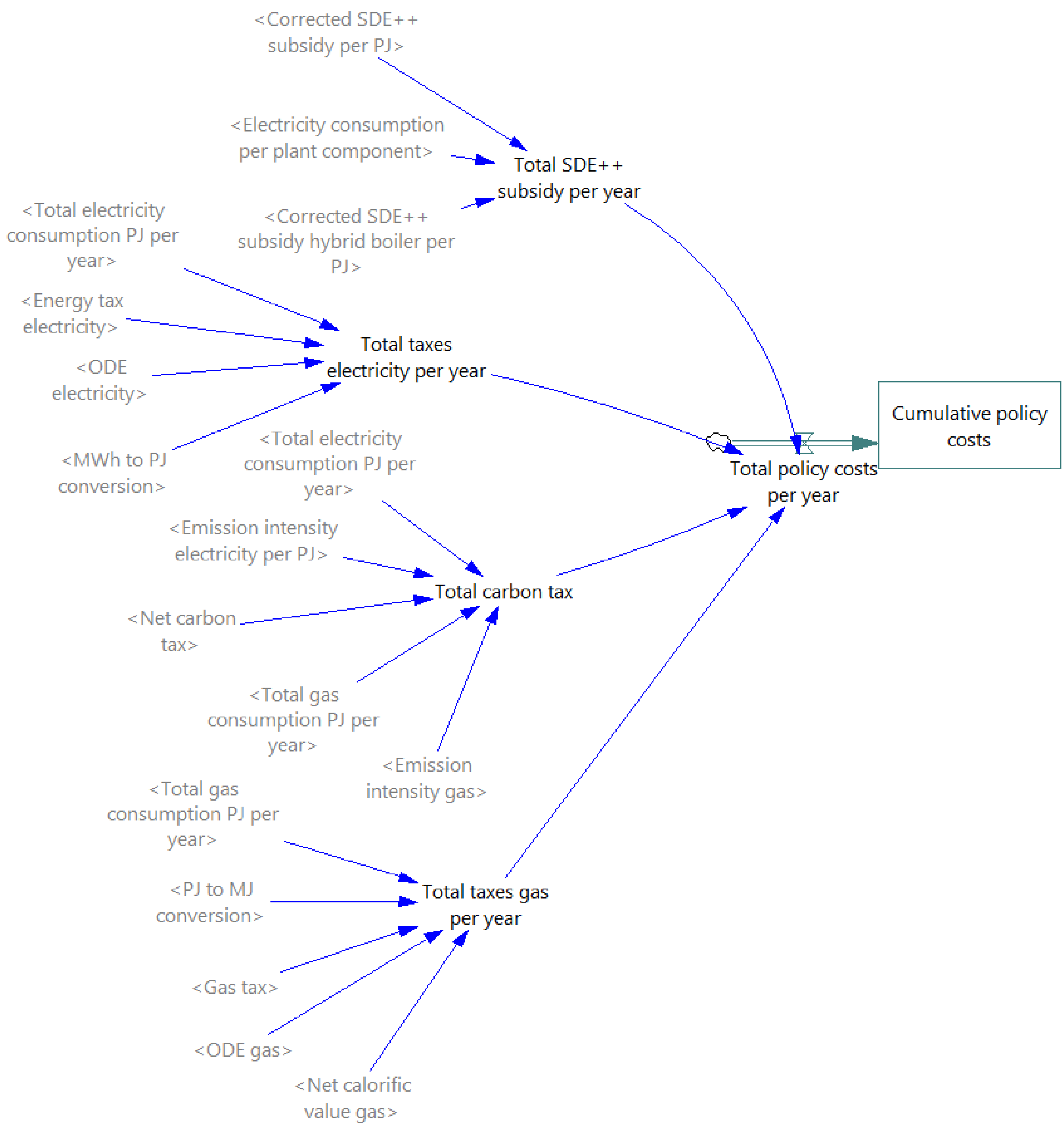

Figure 97: Computation of annual policy costs and stock-flow structure of cumulative policy costs.

D Further details about the model formalization

In this appendix more details are given about the calculation of specific model components, which were introduced in Section 5.3.

D.1 SDE++ subsidy

The SDE++ subsidy (model structure shown in Figure 77) is composed of a *base fee* and a *correction fee*. These are calculated each year by the Netherlands Environmental Assessment Agency for a range of electrification technologies. The base fee is a fixed fee over the duration of the subsidy. The correction fee is determined by the avoided costs related to fossil fuel consumption (Lensink & Schoots, 2020). In the model, the base fee is a policy lever with a fixed value, unlike in reality where PBL performs a calculation of the base fee for specific technologies. However, performing such calculations were deemed outside of the scope of this research. Hence, the SDE++ subsidy is calculated as follows:

$$SDE = base\ fee - correction\ fee \tag{39}$$

$$correction\ fee = EC_{con} \tag{40}$$

where EC_{con} are the energy costs for a conventional retrofit, represented by Equation 4.

D.2 Value loss of residual gas

Naphtha cracking plants consumes gas to fuel its furnaces and boilers but also produce (methane-rich) gas in its process (see Section 4.1.2). This gas is fed back into the system. Hence, only part of the gas demand needs to be imported and often, the majority of the gas is "free" (Wong & van Dril, 2020).
With increasing electrification, the demand for gas decreases. Hence, if the gas production starts to exceed the gas demand, there is residual gas. This residual gas will likely not have the same value as natural gas on the market. In other words, part of its value will be lost. This value loss is voiced as a concern by the industry (Interviews, 2021) as it means the business case for electrification will become less attractive. As a matter of fact, it may be cheaper to continue gas-dependent operations using "free" gas produced in the production process than to waste this gas while importing electricity.

In the model this effect is accounted for by multiplying the gas price with the value factor v, hence obtaining the effective gas price. As long as the gas consumption exceeds the gas production, $v = 1$: the additional gas demand is bought on the market against the gas market price. However, if the gas consumption drops below the gas production level, the effective costs of gas depend on the export value of residual gas. In this case $0 \leqslant v \leqslant 1$. If $v = 1$ gas can be exported against the same value as the market price. Hence, the effective costs of gas for a conventional retrofit are as high as in the case where gas consumption exceeds gas production: were this gas not to be consumed, it could be sold on the market.
However, in the other extreme case where $v = 0$ the residual gas cannot be commercialized: it would better be consumed or its value would be lost. In this case v acts as a disincentive for electrification.

In the model the value v (model structure show in Figure 81) is computed as follows:

$$v = v_{ex} + \frac{1 - v_{ex}}{1 + e^{-\alpha \cdot (f_{im} - 0.1)}} \tag{41}$$

where v_{ex} is the export value of residual gas (as a fraction of the gas price), f_{im} is the gas import fraction (represented by Equation 42 and α represents the speed with which the industry adjusts to the changing gas import fraction. The value of 0.1 indicates that the industry starts to anticipate the value loss of gas once the gas import fraction becomes lower than 10%. This equation represents an S-curve. Applying an S-curve seemed apt because it implies the industry smoothly adjusts to the changing gas import fraction f_{im} instead of abruptly accounting for a change in the value of gas once the net import fraction becomes lower than 0. Moreover, this would cause a discontinuity in the model once f_{im} becomes lower than 0 as this would mean a sudden drop in the value of gas.

$$f_{im} = \frac{C_{gas} - P_{gas}}{C_{gas}} \tag{42}$$

where C_{gas} is calculated using Equation 27 and P_{gas} = 25.6 PJ/year (Wong & van Dril, 2020) is the gas production, which is assumed constant over time as the production capacity is also considered stable and no changes are assumed to occur in the shares of products in the production output (see Section 5.1).

D.3 Efficiency improvements in conventional technologies

The model structure of the computation of efficiency improvements is shown in Figures 78 and 79. It is assumed that efficiency improvements will occur in conventional technologies (Stork et al., 2018; Wong & van Dril, 2020). According to Stork et al. (2018) these improvements are expected to amount to 0.5 - 1% annually. However, if a percentage would be used, efficiencies would improve exponentially, which is not realistic. In the model, it is assumed that the efficiency improves according to a logistic function (Kucharavy & De Guio, 2011; Lotfi et al., 2014; Borucka & Grzelak, 2019). Therefore, only initially the efficiency improvement rate in the model will be equal to the expected efficiency improvement. Hence, in the model the efficiencies of conventional technologies at time t are computed as follows:

$$\eta_t = \eta_0 \cdot \frac{\eta_{max}}{\eta_0 + e^{-\eta_{max} \cdot s \cdot t} \cdot (\eta_{max} - \eta_0)} \tag{43}$$

η_t is the efficiency of a conventional technology (furnace/compressor turbine/boiler) at time t, η_0 is the efficiency in the reference year and η_{max} is the theoretically maximum attainable efficiency, which is fixed. Note that here, η_t represents the notation $efficiency_{con_k}$ used in Section 5.3. Furthermore, t represents time and s is calculated as follows:

$$s = \frac{\ln(f_{eff})}{\eta_0 \cdot (\eta_{max} - \eta_0)} \tag{44}$$

Here, f_{eff} is the efficiency improvement factor, which is 1 plus the expected initial improvement in conventional technologies.

D.4 Boiler capacity adjustment

In the *Capacities* component of the model (see Section 5.3.3) capacity acquisition is modelled. As only retrofits are considered, the total capacity acquisition for each type of installation equals the depreciation rate. What varies is the kind of retrofit: electric or conventional. Hence, the conventional capacity of an installation may decrease, while the electric capacity of that same installation may increase, but the overall output capacity remains the same.

However, the boiler capacity is an exception to this logic. The boilers produce steam for driving the conventional compressor turbines. Hence, when the compressor turbines become electric, less steam is needed. Therefore, the boiler capacity adjusts to the varying steam demand. The model structure of the boiler capacity adjustment can be found in Figure 88. The capacity adjustment is represented by the following equation:

$$CA_{boiler} = \frac{capacity_{desired} - capacity_{utilized}}{T} \tag{45}$$

where $capacity_{desired}$ is the desired boiler capacity, $capacity_{utilized}$ is the utilized boiler capacity and T is the turnaround time.

$capacity_{desired}$ is described by Equation 46 and $capacity_{utilized}$ is described by Equation 48.

$$capacity_{desired} = S_{cracking} + S_{compression} - S_{production} \tag{46}$$

where $S_{cracking}$ is the steam demand for cracking, $S_{compression}$ is the steam demanded by the compressor turbines and $S_{production}$ is the steam produced in the process by the cooling of cracked gas (see Section 4.1.1). $S_{cracking}$ and $S_{production}$ are considered constant: $S_{cracking}$ = 5.1 PJ/year and $S_{production}$ = 6.1 PJ/year. $S_{compression}$ equals:

$$S_{compression} = \frac{capacity_{con_{comp}}}{efficiency_{con_{comp}}} \tag{47}$$

where $capacity_{con_{comp}}$ is the capacity of conventional compressor turbines (see Section 5.3.3) and $efficiency_{con_{comp}}$ is the aggregate efficiency of the installed conventional compressor turbines (see Section D.8).

$capacity_{utilized}$ equals:

$$capacity_{utilized} = OC_{el_{boiler}} + OC_{con_{boiler}} \tag{48}$$

where $OC_{el_{boiler}}$ is the total output capacity of electric boilers (including those operating in hybrid configuration) and $OC_{con_{boiler}}$ (also including those operating in hybrid configuration). Hence, $OC_{el_{boiler}}$ and $OC_{con_{boiler}}$ are represented by the following equations:

$$OC_{el_{boiler}} = capacity_{el_{boiler}} + \frac{N_{load}}{N_{tot}} \cdot capacity_{hy_{boiler}} \tag{49}$$

$$OC_{con_{boiler}} = capacity_{con_{boiler}} - \frac{N_{load}}{N_{tot}} \cdot capacity_{hy_{boiler}} \tag{50}$$

where $capacity_{el_{boiler}}$ is the baseload capacity of electric boilers, $capacity_{con_{boiler}}$ is the baseload capacity of gas boilers and $capacity_{hy_{boiler}}$ is the capacity of hybrid boilers (additional electric boilers operating in hybrid configuration). N_{load} is the number of operating hours of the hybrid boilers (see Section D.7) and N_{tot} is the total number of operating hours per year (which depends on the utilization rate of the plant).

D.5 Share of renewable electricity and emission intensity of electricity

The long-term development of renewable energy sources tends to follow a logistic function, also known as an S-curve (Skoczkowski et al., 2019). In the model the development the share of renewable electricity in the electricity mix is modelled as such. Hence, in the model, the availability of renewable electricity (model structure shown in Figure 80) is represented by the equation:

$$R_t = R_0 \cdot \frac{R_{max}}{R + e^{-R_{max} \cdot z \cdot t} \cdot (R_{max} - R_0)} \tag{51}$$

where R_t is the share of renewable electricity at time t, $R_{max} = 100\%$ (the maximum possible share being 100% obviously), $R_0 = 18\%$ the share in the reference year 2019 (Lensink, 2020). Then, the factor z equals:

$$z = \frac{\ln(P)}{R_0 \cdot (R_{max} - R_0)} \tag{52}$$

In turn, P equals:

$$P = \frac{R_0 \cdot (R_{max} - R_{proj})}{R_{proj} \cdot (R_{max} - R_0)} \tag{53}$$

where R_{proj} is the projected share of renewable electricity in a certain year. In the model this is the year 2030. R_{proj} is considered an exogenous uncertainty. In the reference mode, $R_{proj} = 75\%$, according to the Climate Agreement.

The emission intensity of electricity EI_{elec} is assumed to have a linear relationship to the availability of renewable electricity. It should be noted that this is a rather simple assumption. However, because the relationship between the availability of renewable electricity and the emission intensity is not obvious, a linear relationship was used in lack of another simple alternative. It is assumed that when the availability of renewable electricity reaches 100%, $EI_{elec} = 0$. In the reference year, $EI_{elec,0} = 0.53$ tonne/kWh (PBL, 2020). Therefore:

$$EI_{elec} = a \cdot R_t + b \tag{54}$$

where

$$a = \frac{-EI_{elec,0}}{R_{max} - R_0} \tag{55}$$

and

$$b = EI_{elec,0} - a \cdot R_0 \tag{56}$$

D.6 Net carbon tax

The net carbon tax (model structure shown in Figure 76) is the tax levied by the Dutch government on CO_2-emitting industries. Together with the ETS price, it constitutes the carbon costs paid by the industry (Equation 7). The value of the net carbon tax is based on the carbon levy (Dutch: *nationale CO_2-heffing*) which was introduced by the government in 2021 in order to increase the carbon pricing as the EU ETS price was deemed insufficient to stimulate the industry to curb emissions (Government of the Netherlands, 2021). The carbon levy starts at 30 euro/tonne CO_2 in 2021 and increases linearly up to 125 euro/ton CO_2 in 2030. The net carbon tax companies pay is the difference between the carbon levy and the EU ETS carbon price. Mathematically this principle is represented in the model as follows:

$$net\ carbon\ tax = \begin{cases} carbon\ levy_{eff} - ETS\ price, carbon\ levy_{eff} > ETS\ price \\ 0, carbon\ levy_{eff} \leq ETS\ price \end{cases} \tag{57}$$

According to the principle behind the carbon levy introduced in Section 5.2.3 the effective carbon levy (model structure shown in Figure 75) is calculated as follows:

$$carbon\ levy_{eff} = \left(1 - \frac{DPR}{emissions}\right) \cdot carbon\ levy \tag{58}$$

where *carbon levy* is the "base" carbon levy, which starts at 30 euro/tonne CO_2 in 2021 and increases linearly up to 125 euro/ton CO_2 in 2030. However, since the industry is granted a certain number of dispensation rights (DPR) - or exempted emissions (see section 5.2.3) - the *carbon levy* is reduced. Hence, $carbon\ levy_{eff}$ is lower than *carbon levy*. The number of dispensation rights (with 1 DPR being equivalent to 1 tonne CO_2) equals (NEa, 2020):

$$DPR = production\ output \cdot benchmark \cdot NRF \tag{59}$$

where *production output* is the combined volume of ethylene and propylene produced per year, which is assumed constant at the 2018 value reported for Shell MLO (Wong & van Dril, 2020). *benchmark* is a steam cracking-specific benchmark applied by the Dutch Emissions Authority, reported in number of DPRs per tonne production output. NRF represent the *national reduction factor*, a factor that decreases linearly over time, meant to lower the number of dispensation rights over time. As such, the number of exempted emissions decreases over time, stimulating decarbonization among the industry (NEa, 2020).

D.7 Number of load hours hybrid boiler

The model structure of the calculation of load hours is shown in Figure 73. Like the emission intensity of electricity (see Section D.5), the number of load hours for a hybrid boiler is also assumed to show a linear relationship with the availability of renewable electricity:

$$N_t = m \cdot R_t + c \tag{60}$$

where

$$m = \frac{N_{max} - N_0}{R_{max} - R_{ref}} \tag{61}$$

where N_{max} = 8760 hours/year: the number of hours in a year and N_0 is the number of load hours in the reference year. According to Lensink (2020): N_0 = 1400 hours/year in 2021. R_{max} = 100%, the maximum share of renewable electricity. Because N_0 has a different reference year from R_0, which is recorded as 18% in 2019 (PBL, 2020), this has to be adjusted. Hence, an estimate R_{ref} in the year 2021 is made, based on R_0 and the projected share of renewable electricity in 2030, R_{proj}. Furthermore, c equals:

$$c = N_0 - m \cdot R_0 \tag{62}$$

D.8 Aggregate efficiencies of installed conventional capacities

The total gas consumption is modelled by a co-flow structure (Sterman, 2000) which calculates the aggregate efficiencies of the installed capacities based on the inflow of new capacities with higher efficiencies and the outflow of older capacities with lower efficiencies (see Appendix C, Figure 89). In the stock-flow structure the gas consumption for each installation k is calculated as:

$$C_{gas_k} = \int_t (c_{gas,in_k} - c_{gas,out_k})\, dt \tag{63}$$

where c_{gas,in_k} is gas consumption change due to capacity acquisition and c_{gas,out_k} is the gas consumption change due to capacity depreciation. c_{gas,in_k} is represented by Equation 64 and c_{gas,out_k} by Equation 65.

$$c_{gas,in_k} = \frac{acquisition\ rate_k}{eff_{con_k}} \tag{64}$$

$$c_{gas,out_k} = \frac{depreciation\ rate_k}{eff_{con_{k_{tot}}}} \tag{65}$$

Here, $efficiency_{con_k}$ is the efficiency of new conventional capacities at time t, which is calculated according to Equation 43. $efficiency_{con_{k_{tot}}}$ is the aggregate efficiency of the installed capacity of type k. It equals:

$$efficiency_{con_{k_{tot}}} = \frac{capacity_k}{C_{gas_k}} \tag{66}$$

D.9 Calculation of feedstock costs and credits

For the calculation of the production costs in the model (see Section 5.3.3) the costs of naphtha feedstock and the credits earned by the production of other chemicals have to be taken into account. In Table 2 an overview of these costs can be found.

Table 2: Overview of feedstock costs and credits used in the calculation of production costs.

	Capacity [ktonne/year]	**Price [3] [euro/tonne]**	**Inflation 2017-2019 [4]**	**Corrected price [euro/tonne]**	**Total amount [euro]**
Feedstock costs					
Naphtha	3000 [5]	671.67	1.043432	700.842	$2.10 \cdot 10^9$
Credits					
Hydrogen	45.5 [6]	1343	1.043432	1401.329	$6.38 \cdot 10^7$
Propylene	482.3 [6]	1007.55	1.043432	1051.31	$5.07 \cdot 10^8$
Butadiene, butanes, butenes	309.4 [6]	885.02	1.043432	923.4582	$2.86 \cdot 10^8$
Pygas	682.5 [6]	789.01	1.043432	823.2783	$5.62 \cdot 10^8$
Fuel oil	118.3 [6]	468.42	1.043432	488.7644	$5.78 \cdot 10^7$
Total credits	**1638**				$\mathbf{1.48 \cdot 10^9}$

[3] Source: (Boulamanti & Moya, 2017b)
[4] Source: (Statista, 2021)
[5] Source: (Wong & van Dril, 2020); the reference plant is based on Shell Moerdijk MLO.
[6] Based on an ethylene production capacity of 910 ktonne/year (Wong & van Dril, 2020) and co-products yields obtained from Boulamanti & Moya (2017b)

E Overview of model input parameters

In this appendix the full list of model input parameters can be found with the values for the base case. That means: the variables that are labelled "uncertain" or "policy lever" have been set to certain values corresponding to data (projections) found in various sources. The base case is a "policy-rich" scenario, meaning that it contains policy options based on current, adopted and proposed government policy.

Table 3: Full list of model input parameters with values for the base case. Parameters for which assumptions have been made contain "Assumption" and a number in the source column. The assumptions are further elaborated below the table.

