Interaction between defossilisation of basic industries and relocation

Scenario-based explorative and normative transition pathways to electrification for European basic industries and specific clusters

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DEPT OF TECHNOLOGY AND SOCIETY | FACULTY OF ENGINEERING | LUND UNIVERSITY

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Clemens Schneider

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Abstract:

The steel and chemical production industries are the largest industrial emitters of greenhouse gases in the European Union, together accounting for half of the EU's industrial greenhouse gas (GHG) emissions. A promising strategy for achieving deep GHG emissions reductions is the electrification of these two industries, which would depend on the rapid expansion of renewable electricity supply. Such electrification can be direct, where electrical appliances replace fossil fuel powered ones, or indirect, using renewable hydrogen produced from water by electricity. Both methods of electrification represent a systemic shift for these industrial systems and require a major wave of investment into new process technologies, as well as access to renewable electricity and green hydrogen. Old industrial structures could become stranded as a consequence of shifting energy and feedstock supply in this way.

The thesis focuses geographically on the major region for EU steel and chemical production: the area between the two North Sea ports of Antwerp and Rotterdam in the west and the Rhine-Ruhr area in the east. It studies the technical and economic feasibility of electrification in the steel and chemical production industries (specifically petrochemicals), followed by an analysis of the impact on locational factors and possible spatial reconfigurations of the production system. The analysis builds on scenario methodology with extensive stakeholder engagement and uses different quantitative bottom-up models developed during several projects. To accelerate and facilitate the transformation of the two focal industries in the region, the thesis identifies strategic options for policy makers, steel and petrochemical companies, as well as for infrastructure providers such as port authorities and network operators.

The results obtained demonstrate the feasibility of electrification and its potential to play a crucial role in the defossilised production of steel and petrochemicals, even in a region with a relatively low renewable electricity potential (such as the one studied). The transformation requires a hydrogen infrastructure for steel and petrochemical clusters and increased circularity, especially in the petrochemical industry. Some production steps in the value chain, such as iron making or chemical feedstock production, will have strong incentives to relocate (either partially or fully). However, other factors, such as the benefits of existing assets and the advantages of vertical integration in existing clusters, may discourage the total relocation of entire production chains.

Key words:
steel, petrochemicals, defossilisation, climate-neutral production, electrification, industry clusters

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MADE IN SWEDEN

To my family

Table of Contents

Popular summary

The steel and chemical manufacturing industries are the largest industrial emitters of greenhouse gases in the European Union, together accounting for half of the EU's industrial greenhouse gas (GHG) emissions. Rapid action is required to meet the EU's target of climate neutrality by 2050 and the 2030 targets at both EU and member state levels. If the GHG mitigation in these industries is governed by the EU Emissions Trading System (EU ETS) via a high carbon price alone, this is likely to lead to de-industrialisation. Consequently, active policies at all levels are necessary to enable the steel and petrochemical industries to move towards defossilisation. Policies are required not only at EU level, but also at the national and sub-national levels. This thesis focuses geographically on the major region for EU steel and chemical production: the area between the two North Sea ports of Antwerp and Rotterdam in the west and the Rhine-Ruhr area in the east. In this traditional industrial region, stakeholders are concerned about the risk that climate mitigation poses to their existing industries due to the value added employment opportunities and strong supply chain networks that these industries bring to the region.

A promising strategy for achieving deep GHG emissions reductions is the electrification of these two industries, which would depend on the rapid expansion of renewable electricity supply. Such electrification can be direct, where electrical appliances replace fossil fuel powered ones, or indirect, using renewable hydrogen produced from water by electricity. Both methods of electrification represent a systemic shift for these industrial systems and require a major wave of investment into new process technologies, as well as access to renewable electricity and green hydrogen. Old industrial structures could become stranded as a consequence of shifting energy and feedstock supply in this way.

This doctoral thesis studies the technical and economic feasibility of electrification in the steel and chemical production industries (specifically petrochemicals), followed by an analysis of the impact on locational factors and possible spatial reconfigurations of the production system. The analysis builds on scenario methodology with extensive stakeholder engagement and uses different quantitative bottom-up models developed during several projects. To accelerate and facilitate the transformation of the two focal industries in the region, the thesis identifies strategic options for policy makers, steel and petrochemical companies, as well as for infrastructure providers such as port authorities and network operators.