	Variable type	**Unit**	**Value**	**Source**
Prices				
Electricity market price current	Fixed	euro/MWh	41	PBL (2020)
Electricity market price projection 2030	Uncertain	euro/MWh	50.7	PBL (2020)
ETS carbon price current	Fixed	euro/ tonne$_{CO_2}$	25	PBL (2020)
ETS carbon price projection 2050	Uncertain	euro/ tonne$_{CO_2}$	83.3	Assumption 1
Gas market price current	Fixed	euro/m^3	0.16	PBL (2020)
Gas market price projection 2030	Uncertain	euro/m^3	0.229	PBL (2020)
Cost calculations				
Discount rate	Uncertain	%	15	(Verbeek, 2021)
Exogenous learning rate	Uncertain	-	0.00928	Assumption 2
Export value of residual gas	Uncertain	%	60	Assumption 3
Initial retrofit investment costs per MW electric boiler	Uncertain	euro/MW	$1.15{\cdot}10^5$	Marsidi & Lensink (2020a)
Initial retrofit investment costs per MW electric compressor turbine	Uncertain	euro/MW	$1.375{\cdot}10^6$	Assumption 4
Initial retrofit investment costs per MW electric furnace	Uncertain	euro/MW	$1.14{\cdot}10^6$	Assumption 5
Fixed O&M costs electric per year in percentage of investment costs	Uncertain	%	2	Assumption 6
Fixed O&M costs conventional per year in percentage of investment costs	Fixed	%	5	Assumption 6
Retrofit investment cost per MW boiler	Uncertain	euro/MW	$5.50{\cdot}10^4$	Rutten (2019)
Retrofit investment cost per MW compressor	Uncertain	euro/MW	$7.20{\cdot}10^5$	Rutten (2020)
Retrofit investment cost per MW furnace	Uncertain	euro/MW	$4.75{\cdot}10^5$	Assumption 7
VAT	Fixed	%	21	-
Energy & efficiency				
Efficiency boiler reference year	Fixed	%	85	Wong & van Dril (2020)
Efficiency electric boiler	Fixed	%	99	Marsidi & Lensink (2020a)
Efficiency electric compressor turbine	Fixed	%	95	Interviews (2021)
Efficiency electric furnace	Fixed	%	95	Interviews (2021)
Efficiency improvements in conventional technologies	Uncertain	%/year	0.5	Assumption 8
Efficiency steam turbine reference year (steam-to-work)	Fixed	%	37.6	Assumption 9
Emission intensity gas	Fixed	tonne$_{CO_2}$/PJ	$6.24{\cdot}10^4$	Zijlema (2020)

	Variable type	Unit	Value	Source
Maximum efficiency boiler	Fixed	%	95	Assumption 10
Maximum efficiency furnace	Fixed	%	95	Zimmermann & Walzl (2012)
Maximum efficiency steam turbine (steam-to-work)	Fixed	%	52	Manushin (1997)
Net calorific value gas	Fixed	MJ/m^3	31.65	Zijlema (2020)
Thermal efficiency furnace reference year	Fixed	%	82	Assumption 11
S-curve parameters				
Response delay to gas becoming residual	Uncertain	-	20	Assumption 12
Response delay of investment share to costs ratio	Uncertain	-	20	Assumption 13
Response delay of investment share to costs ratio (hybrid boiler)	Uncertain	-	30	Assumption 13
Renewable electricity				
Emission intensity electricity in reference year	Fixed	$tonne_{CO_2}$/ MWh	0.53	PBL (2020)
Renewables share 100%	Fixed	%	100	-
Renewables share projection in 2030	Uncertain	%	75	PBL (2020)
Renewables share in 2019	Fixed	%	18	PBL (2020)
Renewables share in reference year of emission intensity electricity	Fixed	%	11	PBL (2020)
Zero emission intensity	Fixed	$tonne_{CO_2}$/ MWh	0	-
Plant characteristics				
Amount of steam produced in process	Fixed	PJ/year	6.1	Assumption 14
Amount of steam required for cracking	Fixed	PJ/year	5.1	Assumption 15
Cracker production output (ethylene and propylene)	Fixed	tonne	$1.41 \cdot 10^6$	Assumption 16
Gas production	Fixed	PJ/year	25.6	Assumption 17
Initial output capacity boilers	Fixed	MW	195	Assumption 18
Initial output capacity compressor turbines	Fixed	MW	87	Assumption 19
Initial output capacity furnaces	Fixed	MW	600	Assumption 20
Time interval between turnarounds	Uncertain	year	6	Interviews (2021)
Utilization rate plant	Fixed	%	83	Wong & van Dril (2020)
Capacity acquisition & depreciation				
Acquisition time hybrid boiler	Uncertain	year	1.8	Scholten et al. (2021)
Economic lifetime boilers	Uncertain	year	10	Assumption 21
Economic lifetime compressor turbines	Uncertain	year	10	Assumption 21
Economic lifetime furnaces	Uncertain	year	20	Assumption 21
Initial on-order capacity boilers	Fixed	MW	0	-
Initial on-order capacity compressor turbines	Fixed	MW	0	-
Initial on-order capacity furnaces	Fixed	MW	0	-
Max. percentage of boilers to become hybrid per year	Uncertain	%	2.5	Assumption 22

	Variable type	Unit	Value	Source
Policy				
Base fee SDE++	Policy lever	euro/kWh	0.07	Lensink (2020)
Carbon levy increase rate	Policy lever	euro/ $(\text{tonne}_{CO_2}\cdot\text{year})$	10.56	NEa (2020)
Carbon levy increase rate after 2030	Policy lever	euro/ $(\text{tonne}_{CO_2}\cdot\text{year})$	0	-
Carbon levy initial value (2021)	Fixed	euro/tonne_{CO_2}	30	NEa (2020)
DPR switch	Policy switch	-	1	NEa (2020)
EHS grid connection costs	Policy lever	euro	$3\cdot10^6$	ACM (2020)
Energy tax electricity	Policy lever	euro/MWh	0.56	Belastingdienst (2020)
Gas tax	Policy lever	euro/m^3	0.01281	Belastingdienst (2020)
Increase carbon levy after 2030 switch	Policy switch	-	0	-
NRF initial value	Fixed	-	1.2	NEa (2020)
NRF slope	Fixed	1/year	-0.057	NEa (2020)
ODE electricity	Policy lever	euro/MWh	0.4	Belastingdienst (2020)
ODE gas	Policy lever	euro/m^3	0.0232	Belastingdienst (2020)
Steam cracking levy benchmark	Fixed	1/tonne_{CO_2}	0.681	Ministry of Economic Affairs & Climate (2020)
Variable transport tariff (electric furnace and turbine)	Policy lever	euro/(kW·month)	1.23	ACM (2020)
Variable transport tariff (e-boiler)	Policy lever	euro/(kW·month)	2.00	Liander (2020)
Time-related variables				
Carbon levy end year current policy	Fixed	year	2030	NEa (2020)
Carbon levy start year	Fixed	year	2021	NEa (2020)
Projection year prices	Fixed	year	2030	PBL (2020)
Projection year renewables share	Fixed	year	2030	PBL (2020)
Projection year ETS carbon price	Fixed	year	2050	Aalbers et al. (2016)
Reference year number of load hours with zero emissions	Fixed	year	2021	Lensink (2020)
Reference year prices	Fixed	year	2019	PBL (2020)
Reference year renewables	Fixed	year	2019	Lensink (2020)
Conversion factors				
MWh to PJ conversion	Fixed	MWh/PJ	$2.78\cdot10^5$	-
DPR to emissions conversion	Fixed	tonne_{CO_2}	1	-
Hours per year	Fixed	hour/year	8760	-
kW to MW unit conversion	Fixed	kW/MW	1000	-
MJ to MWs conversion	Fixed	MJ/(MW·s)	1	-
Months per year	Fixed	month/year	12	-
PJ to MJ conversion	Fixed	PJ/MJ	10^{-9}	-
Seconds per hour	Fixed	s/hour	3600	-

A list of assumptions regarding the data presented in Table 3 is provided below.

1. Assumption 1. Based on a linear extrapolation of the 2030 projection reported by PBL (2020) (45.7 euro/tonne in 2030). This extrapolation was performed because for the uncertainty range of the EU ETS carbon prices the 2050 values reported by Aalbers et al. (2016) are used.

2. Assumption 2. Based on an assumed maximum cost reduction in electric technologies of 25% by 2050 (Jansen et al., 2019).

3. Assumption 3. Educated guess based on (Interviews, 2021).

4. Assumption 4. Based on the interviews the investment costs for an electric compressor turbine of 40 MW were assumed to be 55 million euros (Interviews, 2021).

5. Assumption 5. Electric furnaces are not yet on the market and therefore, the investment costs are highly uncertain. Therefore, it is assumed that the investment costs for an electric furnaces initially equal the upper bound of the investment costs for conventional furnaces (see assumption)

6. Assumption 6. Fixed operations & maintenance (O&M) costs of electric technologies are known to be lower than their conventional counterparts (Interviews, 2021). In the model, the fixed O&M costs are expressed as a percentage of the investment costs. As estimation of the fixed O&M costs as a percentage of the investment costs has been made based on a comparison between electric versus conventional boilers. A TNO technology factsheet (Rutten, 2019) reports fixed O&M costs of 4-5% of the investment costs for conventional boilers, which is in line with Wong & van Dril (2020). By contrast, for electric boilers the O&M costs are 2% of the investment costs according to TNO (Marsidi & Lensink, 2020a).

7. Assumption 7. According to Spallina et al. (2017) the share of the furnaces in the bare erected costs (BEC) of the plant are 29.5%. The total BEC of the plant of Shell Moerdijk MLO is estimated by Wong & van Dril (2020) as 409.9 million euros. The total overnight costs (TOC) of a plant can be expressed in terms of the BEC. Following the relation $TOC = 2.36 \cdot BEC$: the TOC equals 967 million euros. Hence, the TOC of the furnaces equal s 285 million euros. Based on an estimated heating duty of 600 MW for cracker furnaces (Interviews, 2021), the investment costs per MW amount to $4.75 \cdot 10^5$ euro/MW.

8. Assumption 8. Stork et al. (2018) reports an autonomous energy effiency improvement of 0.5-1% per year. It is assumed that this applies to efficiency improvements in conventional technologies too.

9. Assumption 9. Wong & van Dril (2020) reports a 19% electric efficiency and a 63% thermal efficiency for steam-driven compressor turbines. According to Manushin (1997): $\eta_e = \eta_t \cdot \eta_T \cdot \eta_m$ where $\eta_e = 19\%$ is the electric efficiency and $\eta_t = 63\%$ is the thermal efficiency. η_T represents the turbine efficiency. Assuming $\eta_m = 95\%$ as some mechanical losses occur (Interviews, 2021): $\eta_T = 32\%$ is the estimated turbine efficiency. This is in line with estimations of industry representatives (Interviews, 2021). This is the gas-to-work efficiency. To obtain the steam-to-work efficiency η_T is divided by the boiler efficiency in the reference year. Hence, a steam-to-work efficiency of 37.6% is obtained.

10. Assumption 10. Aydemir et al. (2015) report that 48% of the boilers in the EU have an efficiency of at least 90%.

11. Assumption 11. Based on an estimated furnace output capacity of 600 MW (Interviews, 2021), a gas consumption of 19.2 PJ/year (Wong & van Dril, 2020) and a plant utilization rate of 83% (Wong & van Dril, 2020).

12. Assumption 12. This parameter represents the parameter α in the logistic function introduced in Appendix D.2. Based on the assumption that the value loss of gas only becomes significant when the net gas import fraction becomes smaller than 10%.

13. Assumption 13. This parameter represents the parameter k in the logistic function introduced in Section 5.3.2. Based on the assumption that investments in electrification only become significant once P_{el} nears 110% of P_{con}, i.e. at $r = 1.1$. At this value $i_{el} = 12\%$.

14. Assumption 14. Estimation based on Wong & van Dril (2020). It is assumed the amount of steam produced in the process remains constant over time.

15. Assumption 15. Estimation based on Wong & van Dril (2020). It is assumed the amount of steam required for cracking remains constant over time.

16. Assumption 16. Estimation based on Wong & van Dril (2020). It is assumed the production volumes of ethylene and propylene remain constant over time. This parameter is used for the calculation of dispensation rights (DPRs) in the carbon levy (see Appendix D.6). It assumed that the benchmark values for steam cracking (Ministry of Economic Affairs & Climate, 2020) only apply to the ethylene and propylene production output, not to the output of other high-value chemicals.

17. Assumption 17. Estimation based on Wong & van Dril (2020). It is assumed the production volume of methane-rich gas remains constant over time.

18. Assumption 18. Only the boiler capacity required for the production of steam for the compressor turbines is considered. Hence, the initial boiler capacity is based on an initial steam demand of 6.1 PJ/year (Wong & van Dril, 2020) and an initial efficiency of 85% (Wong & van Dril, 2020).

19. Assumption 19. Estimation based on an initial steam demand of 6.1 PJ/year (Wong & van Dril, 2020) and values reported by industry representatives (Interviews, 2021).

20. Assumption 20. Estimation based on Wong & van Dril (2020) and Interviews (2021).

21. Assumption 21. Economic life times are assumed to be half of the technical life times. Technical lifetimes are assumed 20 years for boilers (Rutten, 2019), 20 years for compressor turbines (assumed equal to the life time for gas turbines reported by Rutten (2020)) and over 40 years for furnaces (Shell, 2020; Interviews, 2021).

22. Assumption 22. Based on the expectation that a maximum of 5 MW per year could be subject to boiler hybridization in the current configuration (Schure, 2021a).

F Verification & validation analyses

F.1 Analysis of the extreme conditions tests

The following extreme conditions tests have been executed:

1. Electricity price set to 0
2. Electricity price set to an extremely high value (10^{10} euro/MWh)
3. Gas price set to 0
4. Gas price set to an extremely high value (10^{10} euro/m^3)
5. ETS price set to an extremely high value (10^{10} euro/tonne CO_2)
6. Investment costs conventional retrofit set to an extremely high value (10^{10} euro/MW)
7. Investment costs electric retrofit set to an extremely high value (10^{10} euro/MW)

In Figure 98 the simulation results of the extreme conditions for furnace capacities are shown. Figure 99 shows the results for compressors, Figure 100 for boilers, Figure 101 for boiler hybridization and Figure 99 for emissions. In the following the results of these extreme conditions tests are interpreted. First the expectations for each extreme conditions test are outlined, then the results of the test are elaborated.

1. Electricity price set to 0. With an electricity price of 0 logically fast electrification is expected. Hence, the boiler capacity will decrease at a rapid rate as the steam demand is reduced. As a consequence, the short-term rise of emissions is expected to be larger than in the base case as electricity is more emission-intensive than gas in the short term.

From the results it can be observed that for all installations, 100% of the investments are channeled to electrification from the start. This is indicated by the increasing electric capacities. However, after a rapid increase the capacity of electric boilers starts to decrease after 2026 as can be observed in Figure 100 (see the green/-turquoise curves). For hybrid boilers this turning point occurs around 2029 (see the blue curve in Figure 101). This is due to the fact that the overall need for boilers is reduced due to the electrification of compressor turbines.

Regarding emissions, it can be observed that the emissions peak at a higher value than in the the base case (see the blue curve in Figure 103). This is to be expected as due to the low electricity price, electrification happens even though the emission intensity of electricity is still rather large.

2. Electricity price set to an extremely high value. With an extremely high electricity price no electrification is expected. Hence, there is little decrease in emissions.

As expected, the results show there is no electrification in this extreme condition. The capacity of gas boilers does decrease from ≈195 MW to ≈150 MW (purple curve in Figure 100) but this decrease can be attributed to efficiency improvements. As steam-driven compressor turbines become more efficient, the steam demand is reduced, decreasing the required boiler capacity.
These efficiency improvements result in a minor emission reduction (see the green curve in Figure 103).

3. Gas price set to 0. Like test 2, no electrification is expected in the case of a gas price of 0.

From the test results it can indeed be observed that neither furnaces and nor compressor are electrified. Surprisingly though, electrification still occurs for boilers (see the brown curves in Figure 100). Because electric boilers are a relatively mature technology, they feature relatively lower investment costs per MW than the other technologies (see Table 3). Moreover, electric boilers are highly efficient. Apparently, the projected carbon costs lead to a positive business case for electrification even with a 0 gas price. However, in 2033 the electrification comes to a halt and investments are channeled towards gas-fired boilers again, reducing the installed capacity of electric boilers; this is due to the rising electricity price. This effect is also visible in the emissions (see the red curve in Figure 103), which decrease at first but then bounce back.

Remarkably, boiler hybridization in the extreme condition of gas price zero (purple curve in Figure 101) are similar to the the base case (light blue curve in Figure 101). This is counter-intuitive because with a low gas price

one would expect boiler hybridization to pose less of an attractive business case. Upon closer examination, this effect can be attributed to two distinct effects that reinforce each other. First, the costs ratio $P_{hybrid}/P_{gas\ boiler}$ (see section 5.3.2) decreases as with a zero gas price the energy costs for a gas boiler decrease relatively than for a set of boilers operating in hybrid mode because this capacity runs on gas for only part of its load hours. This results in a higher investment share for hybridization compared to the base case. Second, due to the low electrification speed resulting from the low gas price there remains a higher steam demand as the compressor turbines remain largely steam-driven. Hence, there remains a larger hybridization potential.
However, as the number of load hours in which the boiler operate on electricity increases (due to a higher share of renewable electricity) the business case for boiler hybridization becomes less attractive and investments decline.

4. Gas price set to an extremely high value. With an extremely high gas price it is expected that immediately all investments are channelled towards electrification, resulting in a high electrification rate. As a consequence, the short-term rise of emissions is expected to be larger than in the base case as electricity is more emission-intensive than gas in the short term.

As expected, in this extreme conditions indeed investments in conventional capacity are 0 throughout the simulation. As a consequence, all investments are directed towards electrification. This results in a high electrification speed for all technologies. In 2050, 79% of the furnaces (red curves Figure 98) and 95% of the compressor turbines (green curves in Figure 99) is electrified. The electrification for furnaces is relatively lower due to their longer economic lifetime. Due to the strong electrification of compressor turbines, only 9% of the initial utilized boiler output capacity remains in 2050 (see Figure 102.

Regarding emissions, it can be observed that the emissions peak at a higher value than in the other cases (see the blue curve in Figure 103). This is to be expected as due to the high gas price, electrification happens even though the emission intensity of electricity is still rather large. Hence, emissions increases more in the short term. In 2050 though, emissions have decreased by 83%.

5. ETS price set to an extremely high value. In this case, it is expected that at first, the electrification rate may be lower than in the base case as electricity is more emission-intensive than gas. However, as the availability of renewable electricity increases electrification becomes much more attractive compared to the base case due to the high costs for conventional retrofits resulting from the high ETS price.

In fact, however, the results for this extreme conditions test are the same as for extreme conditions test 4. Hence, the initial slowdown in the electrification rate does not occur, indicating that the decrease in the emission intensity of electricity is sufficiently fast to allow for a rapid onset of electrification. Upon inspection, this can be explained by the fact that in the base case the rising electricity price influences the cost ratio between electrification and a conventional retrofit. However, in this extreme condition test this effect is absent because the electricity price is insignificant compared to the ETS price. As such, the high ETS price allows for the decreasing emission intensity of electricity to dominate the investment behavior while in the base case its electrification-stimulating effect is counteracted by the rising electricity price.

6. Investment costs conventional retrofit set to an extremely high value. As expected, the results for this extreme conditions test are the same as for extreme conditions tests 4 and 5.

7. Investment costs electric retrofit set to an extremely high value. As expected, the results for this extreme conditions test are the same as for extreme conditions test 2.

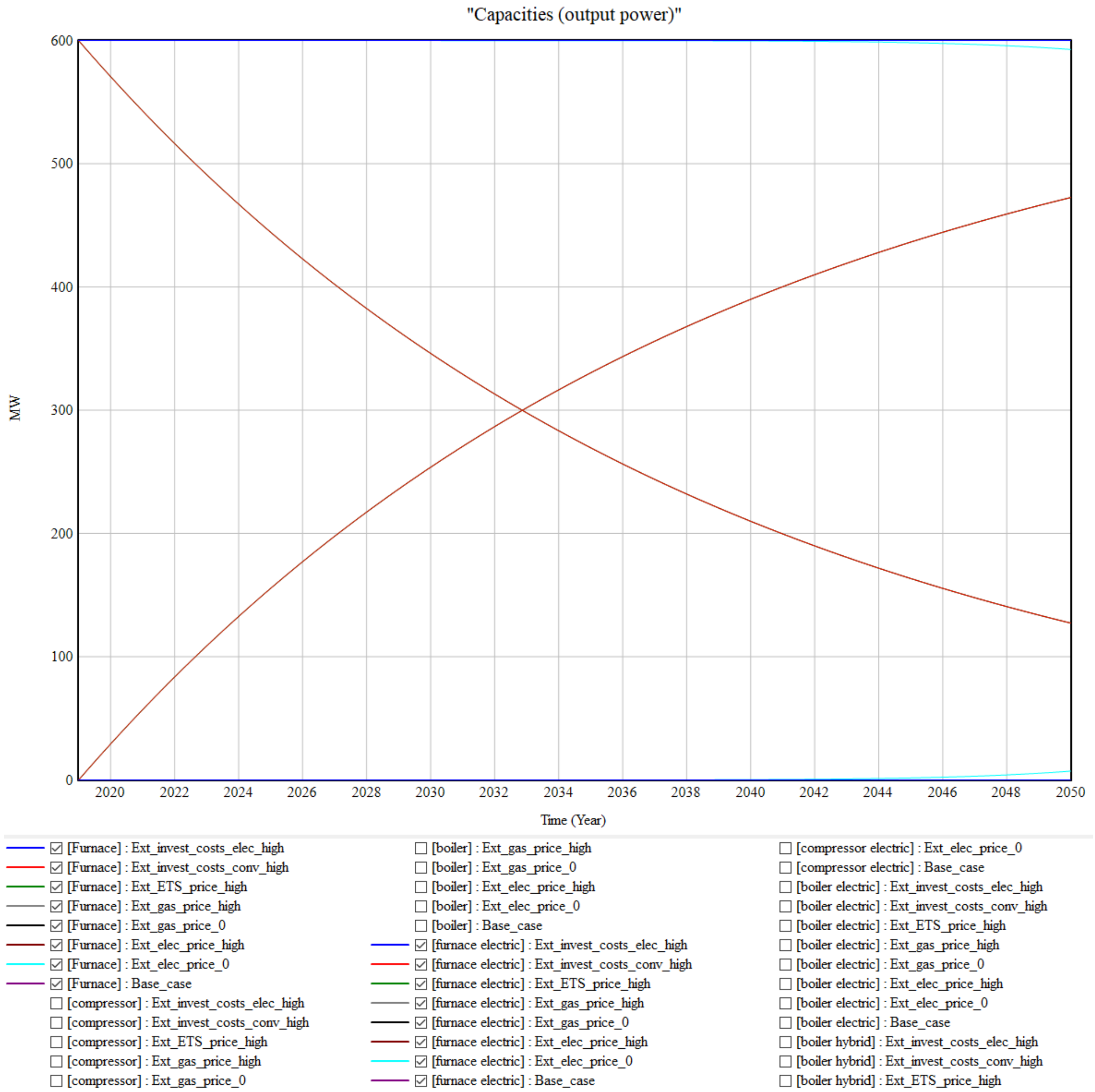

Figure 98: Simulation results of the extreme conditions tests for the capacities of conventional and electric furnaces.

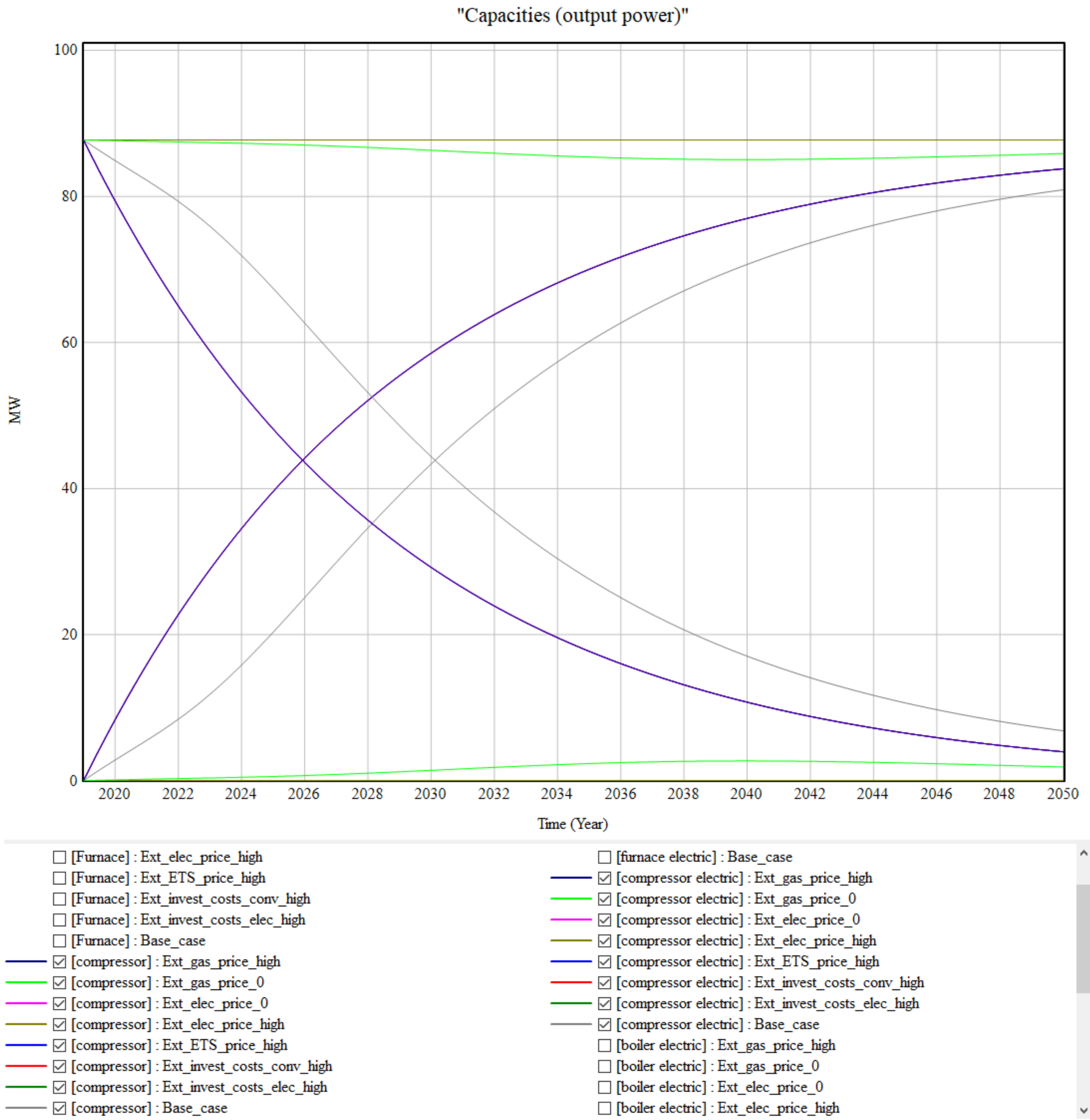

Figure 99: Simulation results of the extreme conditions tests for the capacities of conventional and electric compressor turbines.