In this thesis summary, which is based on the four appended papers, I outline the scope and research questions and develop a set of locational factors that guided my modelling work on the possible relocations of the two production systems.

The results obtained demonstrate the feasibility of electrification and its potential to play a crucial role in the defossilised production of steel and petrochemicals, even in a region with a relatively low renewable electricity potential (such as the one studied). The transformation requires a hydrogen infrastructure for steel and petrochemical clusters and increased circularity, especially in the petrochemical industry. Based on the findings in the four papers, I argue that electrification offers a range of strategic options for proactive stakeholders – but it will have a knock-on effect on location. Some production steps in the value chain, such as iron making or chemical feedstock production, will have strong incentives to relocate (either partially or fully). However, other factors, such as the benefits of existing assets and the advantages of vertical integration in existing clusters, may discourage the total relocation of entire production chains in the steel and petrochemical industries.

Populärvetenskaplig sammanfattning

Produktion avtål- och kemikalier är de två största industriella utsläppskällorna i Europeiska unionen. Tillsammans står de för hälften av industrins utsläpp av växthusgaser. EU:s mål om klimatneutralitet senast 2050 och de kortsiktiga målen för 2030 på både EU-nivå och medlemsstatsnivå kräver snabba åtgärder. Att enbart låta minskningen av utsläppen drivas av EUs system för utsläppsrätter (EU ETS) via ett högt utsläppsrättspris skulle sannolikt leda till avindustrialisering. Det behövs aktiva politiska åtgärder på alla nivåer för att möjliggöra en omställning mot fossilfrihet för dessa två industrier. Åtgärder behövs inte bara på EU-nivå, utan även på nationell och regional nivå. Denna avhandling fokuserar geografiskt på området mellan de två Nordsjöhamnarna Antwerpen och Rotterdam i väster och Rhen-Ruhr-området i öster som är den största industriregionen för stål- och petrokemi i EU. I denna traditionella industriregion är regionala regeringar oroliga för riskerna med vad en klimatomställning skulle innebära för dess industriella bas som bidrar med ett stort ekonomiskt mervärde, sysselsättning och starka industriella försörjningsnätverk till regionen.

En lovande strategi för att uppnå snabba och djupgående minskningar av växthusgasutsläppen är elektrifiering med en samtidig en snabb utbyggnad av förnybar el. Elektrifiering av industrin kan vara direkt, där fossila processer ersätts direkt med elektriska processer, eller indirekt där förnybar vätgas, som produceras med elektricitet från vatten, används i nya processer. En elektrifiering av industrin är ett stort skifte på systemnivå där både fossil energi och, i fallet med petrokemi, även den fossila råvaran behöver bytas ut. En elektrifiering ställer krav på mycket stora investeringar i ny processteknik och anpassning av, eller helt ny, infrastruktur för att understödja denna omställning. Risken med en sådan stor omställning är att stora delar av den befintliga fossila industrin kan bli ekonomiskt olönsam och att existerande industristrukturer förlorar sitt värde.

I denna doktorsavhandling studeras den tekniska och ekonomiska genomförbarheten av en elektrifiering i dessa två industrier och effekterna på dess specifika infrastruktur i regionen. I ett nästa steg analyserades vilken effekt elektrifiering kommer att ha på lokaliseringsfaktorer och om industrien kan förbli konkurrenskraftig. Analysen bygger på scenario-metodik med samarbete med intressenter och använder sig av kvantitativa bottom-up modeller som har utvecklats parallellt under projekten. För att påskynda och underlätta omvandlingen av de två industrierna i regionen identifierar avhandlingen strategiska alternativ för beslutsfattare, stål- och kemiföretag samt infrastrukturleverantörer som hamnmyndigheter eller nätverksoperatörer.

I kappan, baserad på de fyra bifogade artiklarna, motiveras avhandlingens omfattning och dess forskningsfrågor och här utvecklas även en uppsättning lokaliseringsfaktorer som vägledde modelleringsarbetet om möjliga omlokaliseringar.