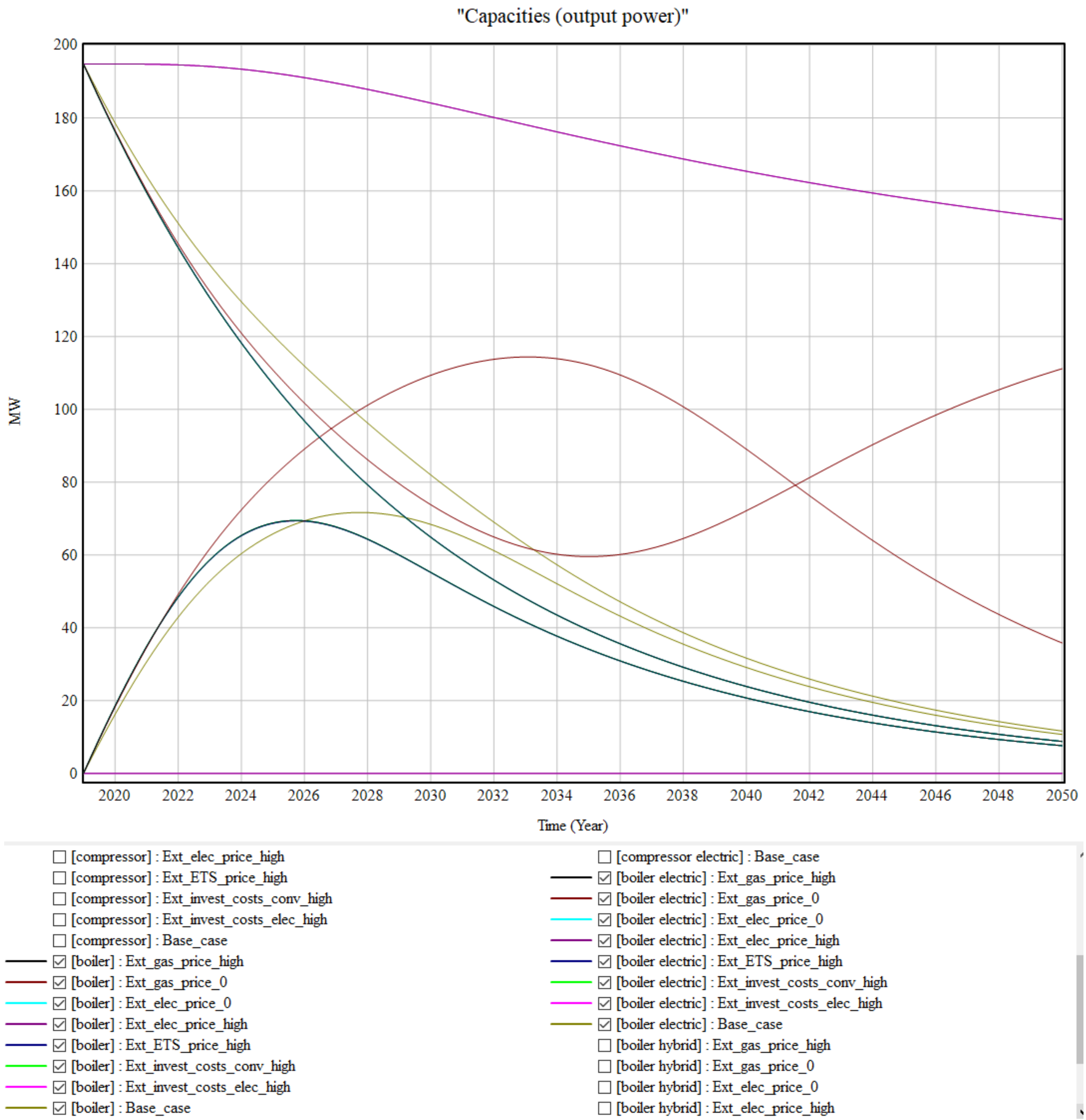

Figure 100: Simulation results of the extreme conditions tests for the capacities of conventional and electric boilers.

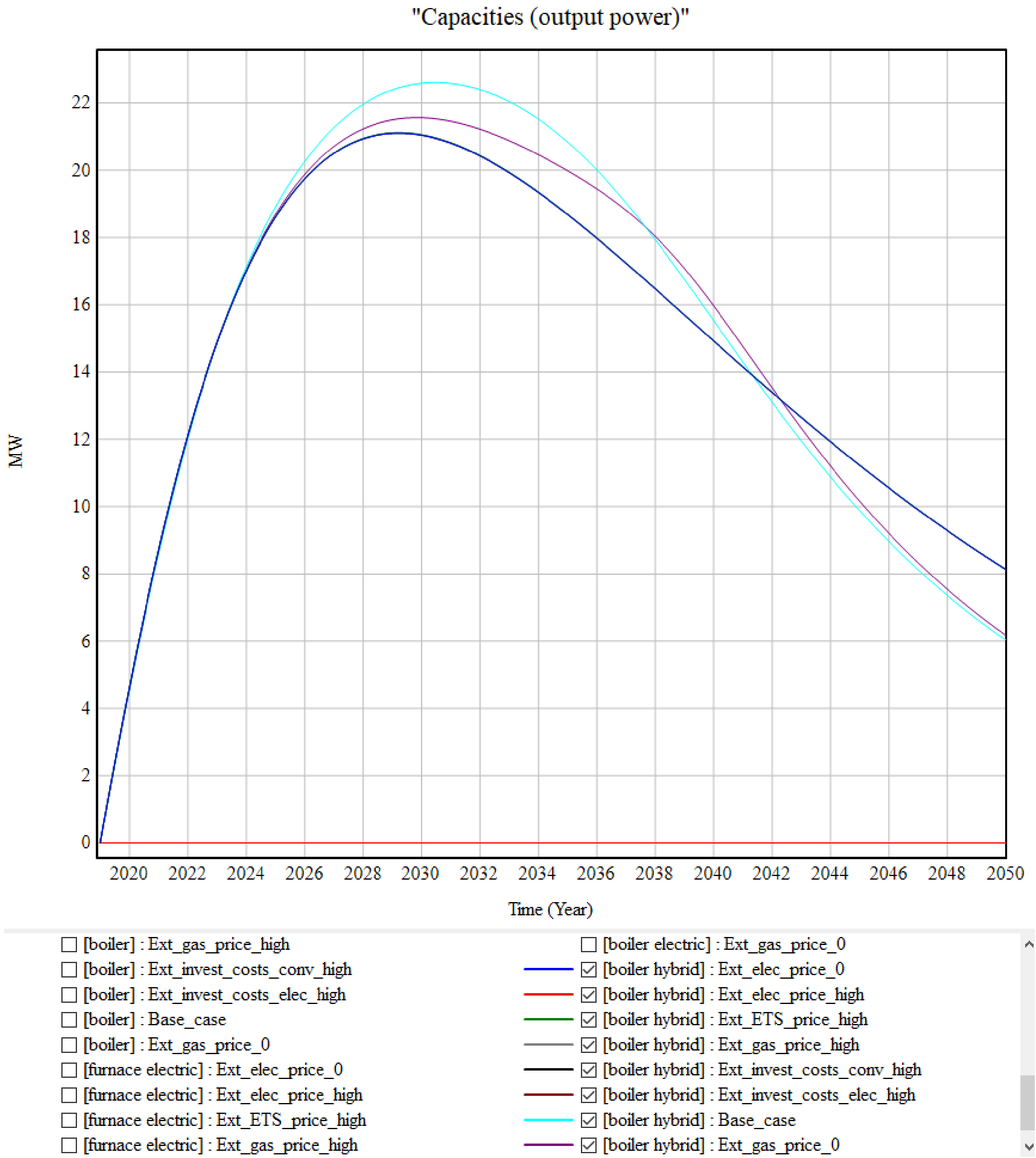

Figure 101: Simulation results of the extreme conditions tests for the capacities of hybrid boilers, i.e. electric boilers placed next to existing gas boilers, operating in a hybrid fashion.

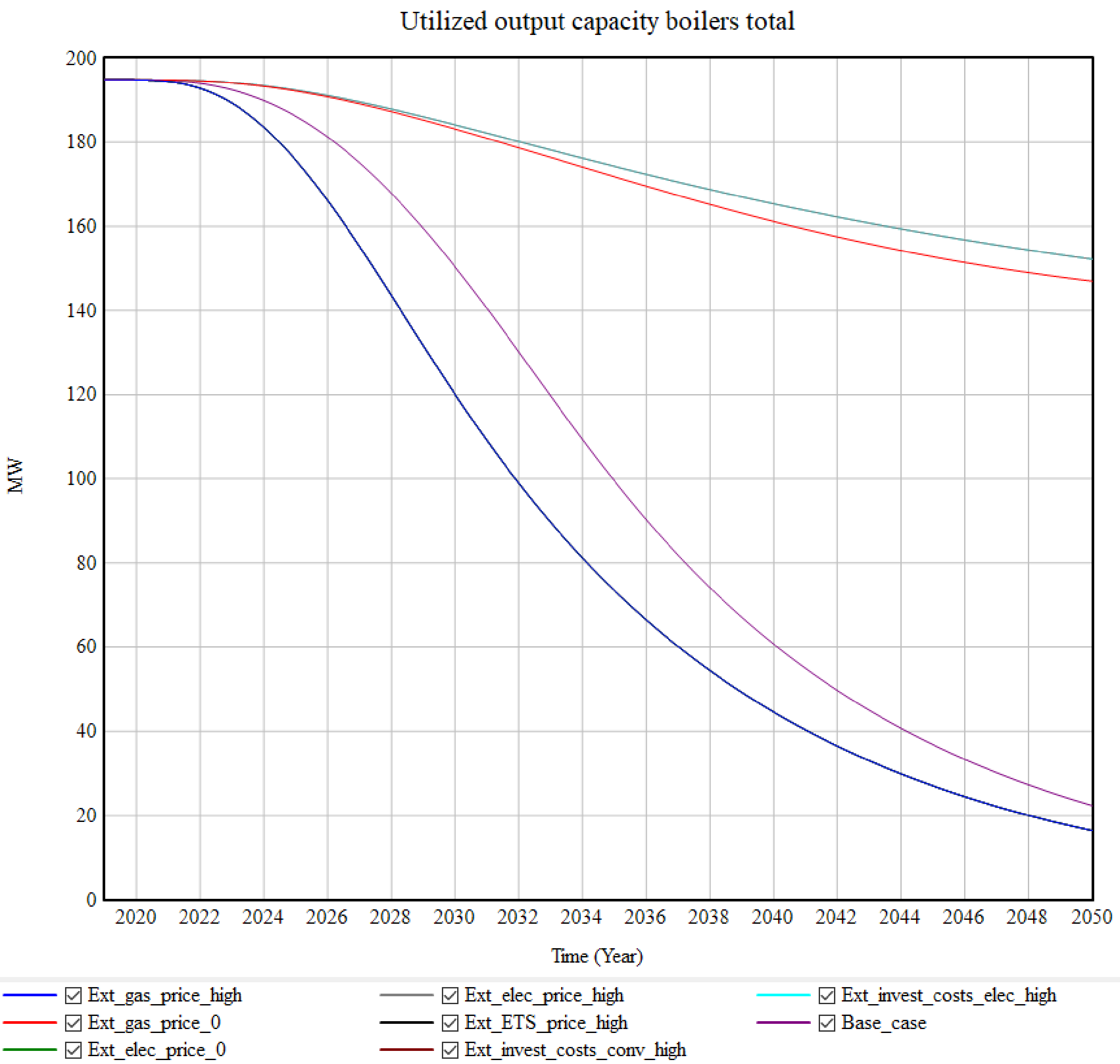

Figure 102: Simulation results of the extreme conditions tests for the utilized output capacity of the boiler installed (both gas boilers and electric boilers).

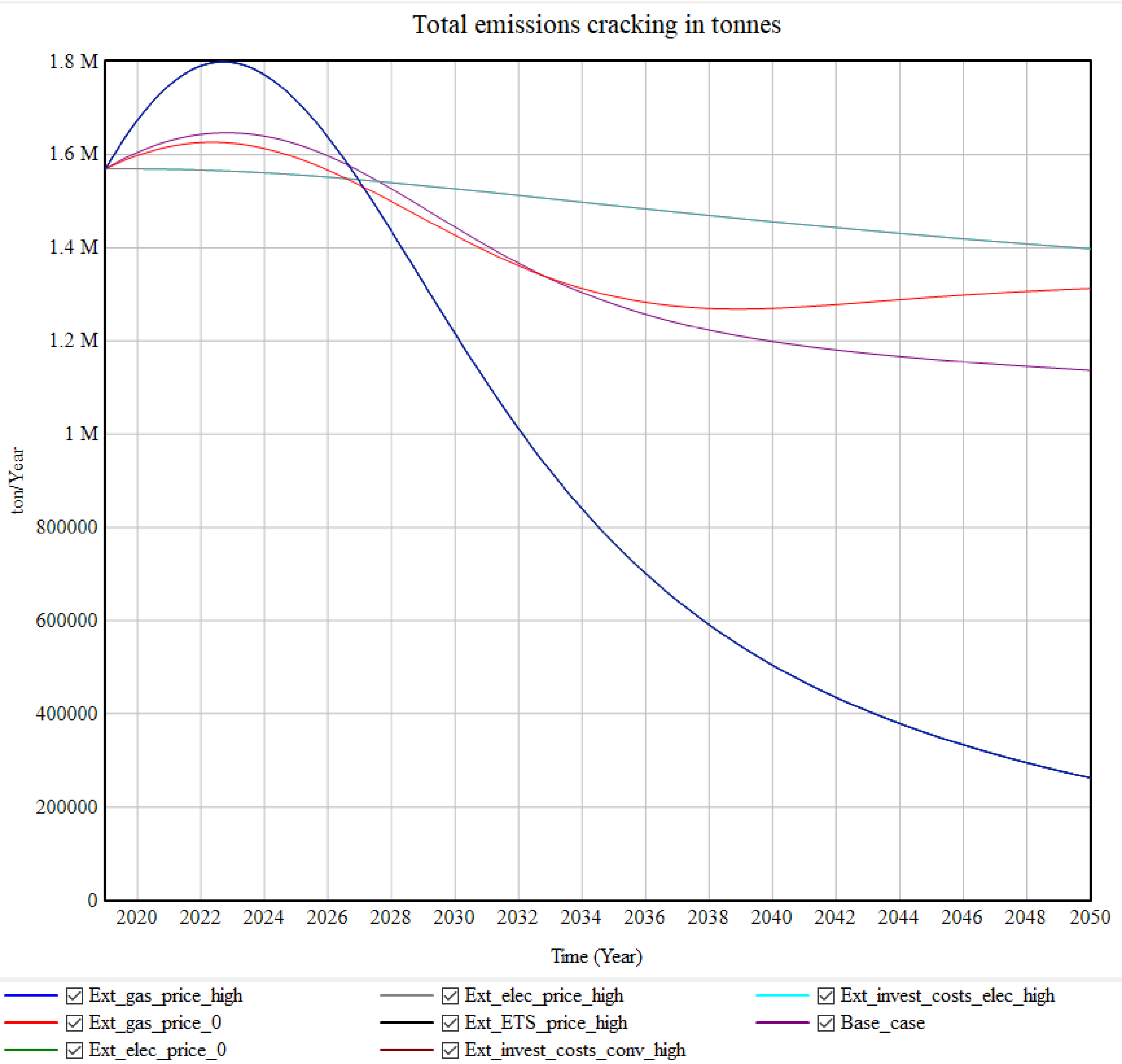

Figure 103: Simulation results of the extreme conditions tests for CO_2 emissions.

F.2 Sensitivity analysis

The following input parameters are varied in the analysis:

1. Electricity market price projection 2030
2. Gas market price projection 2030
3. Exogenous learning rate
4. Initial investment costs per MW: electric furnace, electric compressor turbine & electric boiler
5. Retrofit investment costs per MW: furnace, compressor turbine and boiler
6. Net calorific value gas
7. Response delay of investment share to costs ratio
8. Renewables share projection in 2030
9. Cracker production output (ethylene and propylene)
10. Base fee SDE++

The input parameters above are varied over a bandwidth of -10% to +10% with respect to their base case values (see Appendix E Table 3 for the values of the input parameters in the base case). No radical changes in behavior, or *behavioral sensitivity* as described by Sterman (2000), are expected to occur as a result of the input variations. Analogous to the simulation results of the extreme condition test, the CO_2 emissions are expected to "overshoot" in the short term and "undershoot" in the long term or vice versa as a result of the input variations. As has been described in Section 5.4.1 changes that benefit electrification and thus lead to an emissions reduction in the long term (2050) lead to an emissions increase in the short term due to the emission intensity of electricity being initially higher than the emission intensity of gas. This leads to a increasing-decreasing pattern in the CO_2 emissions curve. Input variations that benefit electrification (such as an electricity price projection of -10%) are expected to amplify this pattern, while input variations that counteract electrification are expected to dampen this pattern. As such, only *numerical sensitivity* is expected: where input variations only affect numerical values of the results. This implies no *policy sensitivity*, where input variations change the desirability of certain policies, is expected either (Sterman, 2000).
In Table 4 the expectations for the results of the sensitivity analysis in terms of the CO_2 emissions pattern are outlined.

Table 4: Expectations for the sensitivity analysis results in terms of the CO_2 emissions curve's pattern. For example: an electricity market price projection 2030 that changes +10% with respect to its base case value is expected to amplify the pattern, featuring lower emissions in the short term relative to the base case but higher emissions in 2050.

	Change with respect to base case	
Input parameter	+10%	-10%
Electricity market price projection 2030	Dampen	Amplify
Gas market price projection 2030	Amplify	Dampen
Exogenous learning rate	Amplify	Dampen
Initial investment costs per MW: electric furnace, electric compressor turbine & electric boiler	Dampen	Amplify
Retrofit investment costs per MW: furnace, compressor turbine and boiler	Amplify	Dampen
Net calorific value gas	Dampen	Amplify
Response delay of investment share to costs ratio	Dampen	Amplify
Renewables share projection in 2030	Amplify	Dampen
Cracker production output (ethylene and propylene)	Dampen	Amplify
Base fee SDE++	Amplify	Dampen

The results of the sensitivity analysis for the CO_2 emissions can be found in Figures 104 and 105. Figure 104 shows the simulation results for the input parameters that lead to *higher* emissions in 2050, while Figure 105

shows the simulation results for the input parameters that lead to *lower* emissions in 2050.
In most cases, the simulation results are as expected with input variations leading to an amplification of the emissions curve's pattern: an overshoot of emissions in the short term but lower emissions in 2050. However, changing *Renewables share projection in 2030* leads to slightly different behavior compared to the other input variations: it leads to a time-wise shift of the initial emissions peak rather than a larger or smaller overshoot. With a lower projected renewables share the emissions curve shifts to the right while with a higher projected renewables share the emissions curve shifts to the left. In the long term, the simulation results converge to the base case. This effect can be attributed to the fact that the impact of the projected renewables share on the emissions is twofold: a higher projected renewables share (1) leads to faster electrification as the carbon costs for electricity are lower and (2) influences emissions directly as the emissions resulting from electricity consumption are lower. Since in all cases the share of renewables approaches 100% it is explainable that in the long term the similation results for a higher/lower projected renewables share converge to the base case.

It should be noted that only the boilers are sensitive to these 10% changes in the input parameters. The electrification of furnaces remains 0 in all cases while the compressor turbines feature fast and complete electrification in all cases. This suggests that electrification of compressor turbines already provide a good business cases, while the electrification of furnaces requires more radical changes in the input parameters to yield a good business case.

In terms of sensitivity, the electricity price projection for 2030 has the largest impact on the CO_2 emissions of the input parameters included, followed by the SDE++ base fee and the projected renewables share in 2030. In Figure 106 the simulation results for these three input parameter CO_2 emissions are shown. As such, Figure 106 shows the bandwidth of the sensitivity analysis.

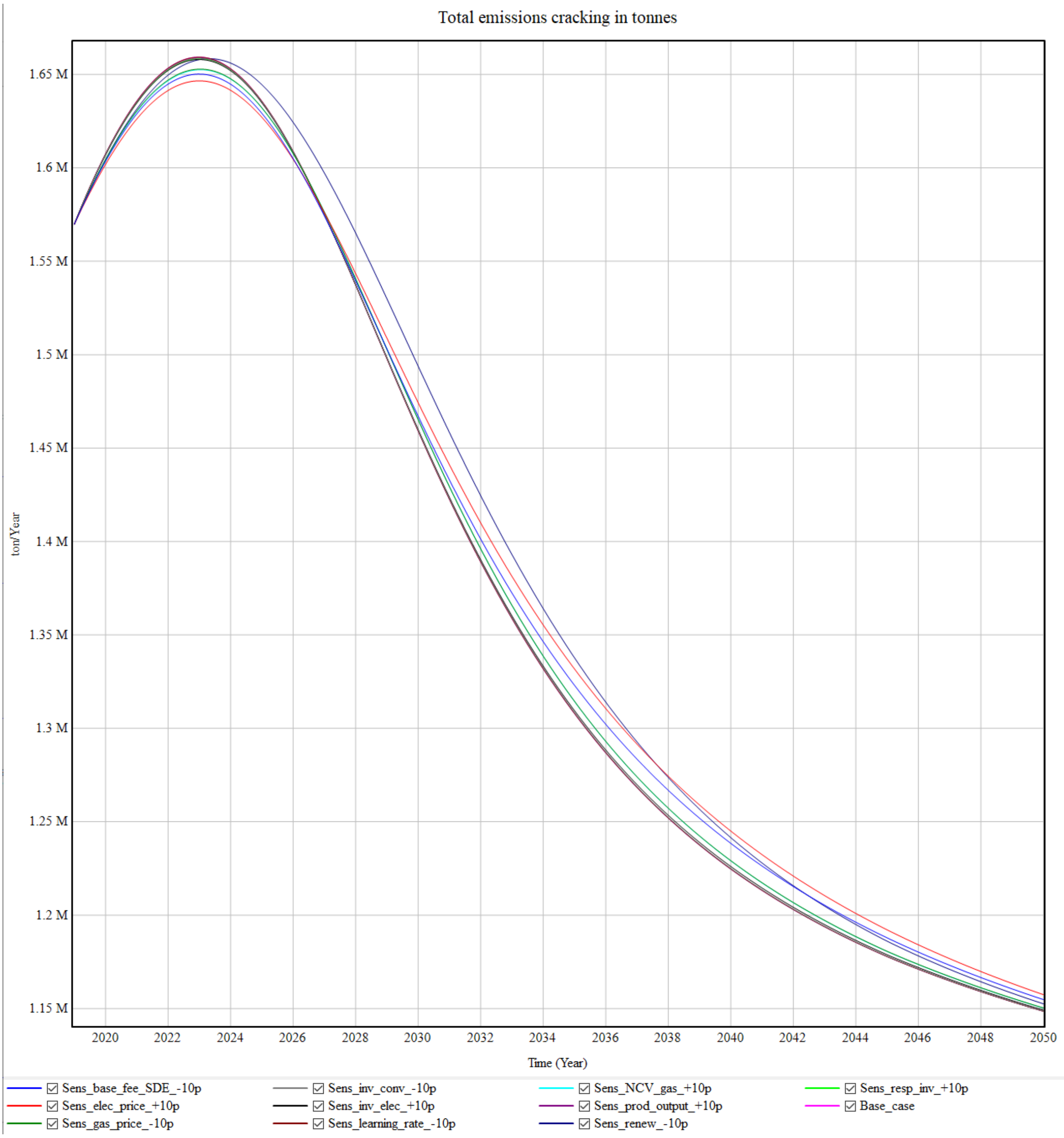

Figure 104: Sensitivity analysis: simulation of emissions [tonnes CO_2 per year] in the electrification model for input parameters that lead to higher emissions in 2050 compared to the base case.