Resultaten visar på möjligheten till elektrifiering och att det är möjligt för både stål- och petrokemiindustrin av bli fossilfria, även i en region som den studerade med en relativt liten potential för förnybar el. Omställningen mot fossilfrihet kräver en vätgasinfrastruktur och även en ökad cirkularitet, framförallt inom petrokemin. Baserat på resultaten i de fyra artiklarna hävdar jag att elektrifiering erbjuder en rad strategiska alternativ för proaktiva intressenter, men att det kommer att påverka lokaliseringsfaktorer. Vissa produktionssteg, som t.ex. reduktion av järnmalm till järn eller fossilfri råvarutillverkning för petrokemin, kommer delvis därför att omlokaliseras. Andra faktorer, som befintliga tillgångar i infrastruktur och fördelarna med vertikal integration i befintliga industrikluster, talar dock emot en fullständig omlokalisering av hela produktionskedjor inom stål- och kemiindustrin.

List of Papers

Paper I

Lechtenböhmer, S., Nilsson L. J., Åhman, M., Schneider, C. (2016) 'Decarbonising the energy intensive basic materials industry through electrification. Implications for future EU electricity demand', *Energy*, 115, pp. 1623-1631. Available at: https://doi.org/10.1016/j.energy.2016.07.110.

Paper II

Schneider, C., Lechtenböhmer, S., Samadi, S. (2020) 'Risks and opportunities associated with decarbonising Rotterdam's industrial cluster', *Environmental Innovation and Societal Transitions*, 35, pp. 414–428. Available at: https://doi.org/10.1016/j.eist.2019.05.004.

Paper III

Schneider, C. (2022) 'Steel manufacturing clusters in a hydrogen economy – Simulation of changes in location and vertical integration of steel production in Northwestern Europe', *Journal of Cleaner Production*, 341, 130913. Available at: https://doi.org/10.1016/j.jclepro.2022.130913.

Paper IV

Schneider, C., Åhman, M., Lechtenböhmer, S., Saurat, M. 'A defossilised EU petrochemical production system: consequences for the meta-cluster in the Antwerp-Rotterdam-Rhine-Ruhr Area', *manuscript submitted*.

Author's contribution to the papers

Paper I

I carried out the literature analysis relating to the specific technologies for assessment. I also undertook the data collection and modelling and calculated energy demands and emissions. I participated in the conceptualisation and wrote the parts in the paper describing the technologies.

Paper II

I conceptualised the paper, was sole modeller in this study and was involved in all stages of scenario building, scenario design and validation. I also carried out most of the analysis and wrote the majority of the paper.

Paper III

I conceptualised and conducted the modelling, did the analysis and wrote the paper.

Paper IV

I conceptualised the paper, sketched the model structure, parametrized the model and did the scenario design, scenario validation and analysis. I wrote most of the paper.

Other relevant papers

List of other relevant articles and reports written during the dissertation (2018-2023)

Schneider, C. (2023) ‘Aus der Gaskrise zu einer anpassungsfähigen klimaneutralen Grundstoffindustrie: Strukturwandel und eine starke industrielle Basis im Bereich der Grundstoffe schließen sich nicht aus‘, *Ifo-Schnelldienst*, 76(3), pp. 26-30. Available at: https://www.ifo.de/publikationen/2023/zeitschrift-einzelheft/ifo-schnelldienst-032023-deindustrialisierung.

Doré, L., Fischedick, M., Fischer, A., Hanke, T., Holtz, G., Krüger, C., Lechtenböhmer, S., Samadi, S., Saurat, M., Schneider, C. and Tönjes, A. (2023) *Treibhausgasneutralität in Deutschland bis 2045: ein Szenario aus dem Projekt SCI4climate.NRW*. Available at: https://www.energy4climate.nrw/fileadmin/Service/Publikationen/Ergebnisse_SCI4climate.NRW/Szenarien/2023/treibhausgasneutralitaet-in-deutschland-bis-2045-szenario-cr-sci4climate.nrw.pdf.

Scholz, A., Schneider, C., Saurat, M. and Theisen, S. (2023) *Das petrochemische System in Deutschland und Westeuropa: regionale Analyse der Polymer-Produktion in Deutschland, den Niederlanden und Belgien; Ergebnisse aus dem Forschungsprojekt "Green Feedstock for a Sustainable Chemistry – Energiewende und Ressourceneffizienz im Kontext der dritten Feedstock-Transformation der chemischen Industrie*. Available at: https://epub.wupperinst.org/frontdoor/deliver/index/docId/8146/file/8146_GreenFeed.pdf.

Schneider, C., Taube, M. and Lorenz, T. (2022) ‘Grüner Wasserstoff in der Industrie: kurzfristige Einsatzpotentiale und langfristige Bedarfe in Deutschland‘, *FVEE Themen 2021*. Available at: https://www.fvee.de/wp-content/uploads/2022/07/th2021_06_01.pdf.

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Merten, F., Nebel, A., Krüger, C., Schneider, C., Scholz, A. and Taubitz, A. (2020) ‘Needs of electricity, hydrogen and carbon infrastructures for greenhouse gas neutral heavy industry clusters in the EU 2050’, *ECEEE Industrial Summer Study proceedings*. Available at: https://www.eceee.org/library/conference_proceedings/eceee_Industrial_Summer_Study/2020/6-deep-decarbonisation-of-industry/needs-of-electricity-hydrogen-and-carbon-infrastructures-for-greenhouse-gas-neutral-heavy-industry-clusters-in-the-eu-2050/2020/6-098-20_Merten.pdf/.

Venjakob, J., Schneider, C. and Arnold, K. (2020): *Konzeption einer Wasserstoffmodellregion Emscher-Lippe*. Available at: https://epub.wupperinst.org/frontdoor/deliver/index/docId/7564/file/WR18.pdf.

Schneider, C., Samadi, S., Holtz, G., Kobiela, G., Lechtenböhmer, S. and Witecka, W. (2019): *Klimaneutrale Industrie: Ausführliche Darstellung der Schlüsseltechnologien für die Branchen Stahl, Chemie und Zement*. Analysis on behalf of Agora Energiewende. Available at: https://static.agora-energiewende.de/fileadmin/Projekte/2018/Dekarbonisierung_Industrie/166_A-EW_Klimaneutrale_Industrie_Ausfuehrliche-Darstellung_WEB.pdf.

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Schneider, C. and Lechtenböhmer. S. (2018) 'Concepts and pathways towards a carbon-neutral heavy industry in the German federal state of North Rhine-Westphalia', *ECEEE Industrial Summer Study proceedings*. Available at: https://www.eceee.org/library/conference_proceedings/eceee_Industrial_Summer_Study/2018/4-technology-products-and-system-optimisation/concepts-and-pathways-towards-a-carbon-neutral-heavy-industry-in-the-german-federal-state-of-north-rhine-westphalia/2018/4-065-18_Schneider.pdf/.

Schneider, C. and Schüwer, D. (2018) *Low-Carbon-Industrie: Elektrifizierung und geschlossene Kohlenstoffkreisläufe*. Technologiebericht 6.4 Low-carbon und ressourceneffiziente Industrie innerhalb des Forschungsprojekts TF_Energiewende. Available at: https://epub.wupperinst.org/files/7067/7067_Low-carbon-Industrie.pdf.

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At the beginning of my PhD, I was still a lone wolf in industry modelling, but that has changed over time. Georg and Mathieu, I owe you a huge debt of gratitude: If you hadn't ventured into industry modelling, we wouldn't have come this far as a team, and I wouldn't have come this far with this PhD. Most importantly, I would not have been able to focus on steel and petrochemicals, which proved fruitful for my PhD. Süheyb, Ylva and Svenja, you continue the modelling at the Wuppertal Institute. Thank you for your passion. With you, industry transformation modelling will reach another level of depth.