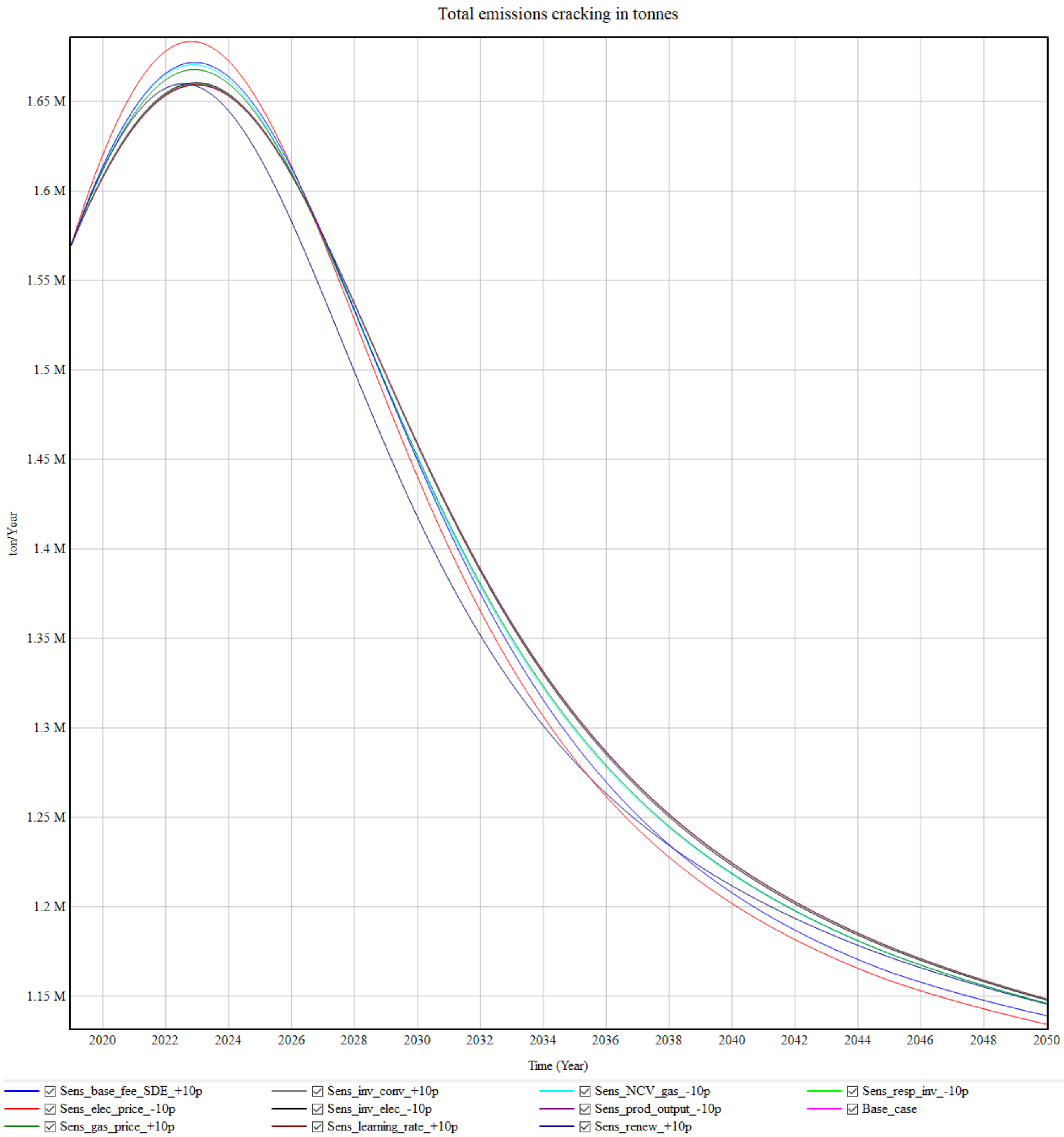

Figure 105: Sensitivity analysis: simulation of emissions [tonnes CO_2 per year] in the electrification model for input parameters that lead to lower emissions in 2050 compared to the base case.

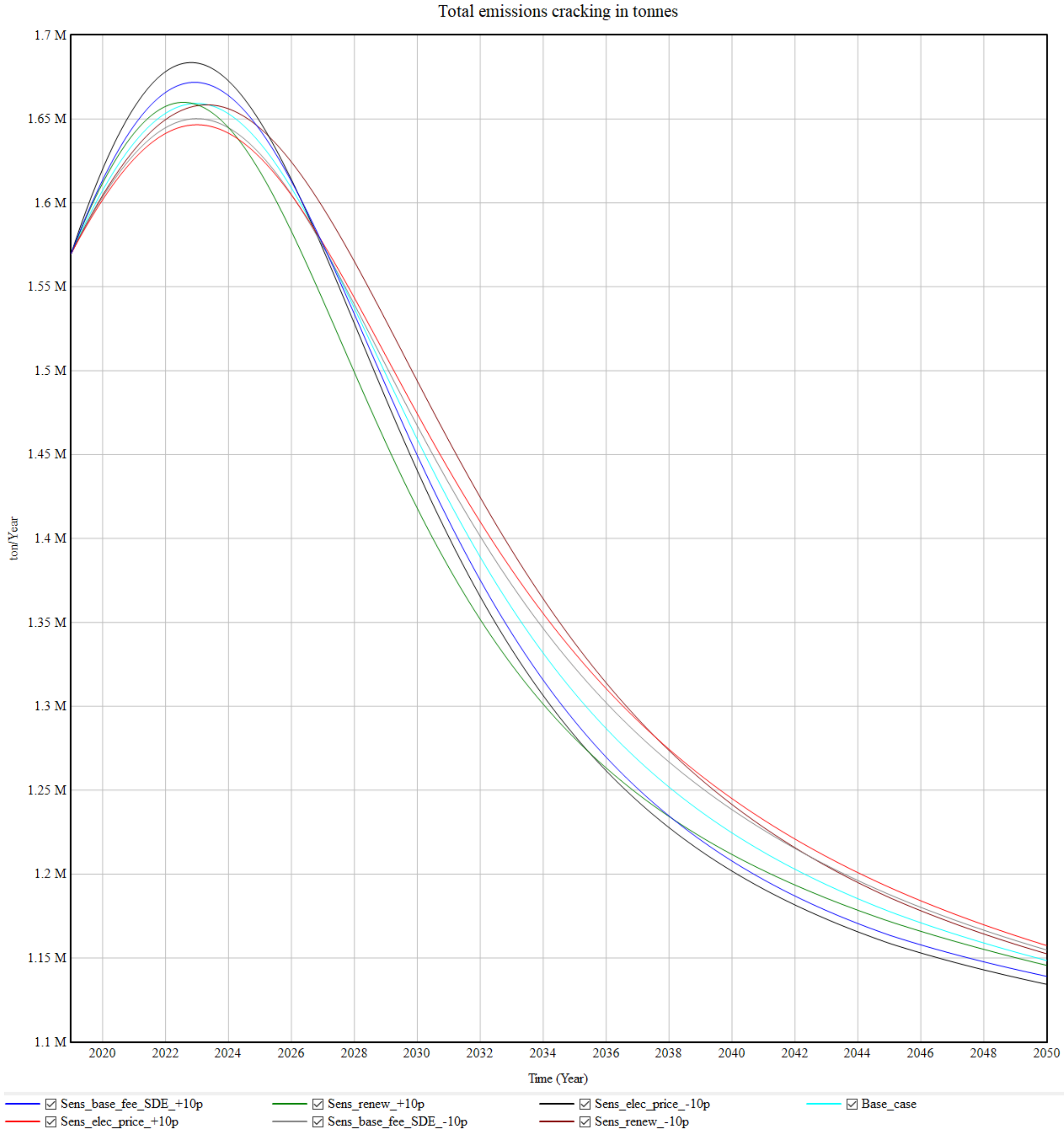

Figure 106: Sensitivity analysis: simulation of emissions [tonnes CO_2 per year] in the electrification model for the three input parameters that introduce the most sensitivity (following from Figures 104 and 105) with their values set at -10% and +10% of their base case values, respectively.

F.3 Face validity test

In a face validity test, experts assess how closely the model resembles the real-world system (Qudrat-Ullah, 2005). In this research, the model has been assessed by Klara Schure, senior consultant at Berenschot, in an interview with the author. This interview has been cited as: Schure (2021b). The face validity test concentrates on three aspects (Shreckengost, 1985; Sterman, 2000):

1. Model structure: does the structure of the model correspond to the structure of the real-world system and does every model component have a real-world counterpart?
2. Model boundary: are the system's most important concepts modelled endogenously?
3. Model behavior: is the behavior of the simulation results of the model representative of how the system behaves or is expected to behave?

Regarding the first aspect, the face validity test points out that the model structure is generally an adequate representation of the real-world system. However, the calculation of the SDE++ subsidy could be improved (Schure, 2021b). The SDE++ subsidy is computed by the Netherlands Environmental Assessment Agency (PBL) based on the so-called "unprofitable top", i.e., the difference between the base fee (the capital expenditures plus the expected operational expenditures corresponding to a particular technology) minus the correction fee (the gas and carbon costs that are avoided due to electrification) (Marsidi & Lensink, 2020b). Thus, in reality, the base fee is calculated based on the costs of a technology. However, in the model the base fee is an input parameter because it acts as a policy option rather than being modelled endogenously. This implies that the base fee is independent of the costs of the technologies considered. Therefore, the SDE++ calculation does not resemble the real-world situation.
Moreover, the SDE++ subsidy in the model is not linked to avoided CO_2 emissions. In reality, the Netherlands Enterprise Agency (RVO) grants SDE++ subsidies based on a ranking of technologies by their subsidy intensity in euro per tonne of avoided emissions (RVO, 2021). Because this ranking cannot be foreseen beforehand, it was not included in the model. Hence, in some cases, technologies are subsidized even though the electricity supply is still more emission-intensive than natural gas (Schure, 2021b).

Concerning the model boundary, it is concluded that most of the system's key concepts are included in the model. The model could be improved by including the product side of the industry. That is, the developments in the ethylene and propylene market and the effect of electrification on the production output (Schure, 2021b). These aspects also emerged from the interviews held among the industry (Interviews, 2021).
Moreover, including the lead times for grid capacity upgrades would have made the model outcomes more realistic. As the model implicitly assumes that the required electricity is readily available, it overlooks the potential delays incurred by required grid capacity upgrades. However, it is also concluded that this not impact the conclusions about policy options as the omission of this aspect does not alter the sequence of the simulation results (Schure, 2021b).
Although the model considers production costs and policy costs it would have been relevant to include *national costs* as an output parameter (Schure, 2021b). National costs, a common concepts in policy studies done by PBL, represent the balance of costs and benefits of certain policy for society as a whole. Moreover, the concept of national costs is broader than just monetary costs and often also incorporates air quality and environmental damage. The reason behind using the concept of national costs can be explained by the following example. The subsidies received by a company yield a financial benefit to that company but need to be levied on other companies or citizens through government intervention. Hence, these companies and citizens experience a combined financial disadvantage that may outweigh the benefit experienced by that one company. This implies the national costs amount to zero. Hence, using the concept of national costs provides insight in the costs and benefits for society as a whole (Koelemeijer & Strengers, 2020). Using the concept of national costs would also elicit under which conditions ethylene production in the Netherlands would remain favorable (Schure, 2021b).

The conclusions about the model behavior are closely connected to the discussion about the model model boundary. The pace of electrification in the reference mode may be rather fast due to the omission of the lead times for grid capacity upgrades. Therefore, emission reduction simulated in the reference mode may be larger than possible in reality (Schure, 2021b).
Moreover, a comment was made regarding the applicability of the model. There are obvious limits for which purposes the model can be used. The model is useful to study which policy could contribute to accelerating electrification on a macro-level. However, it should not be seen as a choice model for electrification or as a possible roadmap for electrification for the industry, i.e. micro-level purposes. Instead, electrification is the

starting point of the model and costs and benefits of electrification are highly scenario-dependent (Schure, 2021b).

G Implementation of EMA in Python

A considerable portion of the code for the implementation of EMA in Python are adaptations of the EMA workbench code provided by Kwakkel (2018), supplemented by additional functions written by the author. A few functions have also been adapted from van der Linden (2020). The code is made available on Github

H Uncertainty and decision spaces in the experiment design

In the context of Exploratory Modelling & Analysis (EMA) the system dynamics model is subjected to experiments, yielding a database of simulation results. In this appendix the design of the experiments is outlined. For each external factor the value ranges are reported in Table 5 and for the policy options in Table 6. Where possible, the value ranges for the uncertain factors have been based on reports and projection such as PBL (2020). However, sometimes assumptions had to be made. These are indicated in the tables and outlined below. For each policy option, the decision space has been explored in the “desirable” direction. That is, only increases in the gas tax are considered, while only reductions in the electricity tax have been considered. The policy bandwidths have been set such that the attainable value are not unrealistically large or small.

Table 5: Overview of the ranges of exogenous factors used for performing experiments with the EMA workbench on the electrification model.

	Unit	**Bottom value**	**Top value**	**Source**
Prices				
Electricity market price projection 2030	euro/MWh	33.3	71.9	PBL (2020)
ETS carbon price projection 2050	euro/ tonne$_{CO_2}$	40	1000	Aalbers et al. (2016)
Gas market price projection 2030	euro/m^3	0.16	0.319	PBL (2020)
Cost calculations				
Discount rate	%	10	15	Assumption 1
Exogenous learning rate	-	0	0.00928	Assumption 2
Export value of residual gas	%	0	100	-
Initial retrofit investment costs per MW electric boiler	euro/MW	$1{\cdot}10^5$	$5{\cdot}10^5$	Marsidi & Lensink (2020a)
Initial retrofit investment costs per MW electric compressor turbine	euro/MW	$1{\cdot}10^6$	$2{\cdot}10^6$	Assumption 3
Initial retrofit investment costs per MW electric furnace	euro/MW	$1.14{\cdot}10^6$	$3{\cdot}10^6$	Assumption 4
OPEX electric per year in percentage of investment costs	%	1	5	Assumption 5
Retrofit investment cost per MW boiler	euro/MW	$9.71{\cdot}10^3$	$5.50{\cdot}10^4$	Rutten (2019)
Retrofit investment cost per MW compressor	euro/MW	$6{\cdot}10^5$	$7.20{\cdot}10^5$	Rutten (2020)
Retrofit investment cost per MW furnace	euro/MW	$3{\cdot}10^5$	$1.14{\cdot}10^6$	Assumption 6
Energy & efficiency				
Efficiency improvements in conventional technologies	%/year	0	1	Assumption 7
S-curve parameters				
Response delay to gas becoming residual	-	5	50	Assumption 8
Response delay of investment share to costs ratio	-	5	50	Assumption 8
Response delay of investment share to costs ratio (hybrid boiler)	-	5	50	Assumption 8
Renewable electricity				
Renewables share projection in 2030	%	40	90	Assumption 9
Plant characteristics				
Time interval between turnarounds	year	5	7	Interviews (2021)
Capacity acquisition & depreciation				
Acquisition time hybrid boiler	year	1	3	Scholten et al. (2021)
Economic lifetime boilers	year	10	20	Assumption 10
Economic lifetime compressor turbines	year	10	20	Assumption 10
Economic lifetime furnaces	year	20	30	Assumption 10
Max. percentage of boilers to become hybrid per year	%	0	2.5	Assumption 11

Table 6: Overview of the ranges of policy levers and grid tariffs used for performing experiments with the EMA workbench on the electrification model.

	Unit	**Bottom value**	**Top value**	**Source**
Policy option				
Base fee SDE++	euro/kWh	0.07	0.14	Assumption 12
Carbon levy increase rate	euro/ (tonne$_{CO_2}$·year)	5.28	21.12	Assumption 13
Carbon levy increase rate after 2030	euro/ (tonne$_{CO_2}$·year)	0	21.12	Assumption 14
DPR switch	-	0	1	-
EHS grid connection costs	euro	$1.5 \cdot 10^6$	$3 \cdot 10^6$	ACM (2020)
Energy tax electricity	euro/MWh	0	0.56	Assumption 15
Gas tax	euro/m^3	0.01281	0.1281	Assumption 16
ODE electricity	euro/MWh	0	0.4	Assumption 15
ODE gas h	euro/m^3	0.0232	0.232	Assumption 16
Variable transport tariff (electric furnace and turbine)	euro/(kW·month)	0	1.23	Assumption 17
Variable transport tariff (e-boiler)	euro/(kW·month)	0	2.00	Assumption 18

A list of assumptions regarding the uncertainty and decision spaces is provided below:

1. Assumption 1. For commercial projects, usually a discount rate of 15% is used. However, strategic investments (sometimes concerning sustainability or decarbonization) tend to feature lower discount rates as low as 10% (Verbeek, 2021).

2. Assumption 2. Based on an assumed maximum cost reduction in electric technologies of 25% by 2050 (Jansen et al., 2019).

3. Assumption 3. Rather arbitrary range taken around the base case value of $1.375 \cdot 10^6$.

4. Assumption 4. As the technology of electric furnaces is not available on the market yet, the investment costs are highly uncertain. The lower bound is assumed to be at least the upper bound of the investment costs of conventional furnaces. The upper bound is chosen rather arbitrarily at $3 \cdot 10^6$ euro/MW.

5. Assumption 5. Fixed operations & maintenance (O&M) costs of electric technologies are known to be lower than their conventional counterparts (Interviews, 2021). In the model, the fixed O&M costs are expressed as a percentage of the investment costs. As estimation of the fixed O&M costs as a percentage of the investment costs has been made based on a comparison between electric versus conventional boilers. A TNO technology factsheet (Rutten, 2019) reports fixed O&M costs of 4-5% of the investment costs for conventional boilers, which is in line with Wong & van Dril (2020). By contrast, for electric boilers the O&M costs are 2% of the investment costs according to TNO (Marsidi & Lensink, 2020a). The lower bound is rather arbitrarily set at 1%. The upper bound is assumed equal 5%: the fixed O&M costs of conventional technologies as a percentage of the investment costs.

6. Assumption 6. Estimation made based on investment sums reported by industry representatives (Interviews, 2021).

7. Assumption 7. Stork et al. (2018) reports an autonomous energy efficiency improvement of 0.5-1% per year. It is assumed that this applies to efficiency improvements in conventional technologies too. 0% is chosen as a lower bound reflecting the worst-case scenario of no efficiency improvements.

8. Assumption 8. Value ranges established by trial and error. At a response delay of 5 the industry responds rather fast to changes in the expected costs and e.g. already channels 8% of its investments in electrification if the present value of electric retrofits is still 50% higher than the present value of conventional retrofits. By contrast, at a response delay of 50 the industry responds abruptly to price expectations and only start to invest in electrification once the present value of electric retrofit equals the present value of conventional retrofits.

9. Assumption 9. Value range chosen rather arbitrarily around the goal of 75% renewable electricity set in the Climate Agreement.
10. Assumption 10. Based on an economic lifetime ranging from 0.5 of the technical lifetime to almost equal to the technical lifetime.
11. Assumption 11. Value range established based on trial and error. The upper bound is based on the expectation that a maximum of 5 MW per year could be subject to boiler hybridization in the current configuration (Schure, 2021a). Higher values would result an excessive pace of boiler hybridization causing much redundant boiler capacity, as steam demand is reduced due to electrification of compressor turbines. 0 is taken as the lower bound, reflecting the scenario the the industry is not inclined to invest in boiler hybridization.
12. Assumption 12. Lower bound chosen the base fee for electric boilers reported by Marsidi & Lensink (2020b). Note that no categories in the SDE++ exist for electric furnaces and electric compressor turbines and hence, a universal base fee was assumed for all three technologies. The upper bound is chosen at twice this base fee. Note that in a new PBL report (Marsidi et al., 2021) a base fee for electric boilers is advised at 0.05 euro/kWh.
13. Assumption 13. The lower bound is arbitrarily set at half the current carbon levy increase rate of 10.56 euro/(tonne·year) (NEa, 2020) and the upper bound at twice this value.
14. Assumption 14. The carbon levy increase rate post-2030 is varied from 0 to twice the current increase rate of the carbon levy (NEa, 2020).
15. Assumption 15. Regarding the electricity tax and ODE electricity, the upper bound is the current value (Belastingdienst, 2020) while the lower bound is arbitrarily set at 0 reflecting a far-reaching fiscal shift favoring electricity consumption.
16. Assumption 16. Regarding the gas tax and ODE gas, the lower bound is the current value (Belastingdienst, 2020) while the upper bound is arbitrarily set at 10 times this value reflecting a far-reaching fiscal shift discouraging gas consumption.
17. Assumption 17. The upper bound is set at the current grid tariff for the HV grid ACM (2020), the lower bound is set at 0.
18. Assumption 18. The upper bound is set at the current grid tariff for the MV grid Liander (2020), the lower bound is set at 0.

I Additional results of the experiments

In this appendix additional results of the experiments performed in Chapter 6 can be found.

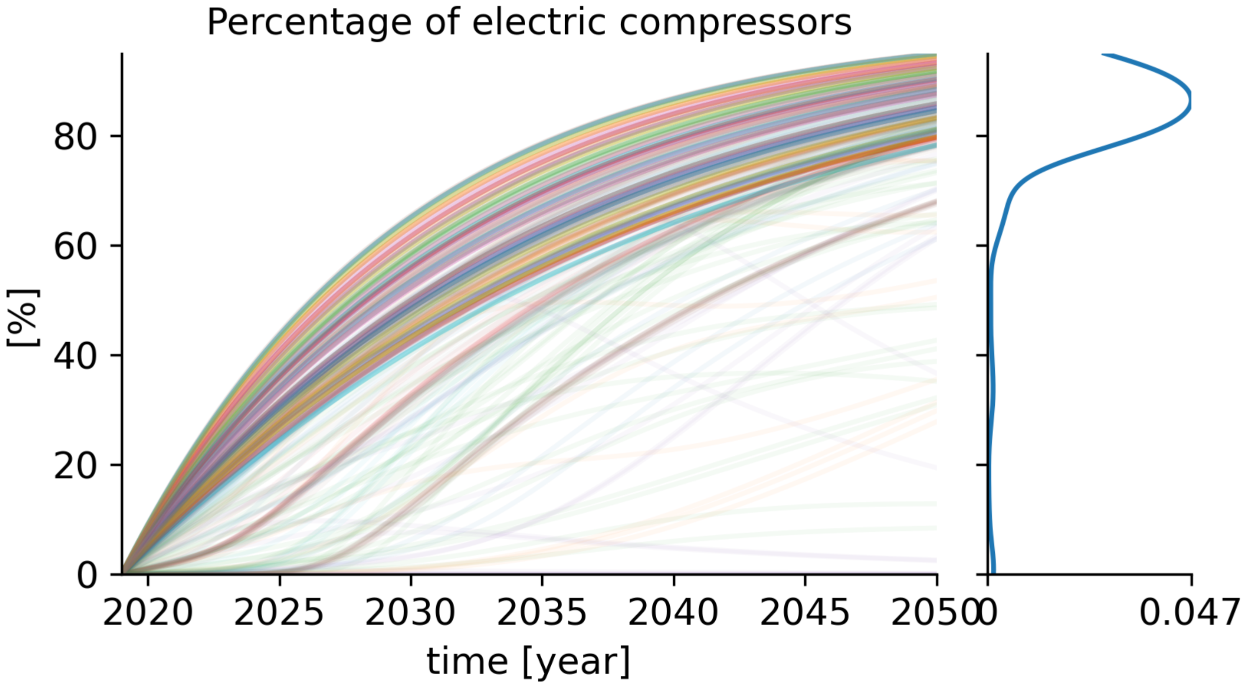

Figure 107: Simulation results for percentage of electric compressors in percentage of the total output capacity. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot.

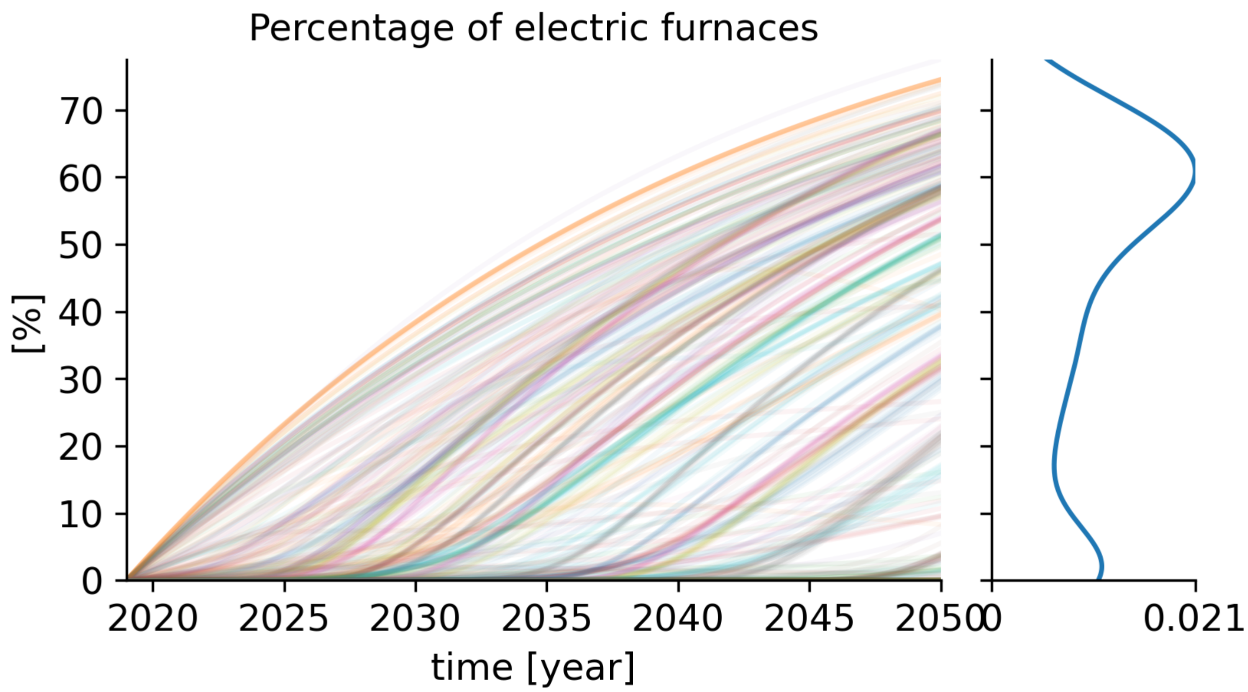

Figure 108: Simulation results for percentage of electric furnaces in percentage of the total output capacity. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot.

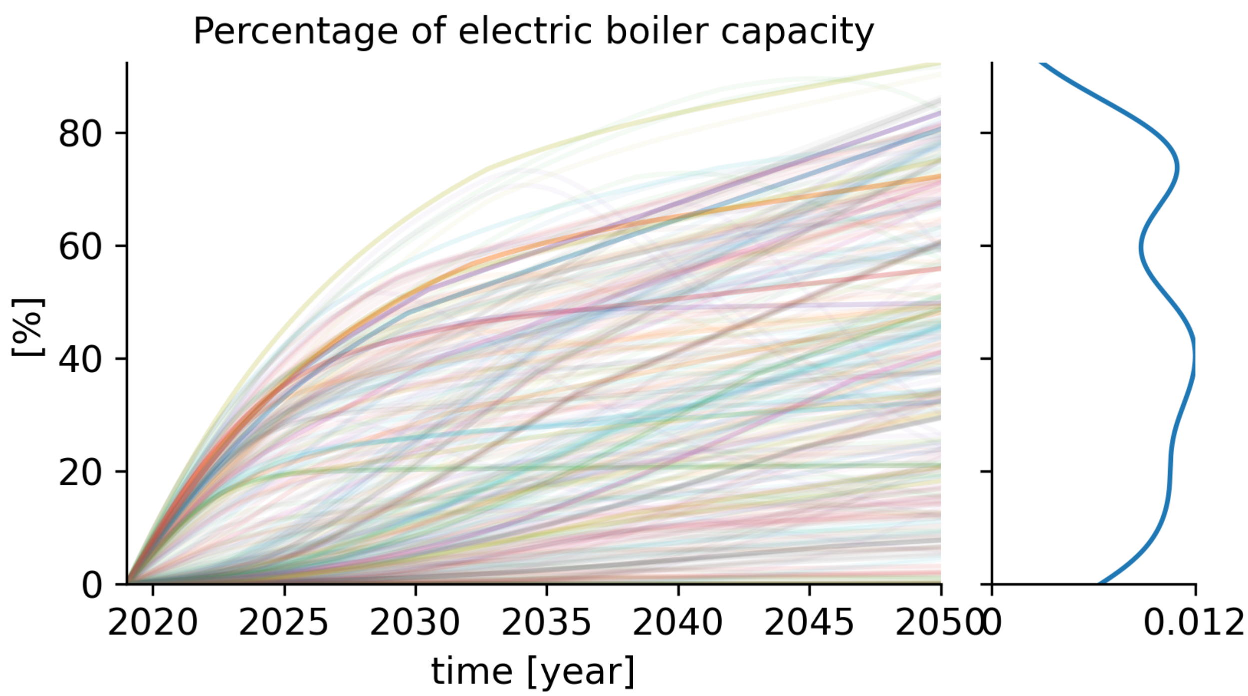

Figure 109: Simulation results for percentage of electric boilers in percentage of the total output capacity. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot.

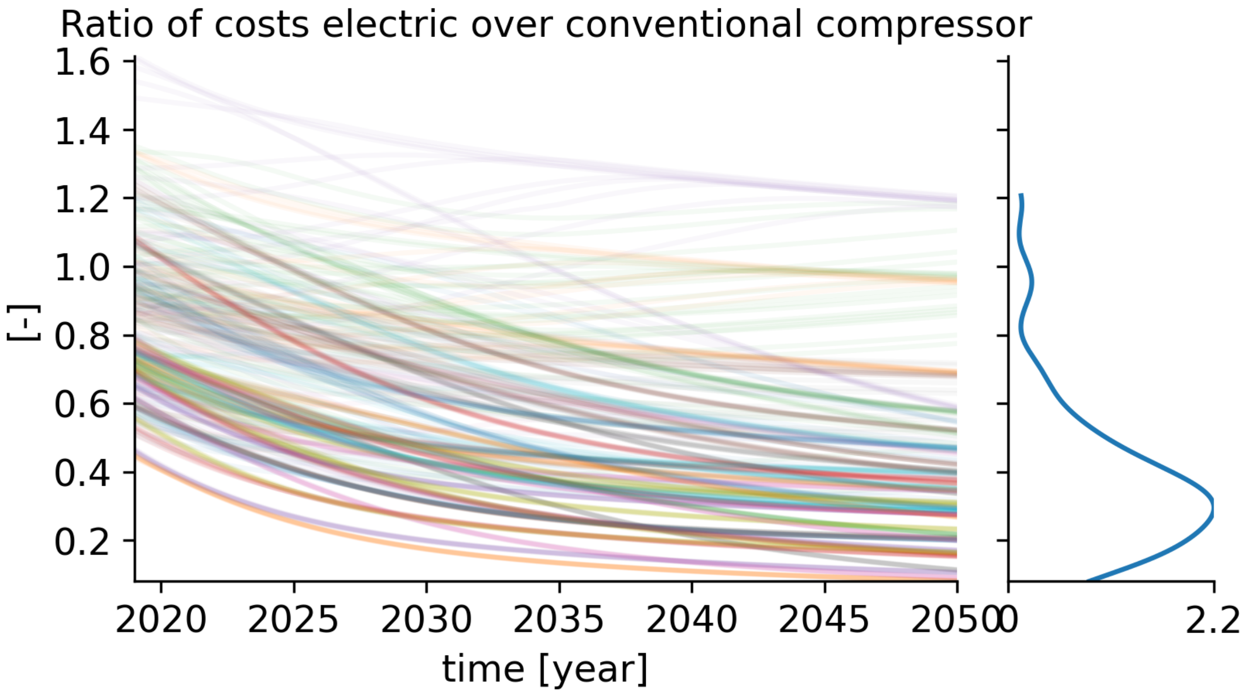

Figure 110: Simulation results for the ratio of the present value for electric retrofits over the present value of conventional retrofit, compressors. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot.

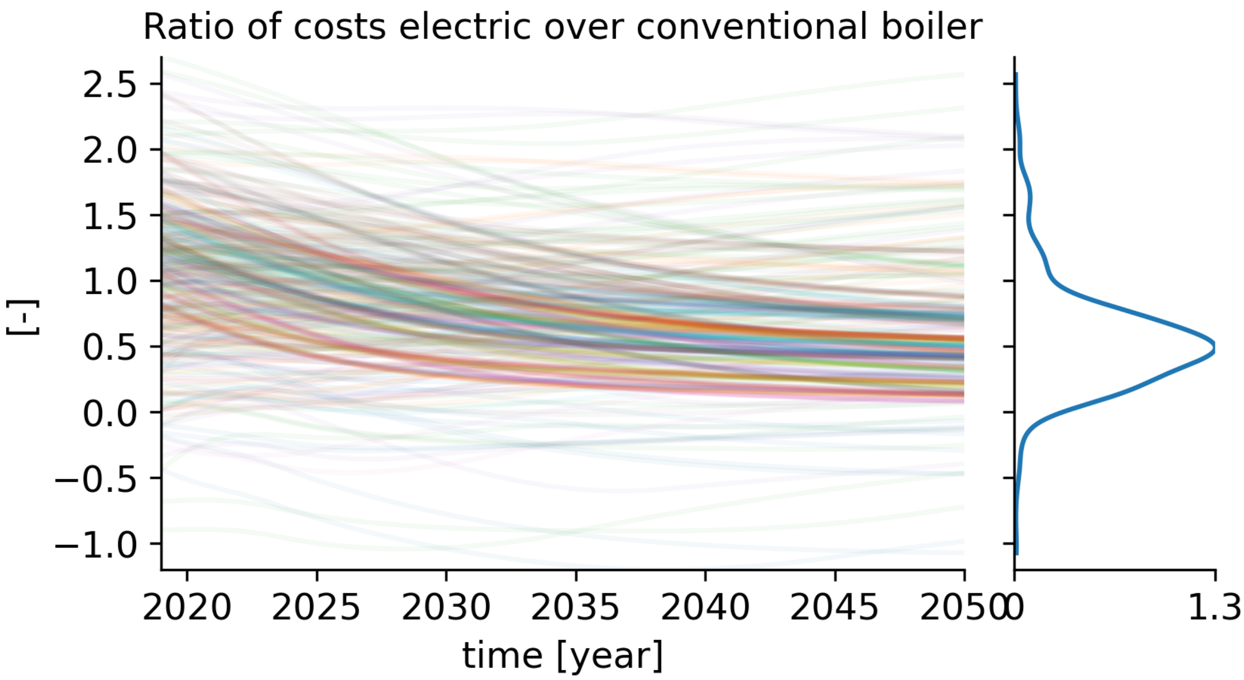

Figure 111: Simulation results for the ratio of the present value for electric retrofits over the present value of conventional retrofit, boilers. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot.

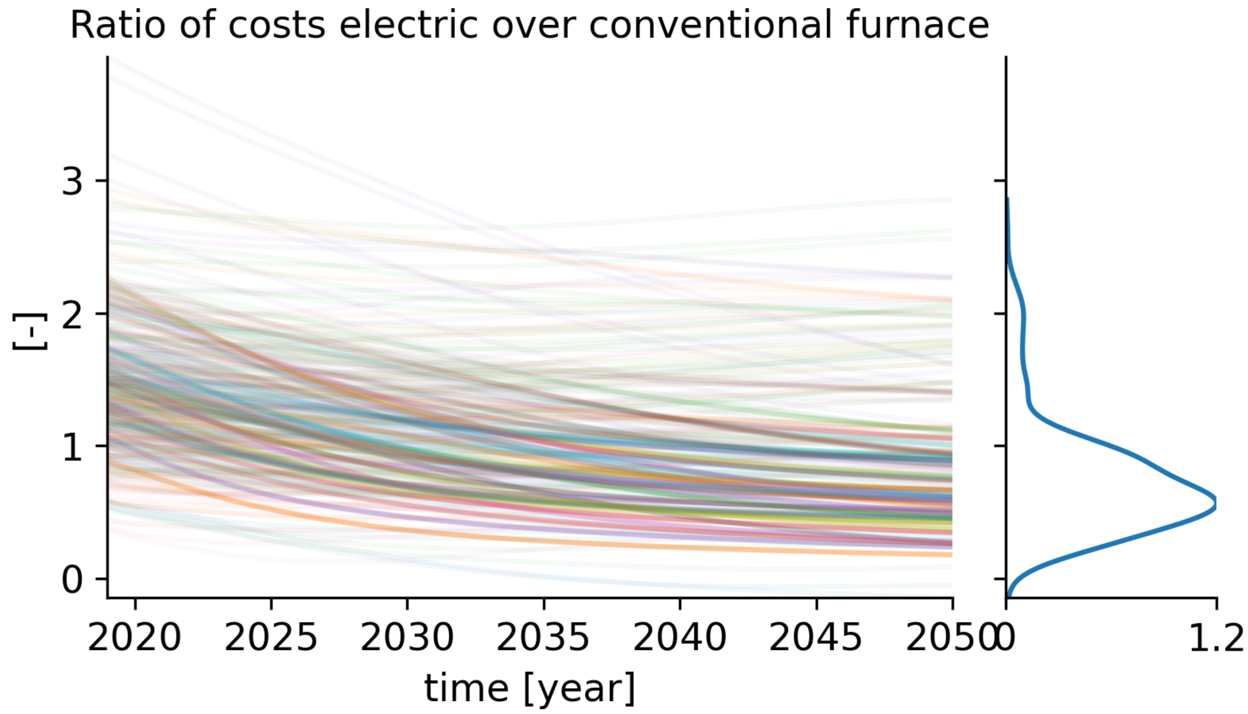

Figure 112: Simulation results for the ratio of the present value for electric retrofits over the present value of conventional retrofit, furnaces. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot.

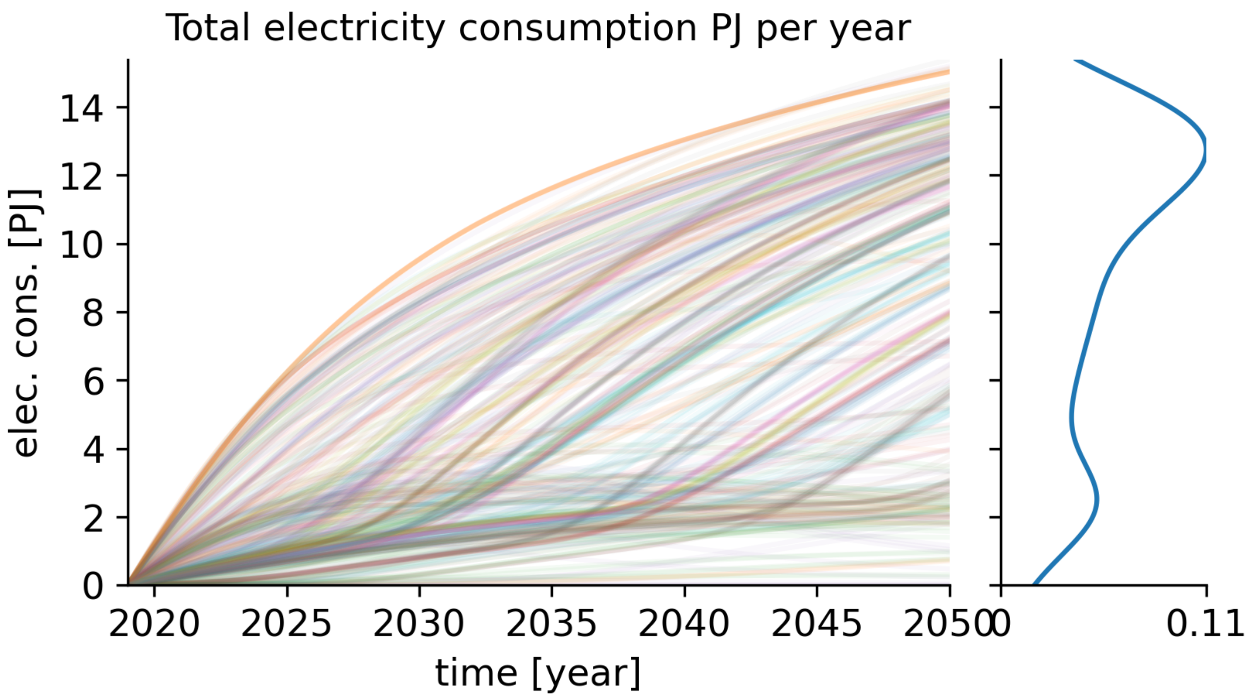

Figure 113: Simulation results for the total electricity consumption. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot.

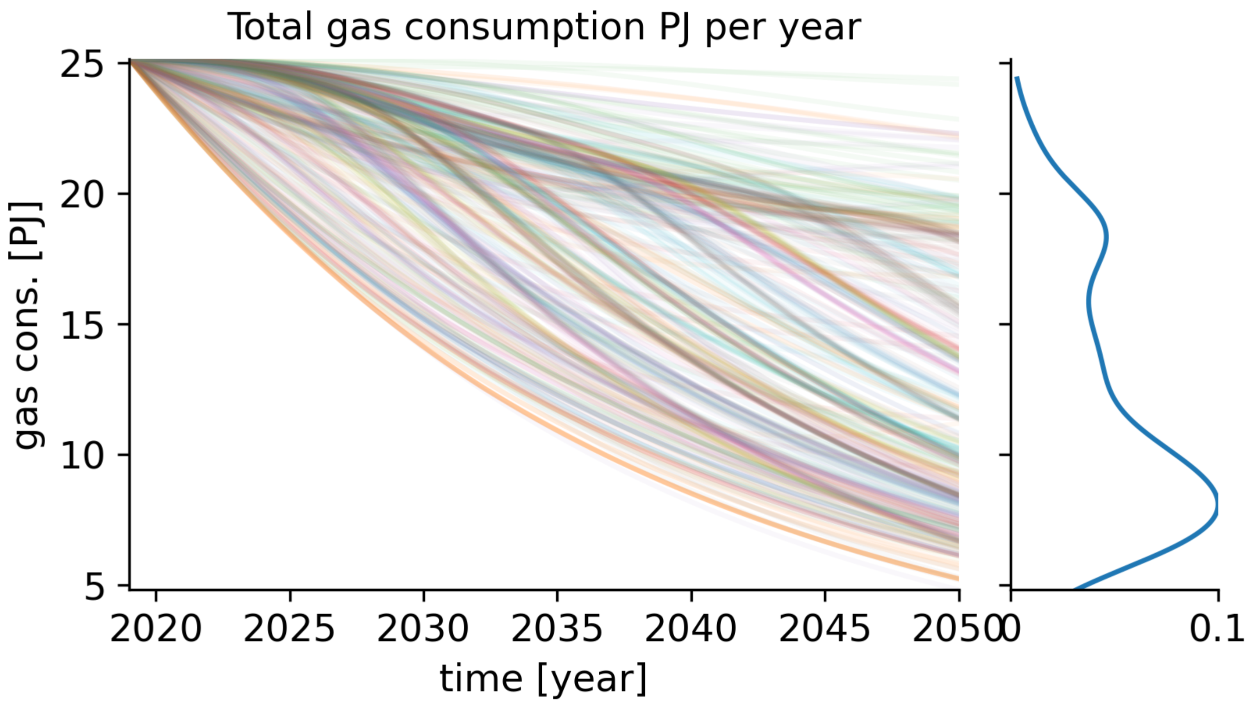

Figure 114: Simulation results for the total gas consumption. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot.

J Robust policy search: further background

In this appendix more details are given concerning the robust policy search performed in Chapter 6.5. First, in Section J.1 the theoretical background of robustness and the multi-objective robust optimization performed in this study will be given. Second, in Section J.2 the concept of robustness metrics will be discussed. Thirs, the selected robustness metrics are outlined in Section J.3.

J.1 Multi-objective robust optimization: theoretical background

Multi-objective optimization problems are optimization problems in which multiple objectives are to be either minimized or maximized (Deb, 2011). The multi-objective optimization problem in this study could be formulated as follows: minimize cumulative CO_2 emissions while also minimizing cumulative production costs and cumulative policy costs. More specifically, this research considers a *constrained* multi-objective optimization problem as the decision parameters considered (policy options and grid tariffs) are not allowed to attain unrealistically high or low values. Instead, they should satisfy certain boundaries as outlined in Appendix H.

The optimal solutions of a multi-objective optimization problem are termed the *Pareto-optimal set*. In turn, a solution is said to be part of the Pareto-optimal set if it is *nondominated* by any of the other solutions considered in the optimization problem. Mathematically, a solution x_1 is regarded as *nondominated* by another solution x_2 if (1) x_1 does not perform worse than x_2 in any of the objective and (2) x_1 performs evidently better than x_2 in at least one of the objectives considered (Deb, 2011). For complex problems, it often proves difficult to find all feasible solutions. Therefore, scholars normally seek the best approximate of the Pareto-optimal set, which is denoted as the *Pareto-approximate set* (Kasprzyk et al., 2013).

However, Pareto-optimal or Pareto-approximate solutions turn out vulnerable, if not extremely vulnerable, to changes in the problem's input parameters (Sniedovich, 2016). Consequently, a solution may perform well in a particular plausible future but its performance may perform (very) badly in another. This feature should definitely be taken into when studying complex systems featuring deep uncertainty, because, as we have seen in Chapter 6, the outcomes of a simulation model representing such a system may strongly depend on uncertain exogenous factors. Therefore, making decisions based on solutions that are deemed Pareto-optimal may not be practical in the context of complex socio-technical systems like electrification in the naphtha cracking industry (Deb & Gupta, 2006).
Therefore, when formulating a multi-objective optimization problem for such systems systems, the concept of *robustness* is introduced. In a multi-objective *robust* optimization problem we seek solutions that perform well across a range of plausible futures instead of a particular plausible future (Lempert, 2002; C. Brown & Asce, 2010; Hine & Hall, 2010; C. Brown et al., 2011). How performance is defined in this regard will be further discussed in Section J.2.

To deal with the intricacies posed by complex socio-technical systems considerable research has been performed over the last few years on multi-objective evolutionary algorithms (MOEAs), a family of algorithms that are fit to deal with constrained, non-linear problems. MOEAs can also deal with decision space features characteristic for complex socio-technical systems, such as large dimensions (Coello et al., 2007; Nicklow et al., 2010; Reed et al., 2013).
Two important concepts related to MOEAs are *convergence* and *diversity*. The higher the convergence of a MOEA, the closer the Pareto-approximate solutions set yielded by the algorithm has come to the theoretical Pareto-optimal front. Diversity, on the other hand, indicates the distribution of the solutions across the entire Pareto front (Kasprzyk et al., 2013).

J.2 Defining robustness: an introduction to robustness metrics

There is no single definition of robustness. In fact, many different robustness metrics exist that capture a variety of decision-maker attitudes, ranging from high to low levels of risk aversion (Giuliani & Castelletti, 2016; McPhail & Maier, 2018). Moreover, decision-maker preferences change over time as they gain new experiences and knowledge related to the system they are trying to influence (Guiso et al., 2013; Giuliani & Castelletti, 2016).
The choice of robustness metric greatly influences the solution of a robust decision-making problem. In fact, different robustness metrics can lead to mutually conflicting solutions. Therefore, in the literature on robustness metrics it is often suggested to consider multiple robustness metrics simultaneously and combine the results

from each of the metrics (Giuliani & Castelletti, 2016; Kwakkel, Eker, & Pruyt, 2016; McPhail & Maier, 2018).