Sascha, special thanks to you for the dedicated leadership of several important projects, but also for the important role in challenging and “translating” my sometimes wild ideas, a role you often took on together with Stefan. Looking beyond the narrow confines of industry modelling has always been important to me, and in this respect, I would like to thank all the electricity market modellers I have had the privilege of working with and from whom I have learned so much about sector coupling. Thank you, Arjuna, Tomke, Tine, Marco and Julie! And thanks to Frank and Dietmar for bringing in the wider context of infrastructures and the heat sector transformation.

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Finally, my very personal thanks to Johannes for always having a sympathetic ear, and once again to Stefan and Max. But it was Ines who listened to most of my self-doubts. You were my support, thank you for all your encouragement and patience with me.

Abbreviations

ARRRA	Antwerp-Rotterdam-Rhine-Ruhr-Area
BECCS	bioenergy use with carbon capture and storage
BF	blast furnace
BOF	basic oxygen furnace
BTX	benzene, toluene and xylenes
Capex	capital expenditures
CBAM	carbon border adjustment mechanism
CCS	carbon capture and storage
CCU	carbon capture and usage
CHP	combined heat and power
DR	direct reduction
DRI	direct reduced iron
EDM	Energy Demand Modelling platform of the Wuppertal Institute
EAF	electric arc furnace
EU ETS	European Union Emissions Trading System
GHG	greenhouse gas(es)
H-DR	hydrogen-based direct reduction of iron ore
HVC	high-value chemicals
LCA	life cycle analysis
LPG	liquefied petroleum gas
LTS	research framework Large Technical Systems
MFA	material flow analysis
NUTS	nomenclature of territorial units for statistics of the EU and the UK
Opex	operational expenditure
SDG	sustainable development goals
STS	science and technology studies
TRL	technology readiness level
TSO	transmission grid operator

1 Introduction

In common with all other sectors, the industrial sector is required to contribute to reducing greenhouse gas emissions and achieving climate neutrality as per the Paris Agreement and the GHG reduction targets adopted by the Euro-pean Union and national governments. The huge cost reductions in renewable electricity supply technologies that became apparent around the 2010s, particularly for wind and solar, combined with the massive potential for renewables identified in Europe and almost everywhere else in the world (Hoefnagels et al. 2011, Hansen, Breyer and Lund 2019, Bogdanov et al. 2021), opened up a new perspective: would it be possible to build new and additional renewable power capacity to replace fossil-based electricity production, fossil fuels and even hydrocarbon feedstock? This new perspective gave rise to the vision of a fully electrified energy system and was later followed by a discussion about the development of new value chains based on renewable electricity, particularly for the steel and petrochemical sectors. These sectors are currently the largest industrial users of fossil carbon and emitters of CO_2 in the EU (see section 2.2). According to recent scenario literature, increased electricity use in all sectors and the related expansion of renewable electricity supply are key to meeting the Paris Agreement targets (European Commission 2021, Ariadne 2021, Tsiropoulos et al. 2020, Prognos, Öko-Institut and Wuppertal Institut 2021).

However, with its high population and industrial density, Northwestern Europe – Europe's steel and chemicals heartland – has a relatively low potential for additional renewable electricity production. Steel and chemical production are economically significant within the region and create considerable employment, not only directly within the two basic industries but also in terms of their multiplying effects (Döhrn and Janssen-Timmen 2011, Limbers, Böhmer and Hoch 2016, Büchel et al. 2022, Sinabell et al. 2022). They are considered as two of Germany’s key industries (among others BMWi 2020, BMWi et al. 2021), supplying the export-oriented automotive and mechanical engineering industries with high-quality steel and plastics. As the automotive and mechanical engineering industries export a large proportion of their goods, the steel and chemical industries are exposed to world markets both directly and indirectly via their main customers. While the export orientation of the German economy in general could be contested from a political or economic standpoint, this PhD thesis takes this industrial legacy with its specialised workforce and innovation systems as a given. In such an environment, the demand for special grades of steel and sophisticated engineering plastics is likely to continue, but in future these products will have to be produced in a climate neutral way. This is not only a normative requirement but is backed by both regulation and consumer demand. This has a significant impact on these basic industries from two different angles:

(1) The European Emissions Trading System (EU ETS) demands the phase-out of CO_2-intensive production in Europe in the mid to longer term, and the EU has introduced a “carbon border adjustment mechanism” (CBAM) to prevent imports of steel with high GHG emissions (European Union 2023). The CBAM will probably extend to plastics in the future.

(2) The downstream manufacturing industries will demand climate neutral materials as they have made commitments to carbon neutral supply chains.[1]

But what are climate neutral (green) materials or climate neutral production systems? While systems analysis often accepts fossil carbon inputs into the industrial metabolism even in the longer term and only requires the carbon to be offset or recycled (or CCS[2] when waste is incinerated), the requirements of life cycle analysis (LCA) can be stricter. According to a strict interpretation, a green (climate neutral) product should not contain any newly extracted fossil carbon, because at least parts of it will be released into the atmosphere as CO_2 at a later point in time (at best after many steps of reuse). Although the term "defossilisation" is not yet well-established in the political and scientific debate, it is used in this thesis (and even in its title) to underline the need to avoid the extraction of fossil carbon. Any fossil carbon in the production system replaced by 'renewable carbon' extracted from the atmosphere (via biomass or CO_2 from direct air capture) contributes to limiting the concentration of CO_2 in the atmosphere and, therefore, to limiting global warming.

Although the two industries studied are different in many respects, there was a strong motivation to treat them together during this doctoral work. In the case of Germany, the Netherlands and Belgium, the steel and petrochemical production industries should not be seen as two separate case studies for illustrating industrial decarbonisation. Instead, these two basic industries in the region should be considered as a common block in their own right, large enough to justify dedicated transmission infrastructure that allows for electrification – such as a European hydrogen backbone and high voltage electricity transmission lines. This type of dedicated backbone infrastructure could enable the two industries to transform

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[1] See for an overview the Net Zero Tracker (https://zerotracker.net/), an open data source project that collates the GHG mitigation targets of companies and also covers scope 3 emissions targets (along the companies’ value chains). Various typical customers of the steel and chemical industries are listed there.

[2] The abbreviation refers to Carbon Capture and Storage.

faster than other sectors and thus contribute significantly to the interim GHG reduction targets, in particular the EU and national 2030 targets.

Germany, the Netherlands and Belgium share the peculiar situation of having economies that are material-intensive, export-oriented and green energy-poor with other export-orientated countries such as South Korea and Japan. This situation provided an incentive to take a closer look at the stability of the industrial complex around steel and plastics production in the context of the transition to climate neutrality. The spatial extent of this heavy industry complex, which is part of the historical "industrial heartland of Europe" stretches from the ports of Rotterdam and Antwerp in the west to the Rhine-Ruhr area in the east and the Upper Rhine in the southeast. In the context of this thesis summary, this region is referred to as the Antwerp-Rotterdam-Rhine-Ruhr Area (ARRRA).

The aim of this thesis is to explore the spatial consequences of an industrial transition towards electrification and defossilisation with a special focus on the ARRRA region. The thesis is problem-oriented, and the identified problem is the lack of knowledge at decision maker level about the necessary actions and possible windows of opportunity to start the transformation in the steel and petrochemical industries. The rationale of this work and the projects on which it is based is to involve local stakeholders from both industries and to accelerate the transformation by increasing their acceptance of electrification, using their existing know-how, reusing the physical assets in the region and disseminating systemic knowledge. The thesis work was part of various road mapping processes for industry branches and specific clusters. As a part of the debate between stakeholders, the thesis work aims to increase the directionality in industrial policy (Nilsson et al. 2021) and to enable decision makers in companies to formulate plans, to invest in specific technologies or to find new partners and infrastructure for the supply of energy or climate neutral raw materials or feedstock.

To this end, the thesis addresses three core research questions:

1) How can European heavy industry become climate neutral by 2050 and what is the possible role of electrification in the climate neutral production systems of basic industries?
2) What sustainable strategies can steel and petrochemical companies in Europe and specific clusters adopt to adapt to climate neutral production and specifically to electrification, and how will these strategies interact with the energy system over time?
3) How strong will clustering benefits and possible relocation effects be due to electrification in the two industries and to what extent can the latter be addressed by policy?