Four main categories of robustness metrics can be distinguished (McPhail & Maier, 2018):

- Expected value metrics (Wald, 1950): these metrics provide an indication of the expected performance (e.g. the mean performance) across a range of plausible futures.
- Metrics of higher-order moments (e.g. skewness and peakedness (Kwakkel, Eker, & Pruyt, 2016)): these metrics are a measure of the variation of performance across a range of plausible futures.
- Regret-based metrics (Savage, 1951), which compares the performance of a particular decision alternative with the performance of another option, such as the best-performing alternative or the median performance.
- Satisficing metrics (Simon, 1956), which calculates the number of plausible futures in which a decision alternative have satisfactory performance. Whether performance is satisfactory or not is based on a certain threshold.

Beside this classification, robustness metrics can be classified according to their levels of risk aversion (McPhail & Maier, 2018). There are many more classifications possible but it is outside of the scope of this study to discuss all the different robustness metrics and their properties in detail.
Based on a review of Giuliani & Castelletti (2016), Kwakkel, Eker, & Pruyt (2016) and McPhail & Maier (2018) three metrics were selected which were chosen such that they reflect a variety types and levels of risk aversion. The selected metrics are outlined in Section J.3.

J.3 Overview of the selected robustness metrics

Regarding the multi-objective robust optimization in this study, three robustness metrics are considered, which were selected based on a literature scan (Giuliani & Castelletti (2016), Kwakkel, Eker, & Pruyt (2016) and McPhail & Maier (2018)). In the following, $f_i(x)$ represents the robustness function as a function of the performance x for performance indicator i. Hence, $f_i(x)$ represents the robustness function for the cumulative CO_2 emissions $f_{CO_2}(x)$, the cumulative production costs $f_{prod.costs.}(x)$ or the cumulative policy costs costs $f_{pol.costs.}(x)$.

1. **Maximin** (Wald, 1950): minimization of worst-case performance across the range of plausible futures. It is an expected value metric with the highest level of risk aversion relative to other metrics studied by McPhail & Maier (2018). Mathematically, the maximin metric is defined as follows (Kwakkel, Eker, & Pruyt, 2016):
$$f_i(x) = \begin{cases} \max(\mathbf{x}_i), & \text{minimization} \\ \min(\mathbf{x}_i), & \text{maximization} \end{cases} \tag{67}$$
where $\mathbf{x}_i$ is a vector containing the performance values of performance indicator i for each plausible future.
2. **Undesirable deviations** (Kwakkel, Eker, & Pruyt (2016)[7]): minimization of undesirable deviations from the median performance. Regret-based metric with a high level of risk aversion, but lower than maximin (McPhail & Maier, 2018). The undesirable deviations metric is defined as follows:
$$f_i(x) = \begin{cases} -\mu_i, \sum\limits_{k=1}^{k} (x_k - q_{50})^2 \; [x_k > q_{50}], & \text{minimization} \\ \mu_i, \sum\limits_{k=1}^{k} (x_k - q_{50})^2 \; [x_k < q_{50}], & \text{maximization} \end{cases} \tag{68}$$
where μ_i is the mean performance of performance indicator i, x_k is the performance of performance indicator i in plausible future k and q_{50} is the median performance of performance indicator i. Note that this metric only considers the worst half of the outcomes: the performance scores x_k above the median performance q_{50} in case of minimization and the performance scores x_k below the median performance q_{50} in case of maximization. Further note that this metric effectively doubles the number of objectives as the mean μ_i and the deviation are formulated as separate objectives.

[7]Adaptation from Takriti & Ahmed (2004)

3. **Percentile-based peakedness** (Kwakkel, Eker, & Pruyt (2016)[8]): minimization of the *kurtosis*, a measure of peakedness, of performance across the range of plausible futures. This metric is mathematically defined as:

$$f_i(x) = \begin{cases} -\mu_i, \frac{q_{90}-q_{10}}{q_{75}-q_{25}}, & \text{minimization} \\ \mu_i, \frac{q_{90}-q_{10}}{q_{75}-q_{25}}, & \text{maximization} \end{cases} \tag{69}$$

where q_{10}, q_{25}, q_{75} and q_{90} are the 10^{th}, 25^{th}, 75^{th} and 90^{th} percentiles of the range of outcomes for performance indicator i, respectively. A higher kurtosis $\frac{q_{90}-q_{10}}{q_{75}-q_{25}}$ is an indication of a distribution of outcomes of performance indicator i that has a stronger peak-shape around the mean.

[8] Adaptation from Voudouris et al. (2014)

K Background analyses for the robust policy search

In this appendix the additional results of the multi-objective are presented. First, in Section K.1 the analysis of the outcomes of the robust optimization is presented which is the basis for the selection of the candidate policies in Section 6.5.2. Section K.2 contains the simulation outcomes of the experiments performed using the candidate policies.

K.1 Analysis of the outcomes of the robust optimization

As discussed in Section 6.5.1 the robust optimizations yielded three databases of robust policies, one for each optimization. These databases were analyzed based on parallel coordinate plots. From this analysis, a subset of 21 policies was selected that have been subjected to further simulation. In this section a few examples of parallel coordinate plots are displayed that were used for the selection of candidate policies. Each plot shows a subset of the results of one of the multi-objective robust optimizations. Based on the characteristics of each subset the candidate policies for performing the experiments were selected. These policies were selected such that they are representative for the diversity of the robust results. The selected policies are distributed over the robust optimizations as follows:

- Policies 0-4: robust optimization 1
- Policies 5-15: robust optimization 2
- Policies 16-20: robust optimization 3

K.1.1 Parallel coordinate plots for robust optimization 1

The results from robust optimization 1 were divided into 11 subsets, based on their outcomes for the maximum emissions. In Figures 115 and 116 two subsets of results are shown.

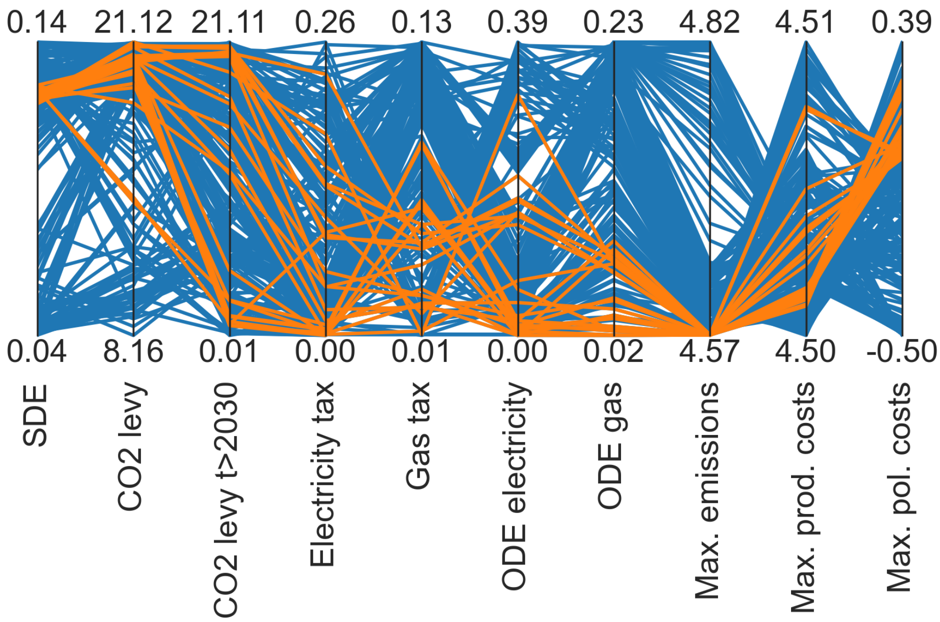

Figure 115: Parallel coordinate plot of subset 1 of the robust results from the multi-objective robust optimization based on robustness metric 1 (maximin). Each line represents a robust policy: the position of the line on a particular axis represent the value for the corresponding policy option. On the left side the policies are shown, to the right the outcomes of the optimization are displayed. Note that the grid tariffs and the DPR switch are not shown.

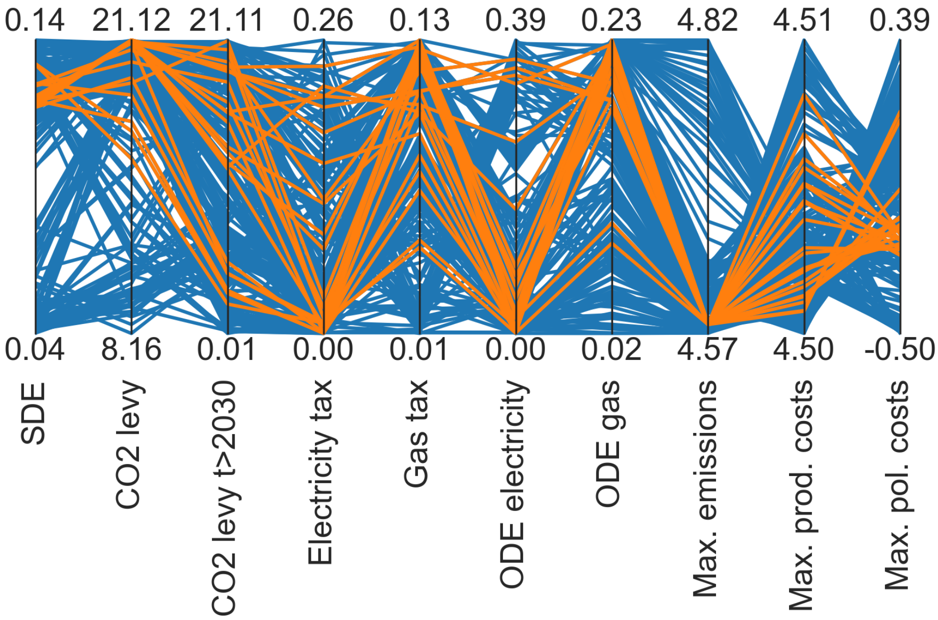

Figure 116: Parallel coordinate plot of subset 2 of the robust results from the multi-objective robust optimization based on robustness metric 1 (maximin). Each line represents a robust policy: the position of the line on a particular axis represent the value for the corresponding policy option. On the left side the policies are shown, to the right the outcomes of the optimization are displayed. Note that the grid tariffs and the DPR switch are not shown.

K.1.2 Parallel coordinate plots for robust optimization 2

The results from robust optimization 2 were divided into 39 subsets, based on their outcomes for deviations in emissions. Figures 117 to 120 show 4 subsets of results.

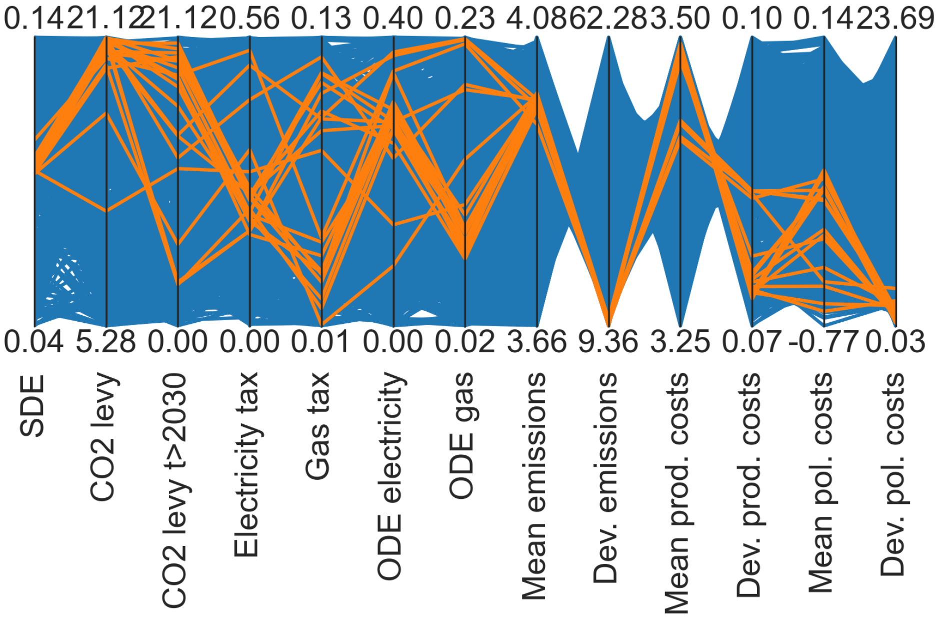

Figure 117: Parallel coordinate plot of subset 1 of the robust results from the multi-objective robust optimization based on robustness metric 2 (undesirable deviations). Each line represents a robust policy: the position of the line on a particular axis represent the value for the corresponding policy option. On the left side the policies are shown, to the right the outcomes of the optimization are displayed. Note that the grid tariffs and the DPR switch are not shown.

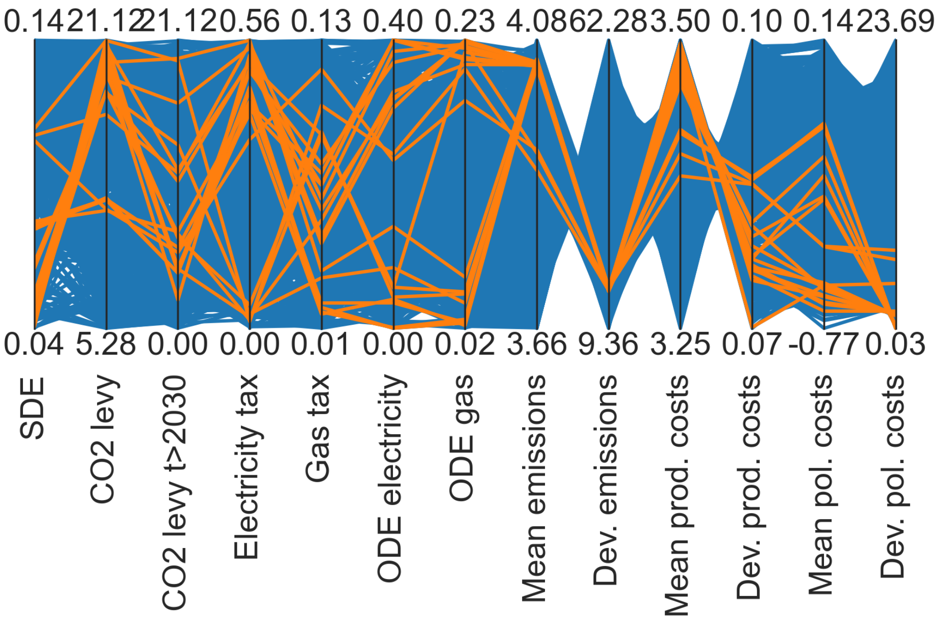

Figure 118: Parallel coordinate plot of subset 2 of the robust results from the multi-objective robust optimization based on robustness metric 2 (undesirable deviations). Each line represents a robust policy: the position of the line on a particular axis represent the value for the corresponding policy option. On the left side the policies are shown, to the right the outcomes of the optimization are displayed. Note that the grid tariffs and the DPR switch are not shown.

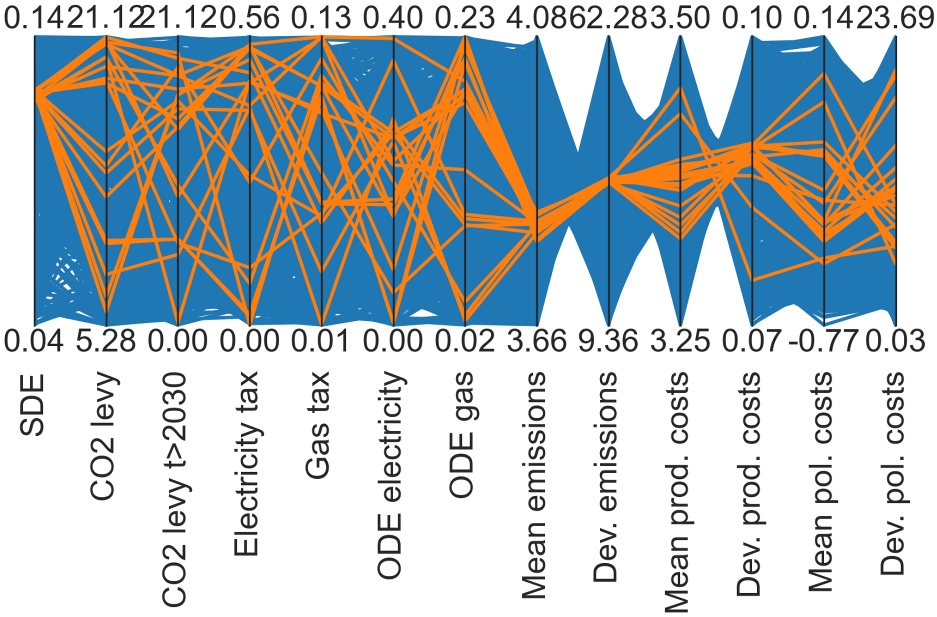

Figure 119: Parallel coordinate plot of subset 3 of the robust results from the multi-objective robust optimization based on robustness metric 2 (undesirable deviations). Each line represents a robust policy: the position of the line on a particular axis represent the value for the corresponding policy option. On the left side the policies are shown, to the right the outcomes of the optimization are displayed. Note that the grid tariffs and the DPR switch are not shown.

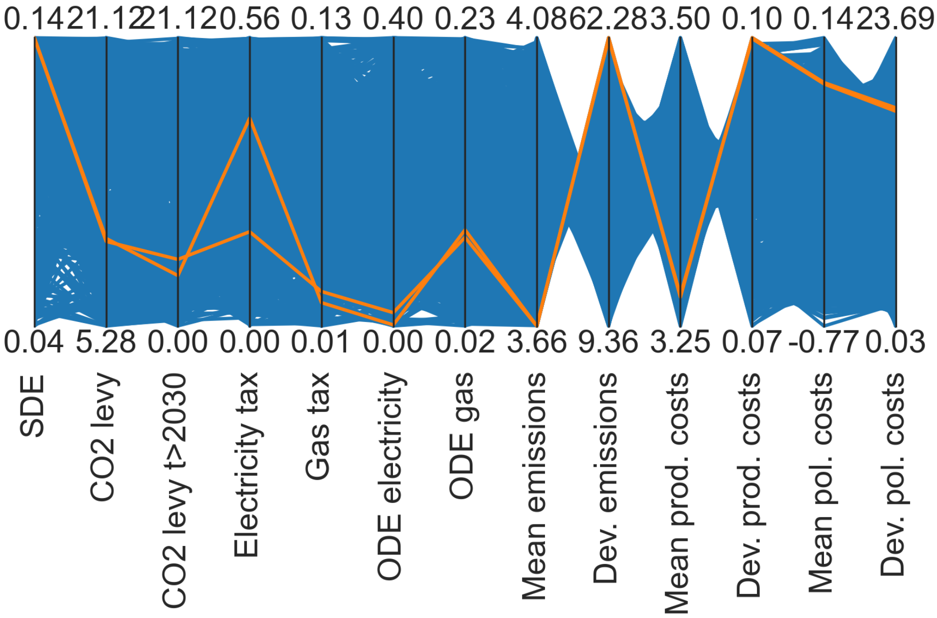

Figure 120: Parallel coordinate plot of subset 4 of the robust results from the multi-objective robust optimization based on robustness metric 2 (undesirable deviations). Each line represents a robust policy: the position of the line on a particular axis represent the value for the corresponding policy option. On the left side the policies are shown, to the right the outcomes of the optimization are displayed. Note that the grid tariffs and the DPR switch are not shown.

K.1.3 Parallel coordinate plots for robust optimization 3

The results from robust optimization were divided into 15 subsets, based on their outcomes for the peakedness in the outcome distribution of emissions (denoted P emissions). Figures 121 to 123 show three subsets of results.

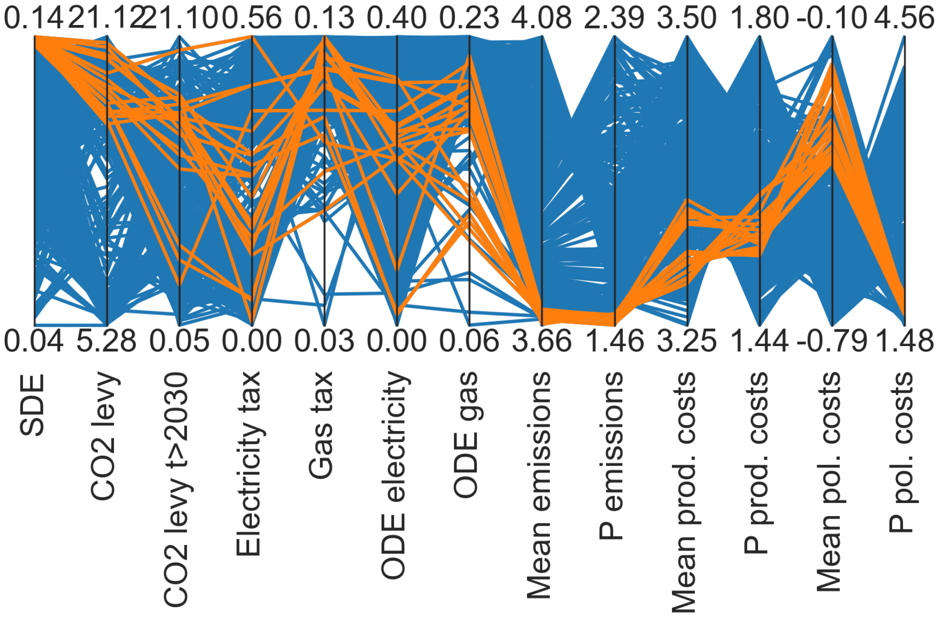

Figure 121: Parallel coordinate plot of subset 1 of the robust results from the multi-objective robust optimization based on robustness metric 3 (percentile-based peakedness). Each line represents a robust policy: the position of the line on a particular axis represent the value for the corresponding policy option. On the left side the policies are shown, to the right the outcomes of the optimization are displayed. Note that the grid tariffs and the DPR switch are not shown.

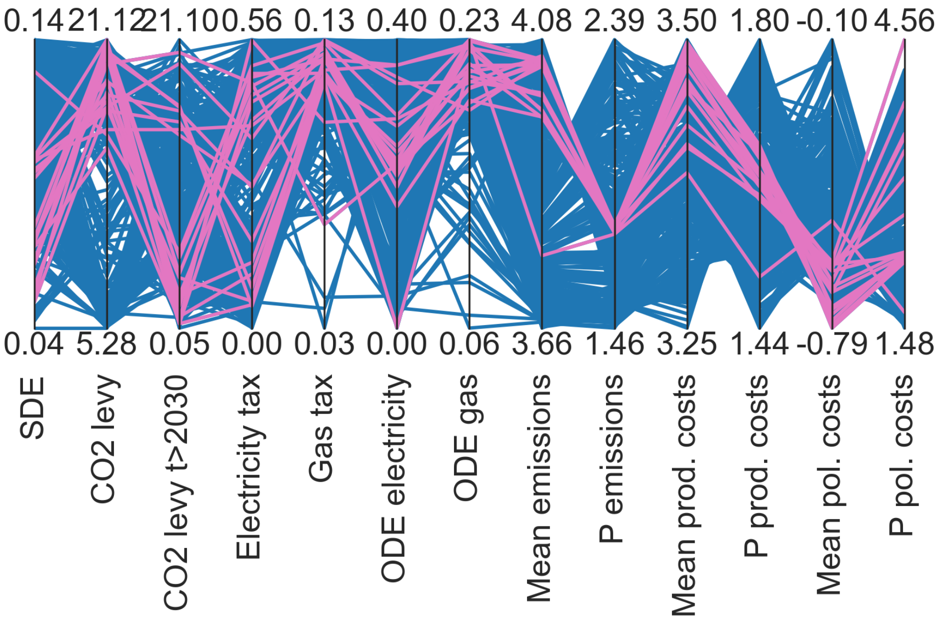

Figure 122: Parallel coordinate plot of subset 2 of the robust results from the multi-objective robust optimization based on robustness metric 3 (percentile-based peakedness). Each line represents a robust policy: the position of the line on a particular axis represent the value for the corresponding policy option. On the left side the policies are shown, to the right the outcomes of the optimization are displayed. Note that the grid tariffs and the DPR switch are not shown.