All three research questions are directed to the future. To cope with the related high uncertainty, the scenario method (a core method for future studies) was used

(Wilson 1978, Becker 1983, Steinmüller 1997) to serve the purpose of dealing with an uncertain future. By applying this method, I cannot claim to acquire insights that are either true or are clearly falsifiable. Instead, this work contributes to the research by increasing the transparency about decision options and possible decision windows for decision makers in companies, trade unions and policymaking.

For the first two research questions, it was possible to follow established concepts of explanatory technology bottom-up modelling. However, when this PhD research started there were no adequate tools or available criteria sets to address the third research question. Conceptual thinking about potential relocations in value chains due to electrification is now evolving (Samadi et al. 2021, Day 2022, Samadi, Fischer and Lechtenböhmer 2023) and a limited number of techno-economic case studies have been published (Gielen et al. 2020, Devlin and Yang 2021, Egerer et al. 2023). Toktarova et al. (2022) have developed a model to analyse the locations of future DRI and steel production within a European region, but with an electricity system focus rather than a production system focus. In this new research field, this PhD work presents a modelling toolbox and related scenario analysis for forces that could potentially shape or re-shape the future geography of production.

The quantitatively modelled scenarios developed during the PhD thesis apply to different approaches, one of which – according to Börjeson et al. (2006) – can be classified as 'explanatory' and the other as 'optimising'. The first two research questions were addressed through explanatory modelling, which requires the discussion of many assumptions, preferably in a transdisciplinary context with stakeholders. The highly exploratory third research question was analysed using a mix of explanatory and optimisation approaches. Optimisation approaches require a strict theoretical background, as the endogenisation of decisions in the model requires clear rules and a clear definition of the relationships between variables. The theoretical framework for the applied cost-optimisation approach was neoclassical economic theory, with its main simplifying assumptions of perfect information about the present (but not necessarily the future) and the homo-economicus paradigm (utility maximisation and rational choice). The scenario work required a range of supporting methods, consisting of technology assessment, systems analysis and stakeholder workshops, the latter being the main qualitative method used. These are described in more detail in chapter 4.

Chapter 2 provides a detailed rationale for the research focus, illustrating its relevance for policy and research. Chapter 3 develops the principles that guided the study of the relationship between electrification and relocation. The general methodological approach is presented in chapter 4, but the more specific methodological developments applied in the four papers are explained in further detail in chapter 5, which focuses on the research process and its results. The final chapter presents reflections and conclusions on the whole PhD journey in the context of the related transformative research flow and suggests further research.

2 Scope and motivation

2.1 Sector focus: steel and petrochemicals

During the course of the PhD, I focused on the two industry branches that are the biggest industrial emitters of CO_2 in the EU: the iron and steel industry and the chemical industry. Figure 1 reveals that their energy and process-related emissions alone account for half of the industrial emissions in the EU-27. The actual carbon footprint of the two industries is even higher. The petrochemical industry's products contain fossil carbon, which is often incinerated at the end of the life of a product, whether in Europe or somewhere else in the world, whether after six months in the case of packaging or more than fifty years later in the case of building materials (Geyer, Jambeck and Lavender Law 2017). Taking the respective carbon throughputs into account, the two sectors account for as much as 60% of the EU's total carbon footprint.