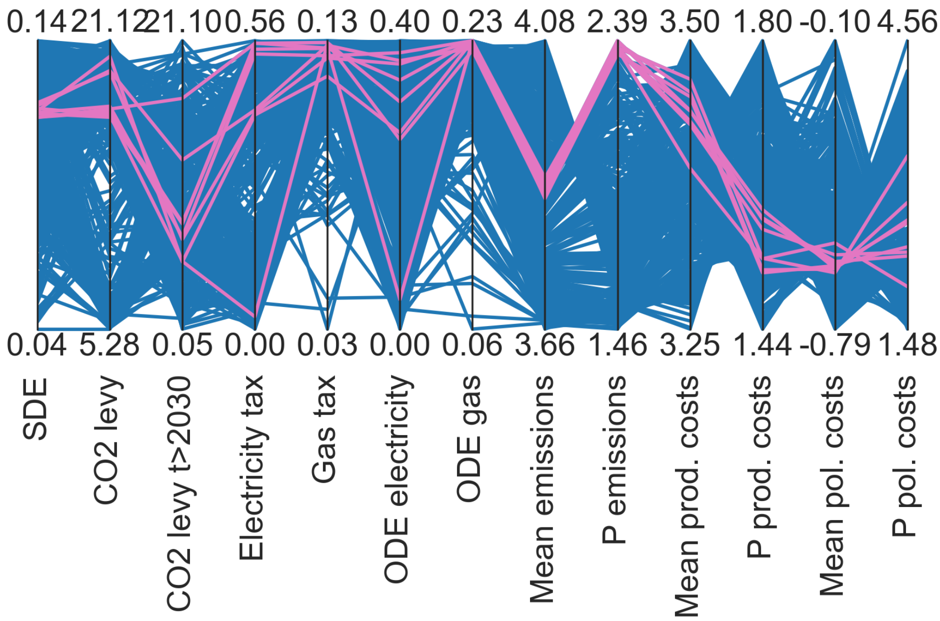

Figure 123: Parallel coordinate plot of subset 3 of the robust results from the multi-objective robust optimization based on robustness metric 3 (percentile-based peakedness). Each line represents a robust policy: the position of the line on a particular axis represent the value for the corresponding policy option. On the left side the policies are shown, to the right the outcomes of the optimization are displayed. Note that the grid tariffs and the DPR switch are not shown.

K.2 Visual analysis of the simulation results

The subset of 21 policies that were selected based on the parallel coordinate plots presented in Section K.1 were fed back into the simulation model through the performance of experiments. This yielded a database of simulation results which was then subjected to visual analysis. Below the results can be found for each of the key performance indicators. The results have been divided over 4 subsets of policies: (1) policies 0-4, (2) policies 5-10, (3) policies 11-15 and (4) policies 16-20.

K.2.1 Cumulative CO_2 emissions

Regarding the cumulative CO_2 emissions it can be clearly seen in Figure 124 that some policies result in fewer deviations but at the expense of a higher concentration of results at the top of the emissions spectrum. By contrast, other policies result in a higher concentration on the lower end of the spectrum but show considerable deviations towards the higher end of the spectrum. With regard to emissions, the latter is deemed favorable because these policies result in a higher probability of the emissions attaining lower values, though the risk of high emissions still exist. From the analysis of Figures 125 to 128 it is concluded that regarding emissions policies 15 and 16 are the best-performing policies.

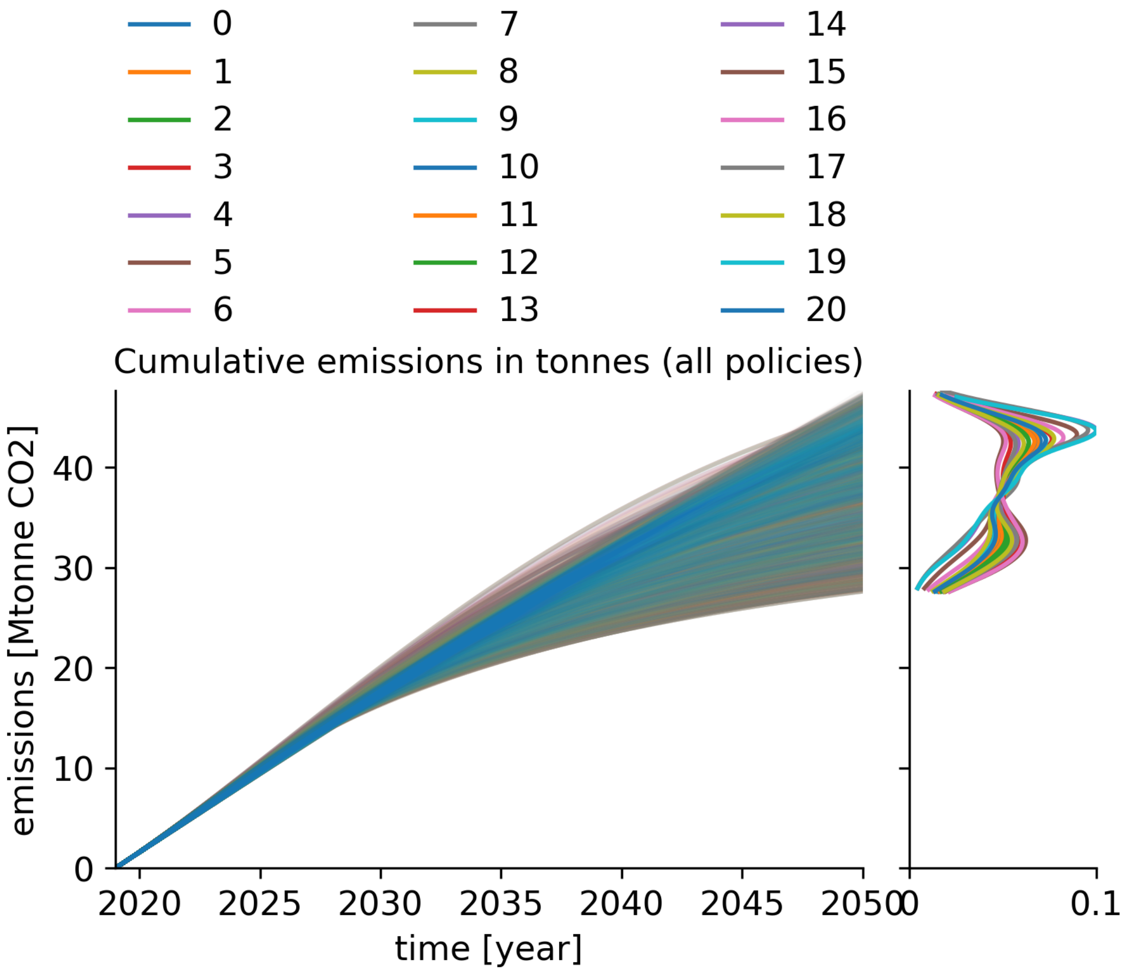

Figure 124: Simulation results for the cumulative CO_2 emissions associated to naphtha cracking for the reference plant, including all of the 21 selected robust policies. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

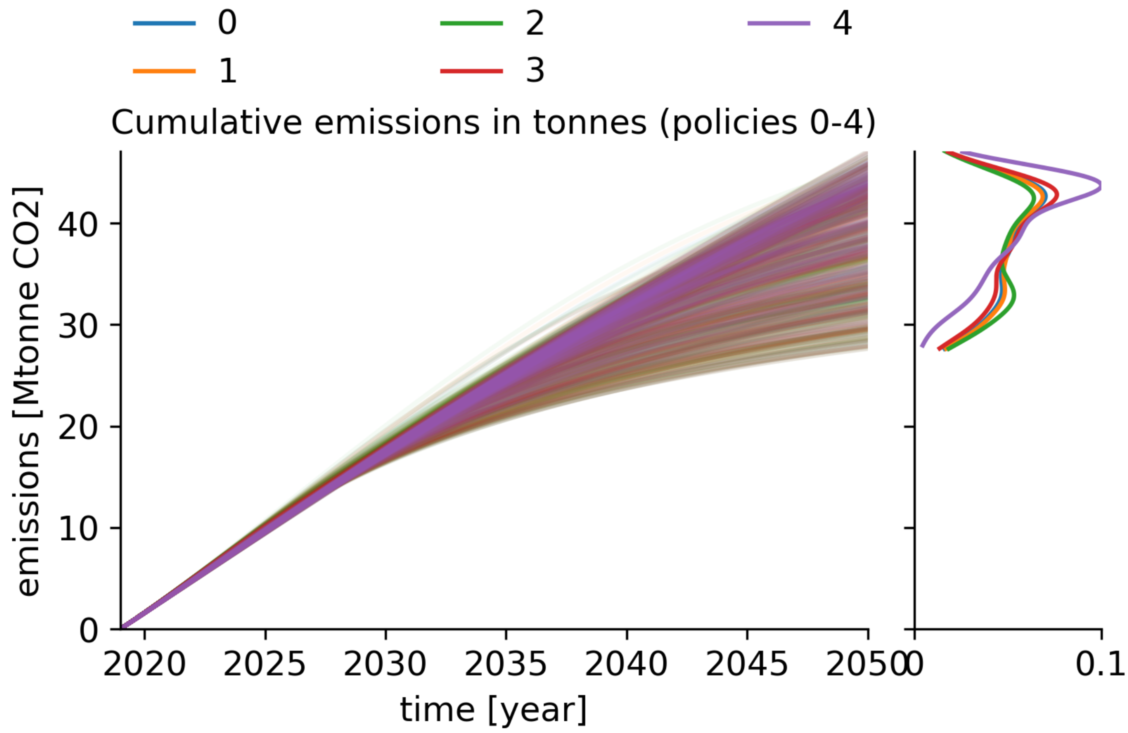

Figure 125: Simulation results for the cumulative CO_2 emissions associated to naphtha cracking for the reference plant, for selected robust policies 0-4. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

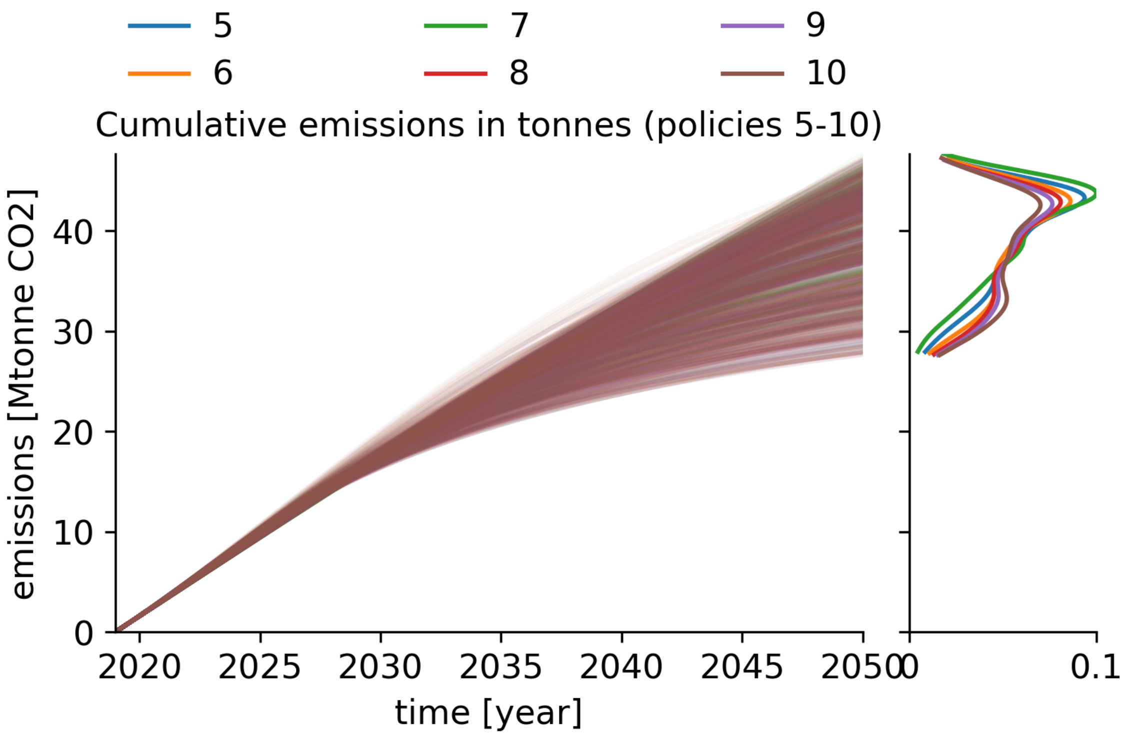

Figure 126: Simulation results for the cumulative CO_2 emissions associated to naphtha cracking for the reference plant, for selected robust policies 5-10. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

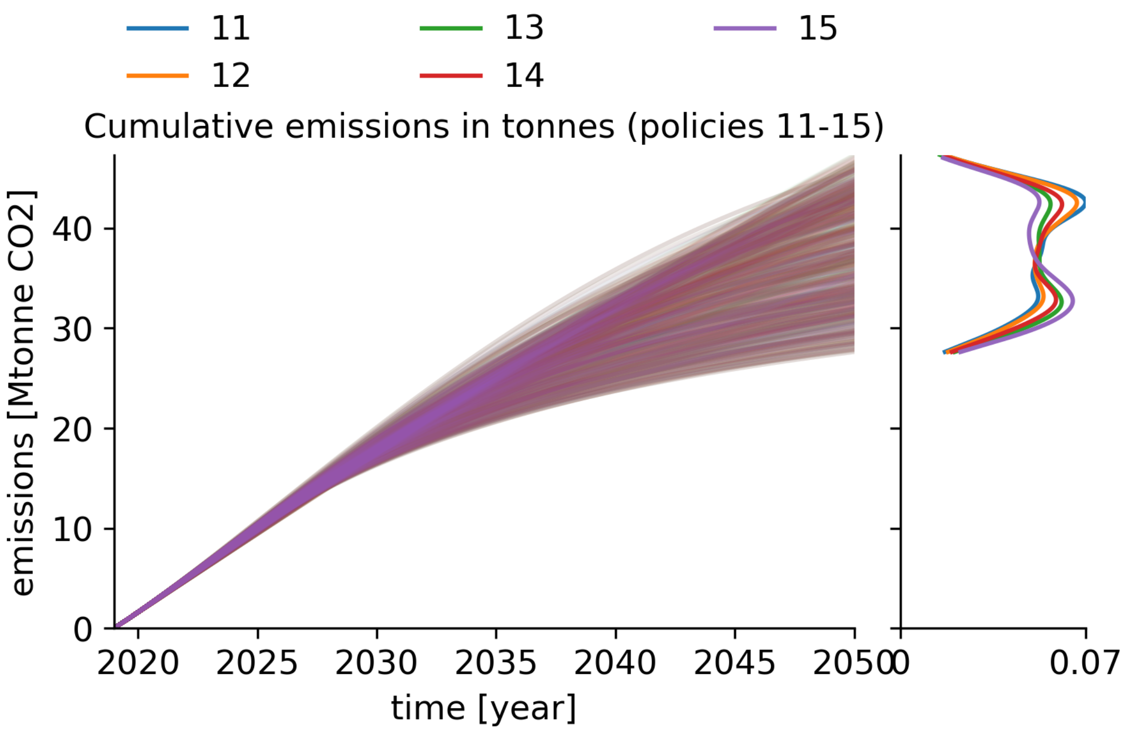

Figure 127: Simulation results for the cumulative CO_2 emissions associated to naphtha cracking for the reference plant, for selected robust policies 11-15. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

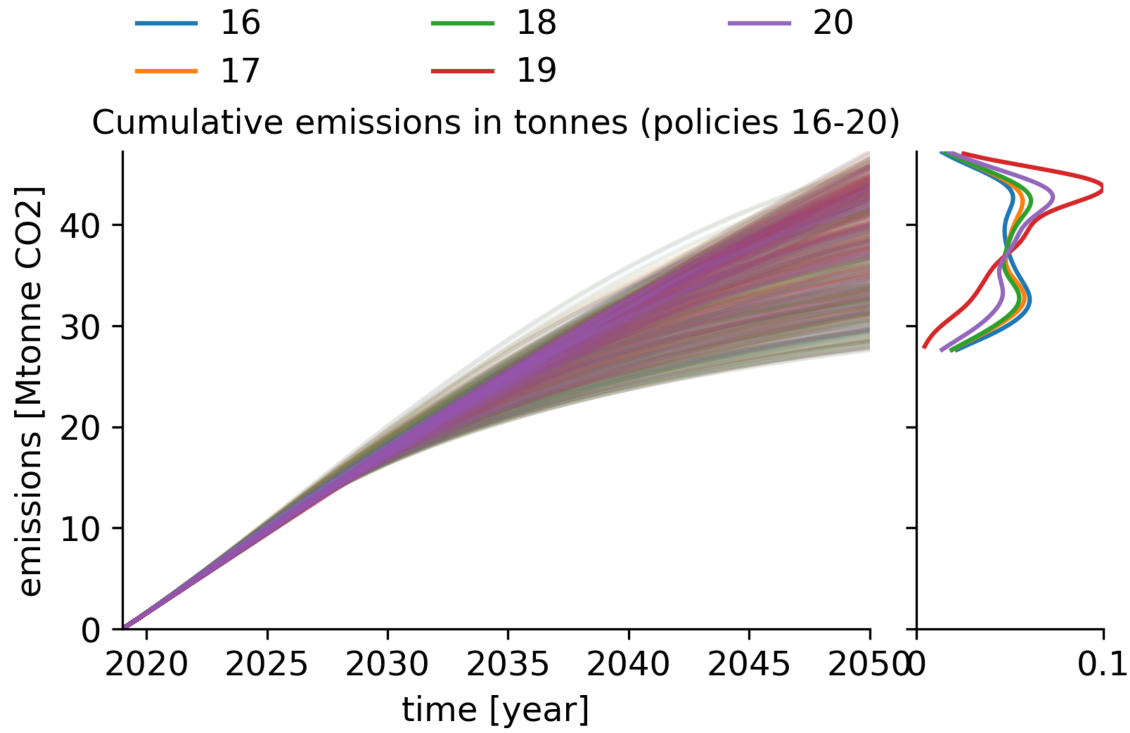

Figure 128: Simulation results for the cumulative CO_2 emissions associated to naphtha cracking for the reference plant, for selected robust policies 16-20. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

K.2.2 Cumulative production costs

From the simulation outcomes for the cumulative production costs shown in Figure 129 it can be seen that all policies result in a more or less equal concentration of outcomes of the higher end of the spectrum. However, considering the lower hand of the spectrum on the one hand policies are observed that show a higher peak and larger minimum values. On the other hand, there are policies that result in outcomes being more spread towards the lower end of the spectrum. The latter policies are clearly more favorable as they result in a higher probability of the production costs attaining low values. From analyzing Figures 130 to 133 it can be observed that these best-performing policies are policies 10, 13, 14 and 15.

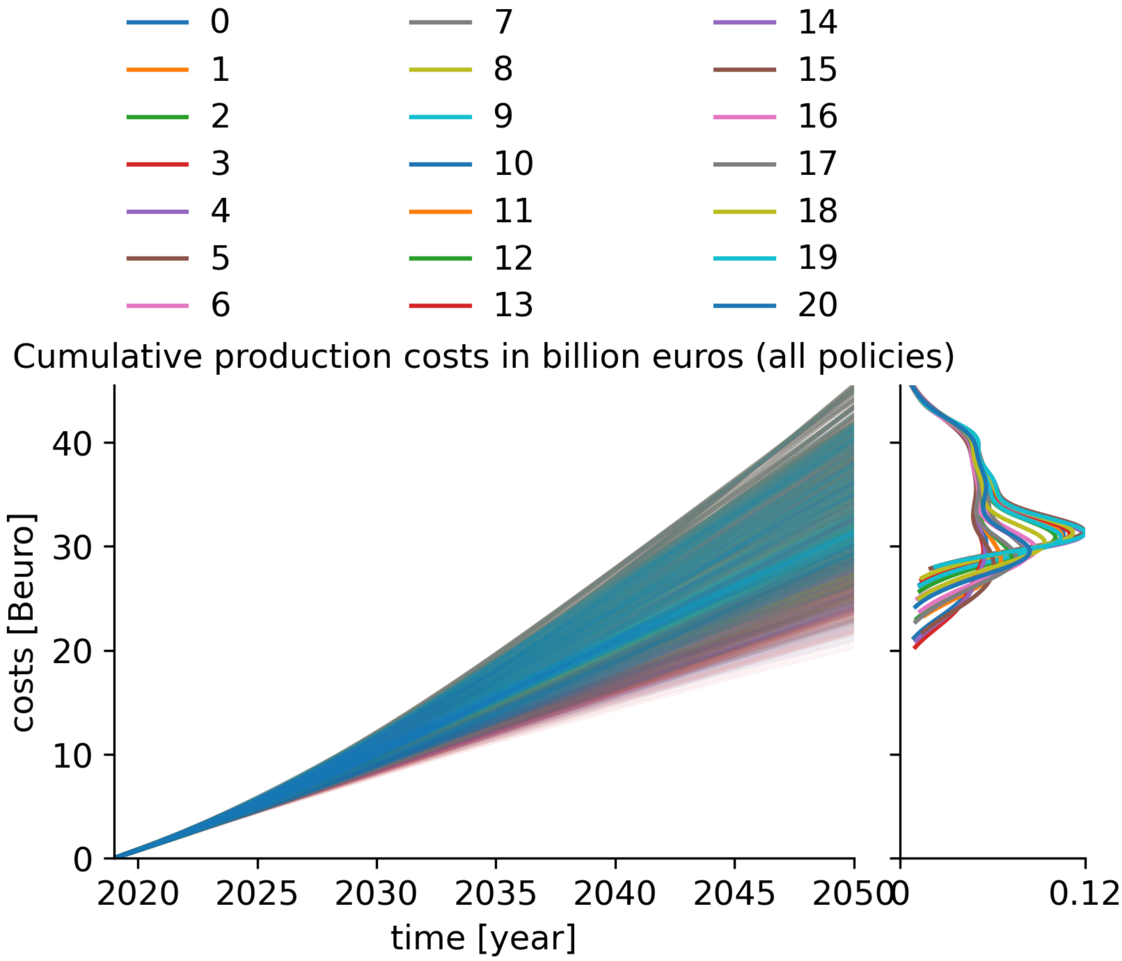

Figure 129: Simulation results for the cumulative production costs associated to naphtha cracking for the reference plant, including all of the 21 selected robust policies. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

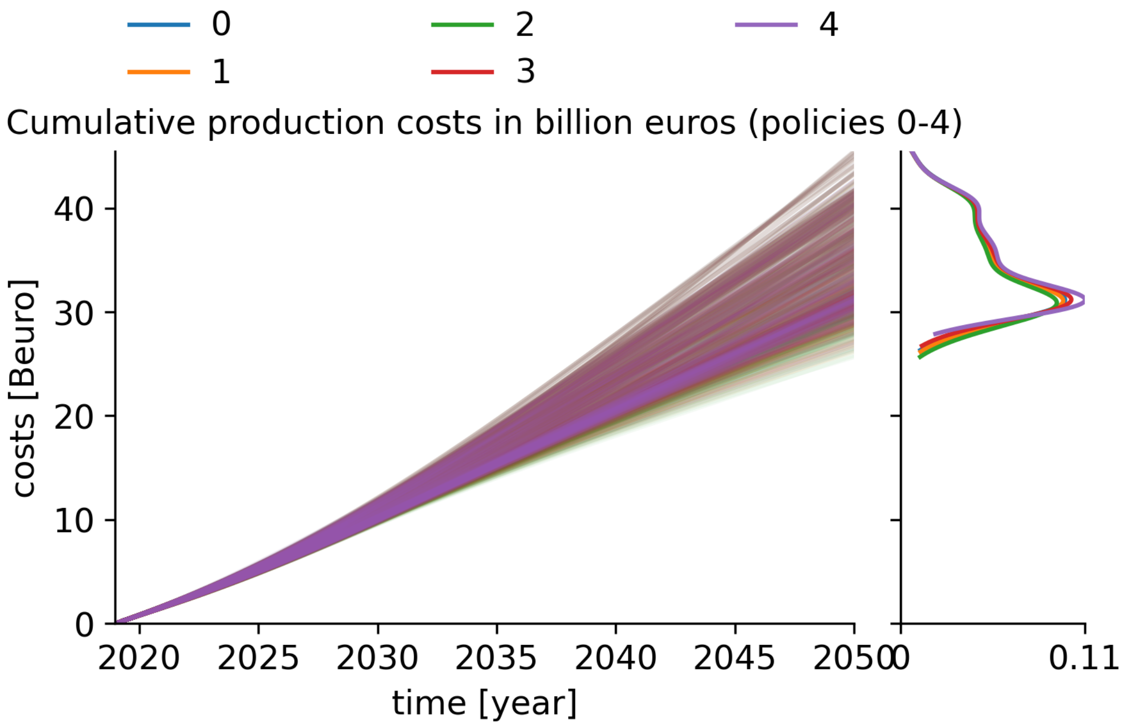

Figure 130: Simulation results for the cumulative production costs associated to naphtha cracking for the reference plant, for selected robust policies 0-4. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

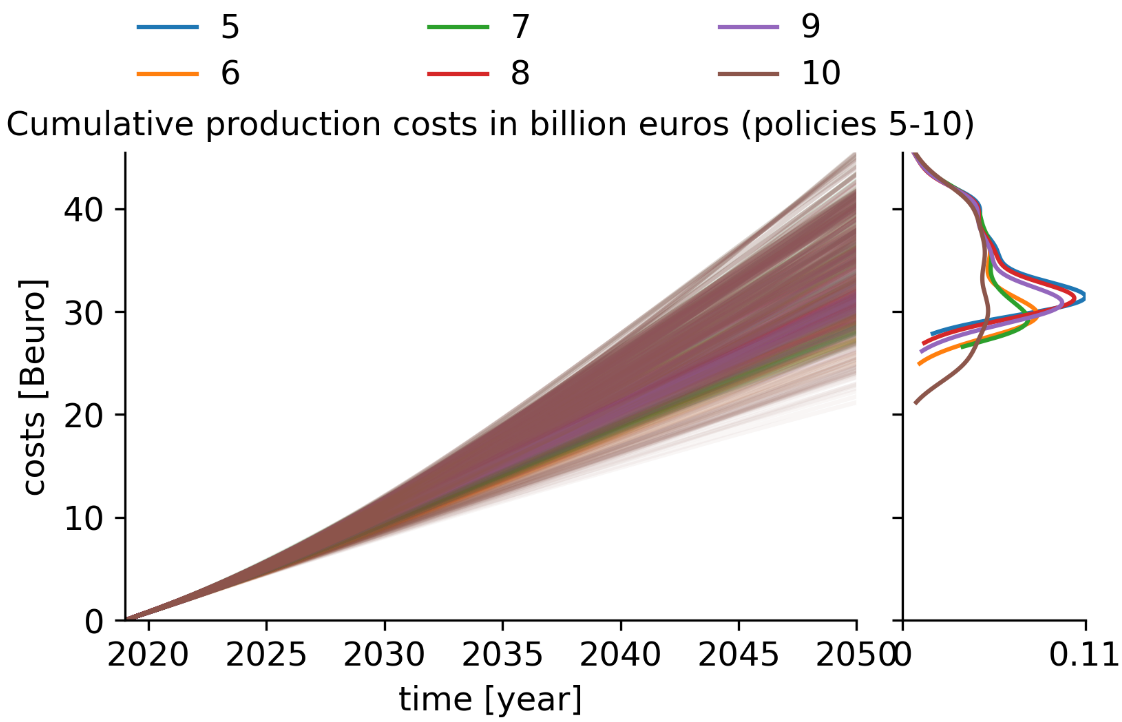

Figure 131: Simulation results for the cumulative production costs associated to naphtha cracking for the reference plant, for selected robust policies 5-10. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

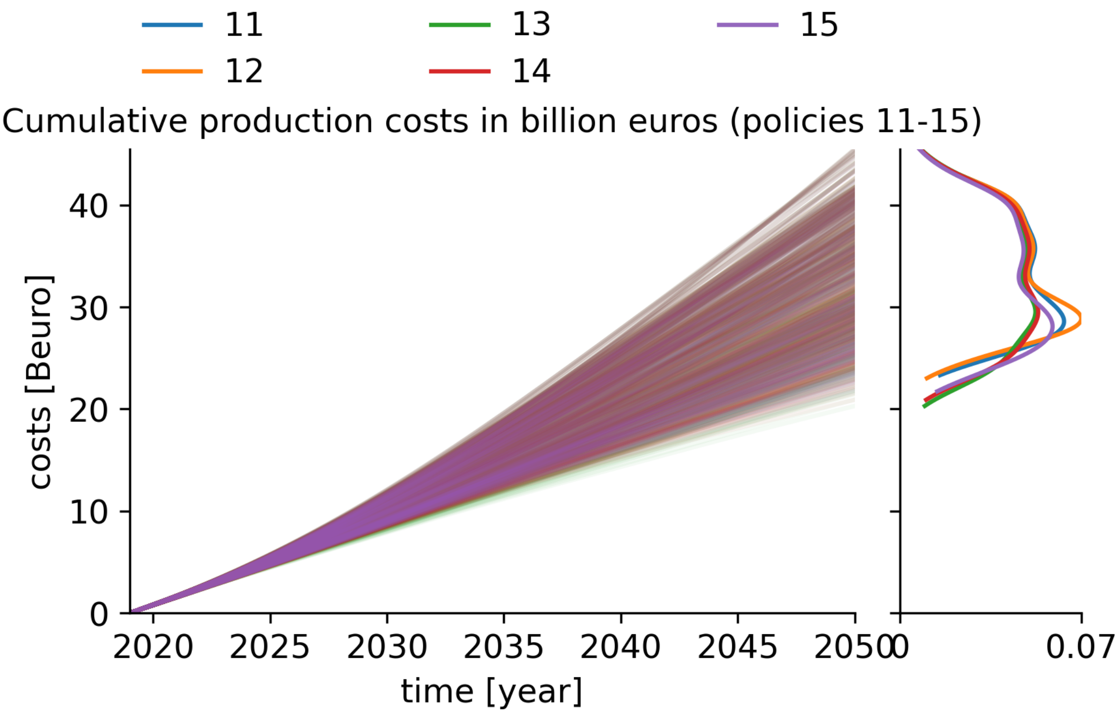

Figure 132: Simulation results for the cumulative production costs associated to naphtha cracking for the reference plant, for selected robust policies 11-15. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

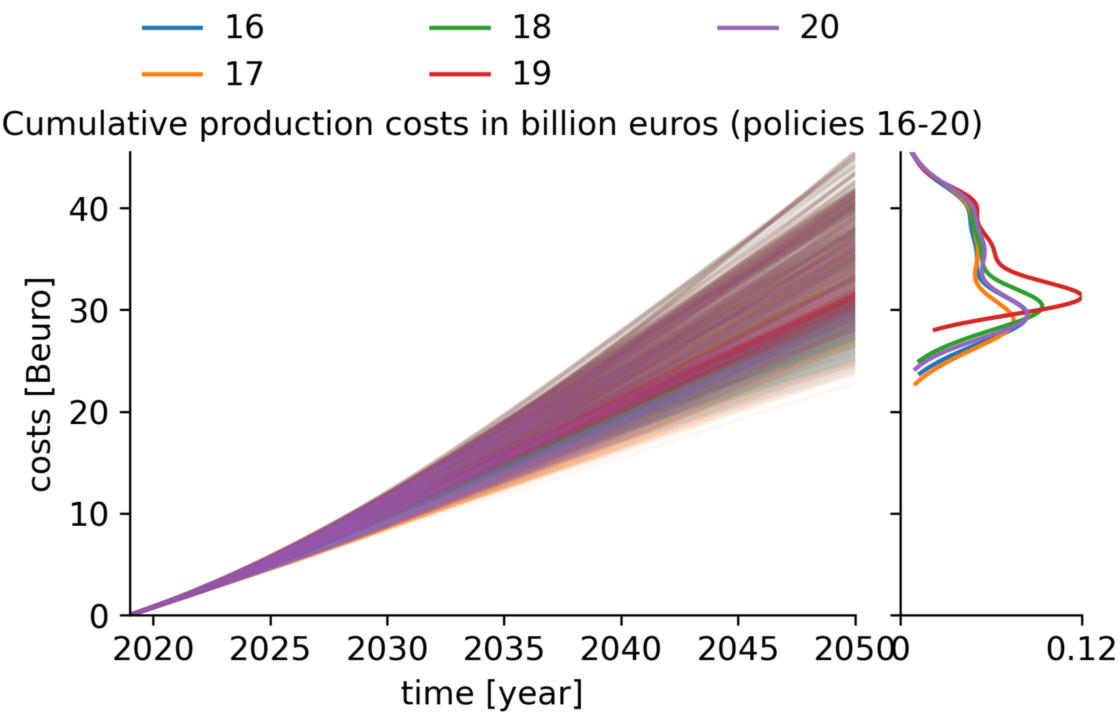

Figure 133: Simulation results for the cumulative production costs associated to naphtha cracking for the reference plant, for selected robust policies 16-20. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

K.2.3 Cumulative policy costs

Compared to the cumulative CO_2 emissions and the cumulative production costs, the outcomes for the cumulative policy costs show less overlap and can be more easily distinguished on the spectrum. From analysis of Figures 135 to 138 it is concluded that policies 3 and 4 are the best-performing with regard to policy costs as they result in the highest concentration of outcomes on the lower end of the spectrum.

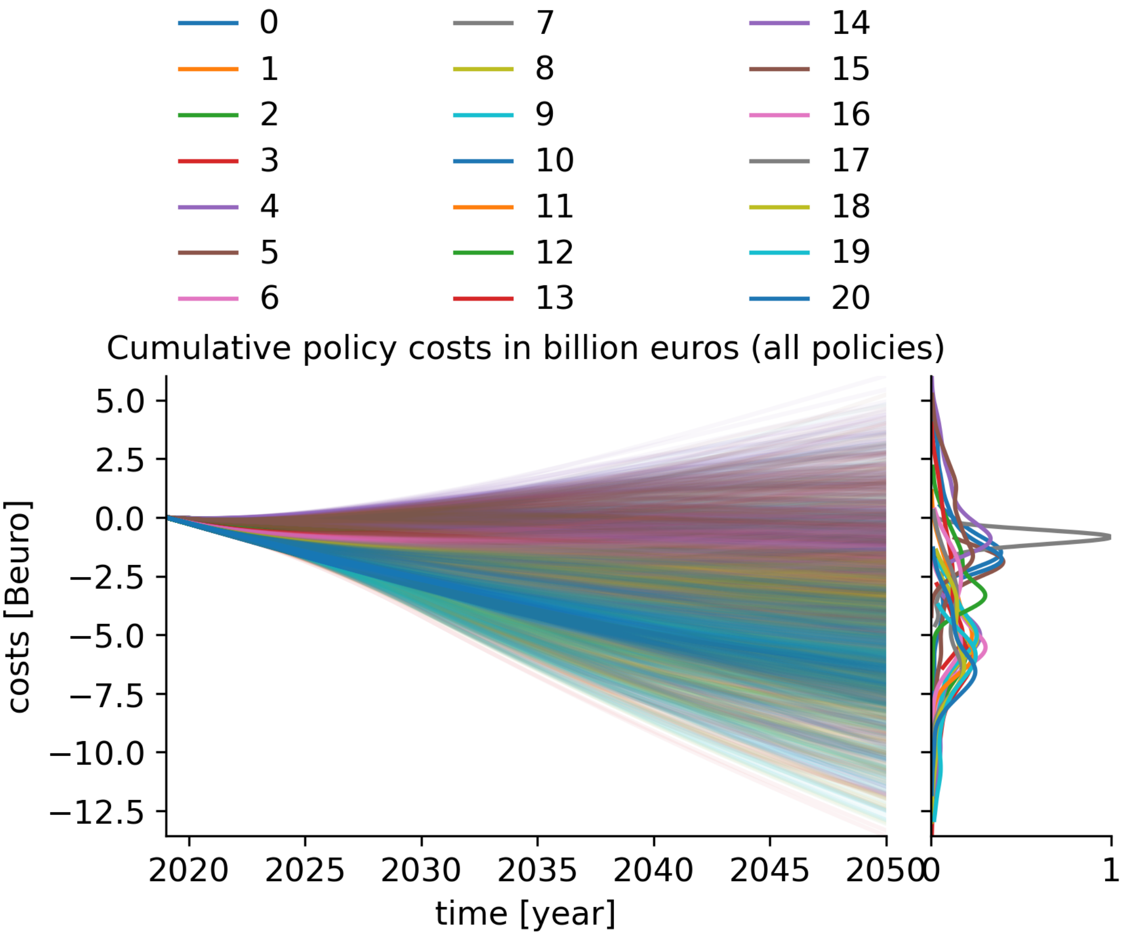

Figure 134: Simulation results for the cumulative policy costs associated to naphtha cracking for the reference plant, including all of the 21 selected robust policies. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

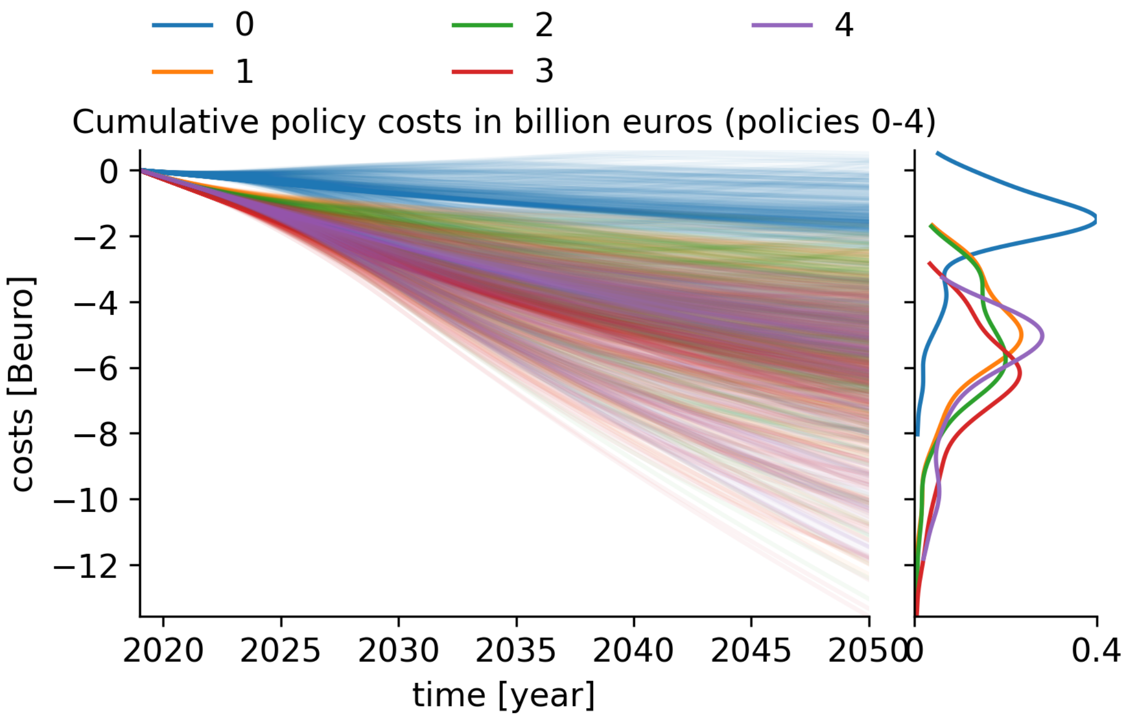

Figure 135: Simulation results for the cumulative policy costs associated to naphtha cracking for the reference plant, for selected robust policies 0-4. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

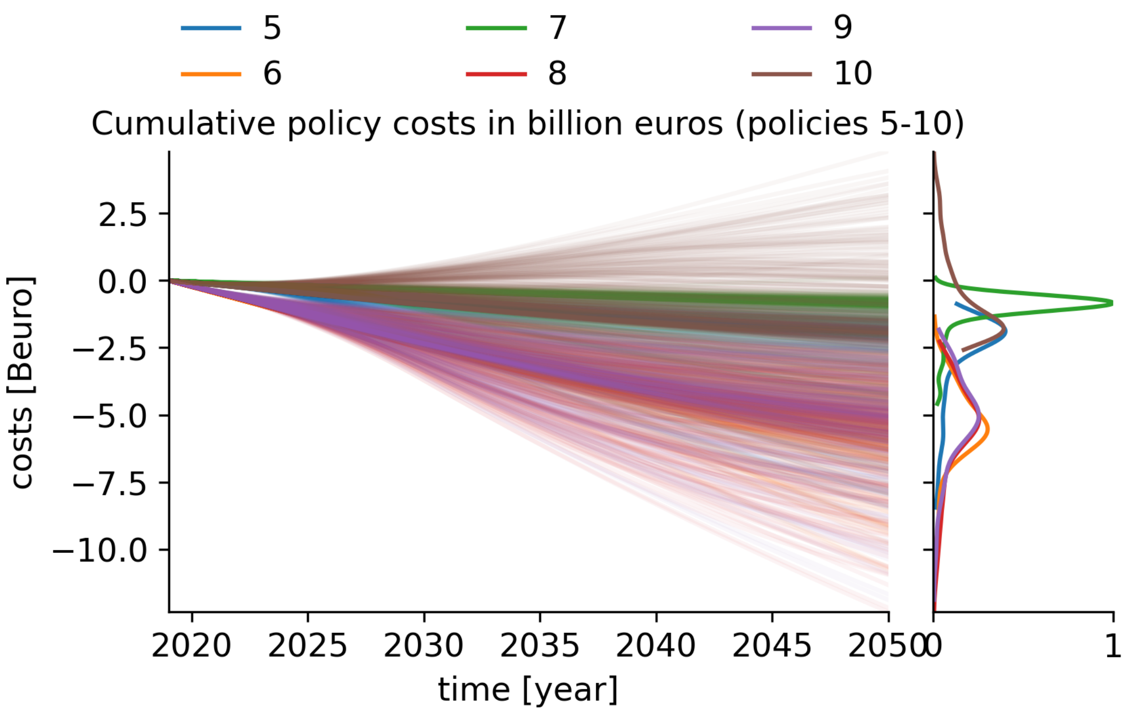

Figure 136: Simulation results for the cumulative policy costs associated to naphtha cracking for the reference plant, for selected robust policies 5-10. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

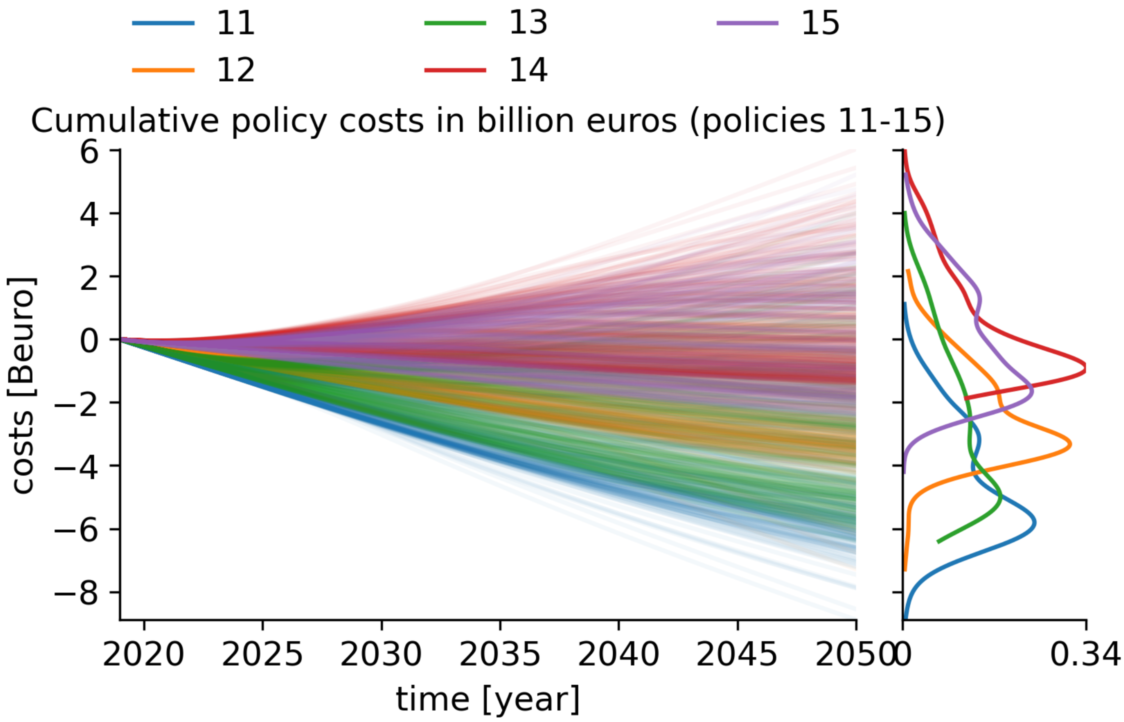

Figure 137: Simulation results for the cumulative policy costs associated to naphtha cracking for the reference plant, for selected robust policies 11-15. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.

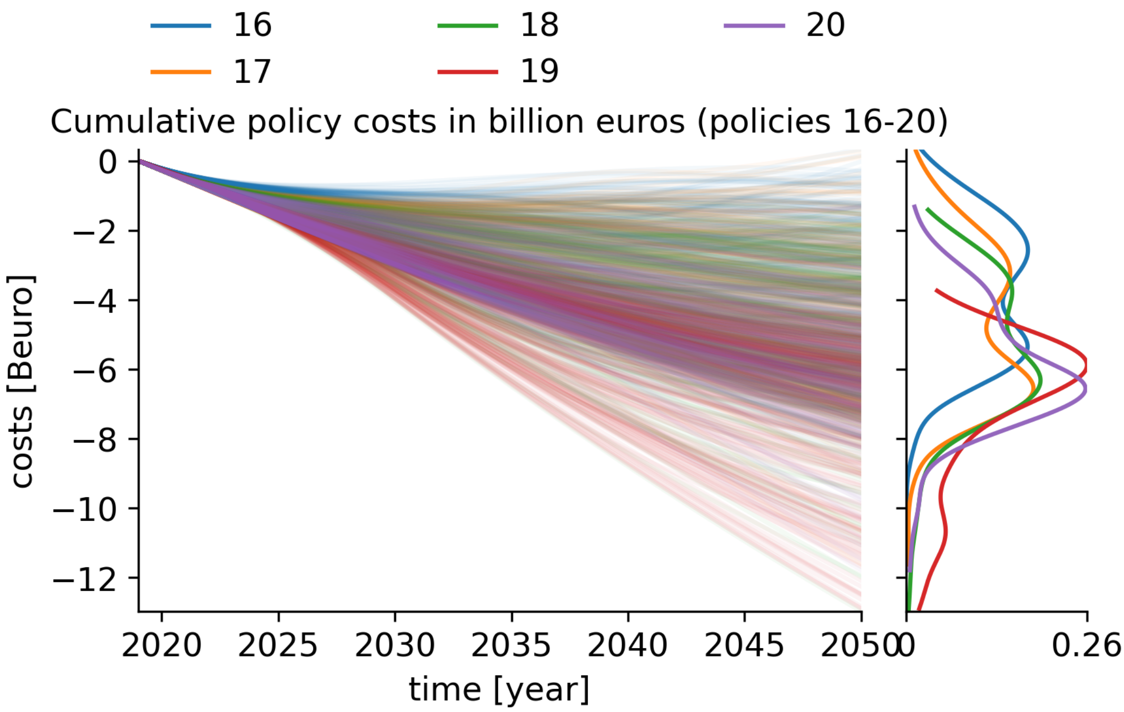

Figure 138: Simulation results for the cumulative policy costs associated to naphtha cracking for the reference plant, for selected robust policies 16-20. To the right the distribution of the simulation outcomes are shown by means of a Kernel density estimation (KDE) plot, which shows the distribution of the outcomes for each of the policies.