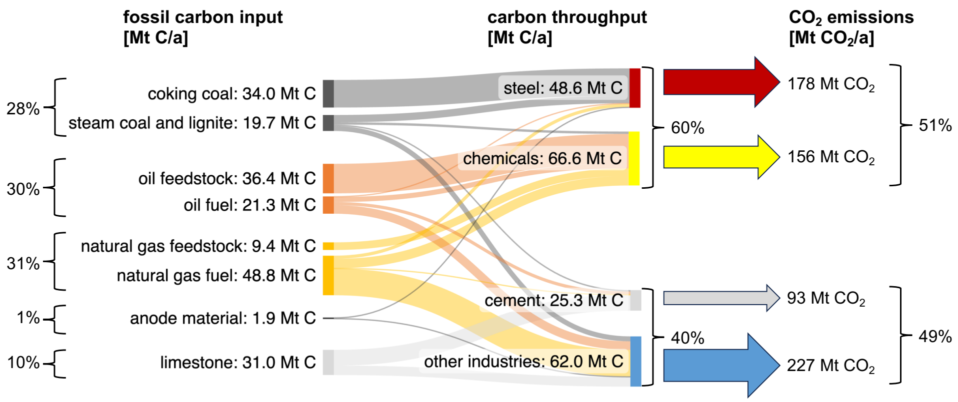

Figure 1: Fossil carbon flows entering the industry sector in the EU-27 in 2018 and the resulting CO_2 emissions. Source: own calculations based on Eurostat, EEA and modelling results obtained in project 12 (see Table 1 below).

In Europe, natural gas is generally the largest supplier of carbon to the industrial production system, but its use is very broad with the majority used as fuel in a wide variety of production processes (Figure 1). Oil and coal use accounts for similar quantities of carbon equivalent as gas, but their use is much more process-specific. Coal, as a reduction agent, and oil, as a feedstock, are the most relevant carbon carriers for the steel and chemical industry. Due to long-lasting assets (with the associated high risks for investors), high mitigation costs and risks of carbon leakage, the steel and chemical sectors have been flagged as “harder-to-abate sectors” by the Energy Transitions Commission (2018). Within the chemical sector, the focus of this PhD is on 'petrochemicals'. The petrochemical industry, in the sense studied, includes the production of hydrocarbons (organic and non-organic) and their successors, i.e., mainly polymers. The production of ammonia is sometimes misleadingly included in the petrochemical sector but it was not the focus of this PhD.[3] However, producing around 27 Mt CO_2 emissions, ammonia production represents a significant part of the chemical industry in regard to GHG emissions.[4] The non-metallic industry (and cement in particular) also belongs to the class of “harder-to-abate” industries and likewise accounts for a high share of total carbon throughput and CO_2 emissions. The spatial organisation of these industries is, however, very different from iron and steel and petrochemicals, with close-to-market production and local limestone resources being more relevant. Therefore, these industries are not covered in this thesis.

In summary, this thesis specifically focuses on the steel and petrochemicals sectors due to: (1) their overall relevance for GHG mitigation; and (2) their similarities in terms of their exposure to international competition. These aspects allow for cross-sectoral comparisons and general conclusions to be drawn. A third motivation for the selection of the two industries is their clustering within the European industrial heartland, the ARRRA, which will be illustrated in the following section.

2.2 The relevance of the ARRRA for the two sectors within Europe

The main activities in Europe’s steel and petrochemical industries are located in the region covering the North Sea ports of Rotterdam and Antwerp and their hinterland, which extends deep into Western Germany. Geographically, the area of focus comprises four European regions, as highlighted in the map displayed in Figure 2. The PhD thesis work is based on projects on each of these four entities (see Table 1). In the following, this region will be referred to as the Antwerp-Rotterdam-Rhine-

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[3] As ammonia production currently uses natural gas as its main feedstock and as its downstream products are mainly inorganic and do not necessarily contain carbon, ammonia production was considered only in so far as it is needed to produce polymers. The fertiliser industry, which is the main producer and consumer of ammonia, was not a focus of this work. It has other technological and logistical options than the petrochemical industry to become climate neutral (IEA 2021a).

[4] The volume of 27 Mt of CO_2 emissions is calculated based on Eurostat’s reported production volume in the EU-27 in 2018 of 12.5 Mt of nitrogen equivalent and the (scope 1) emissions factor of 1.8 t CO_2/t ammonia calculated by Material Economics (2019).

Ruhr-Area (ARRRA), as it comprises the EU's two most important North Sea ports and the part of their hinterland that is interconnected via pipeline infrastructure and the River Rhine as Europe's most powerful logistical backbone in inland navigation. The map shows the extension of the industrial production logistics system from the North Sea ports in the West to Cologne and Gelsenkirchen in the East, and BASF's main site and headquarters in Ludwigshafen far up the River Rhine in the Southeast. This region accounts for 22% of the EU-27's primary steel production[5] and 49% of its high-value chemicals.[6]

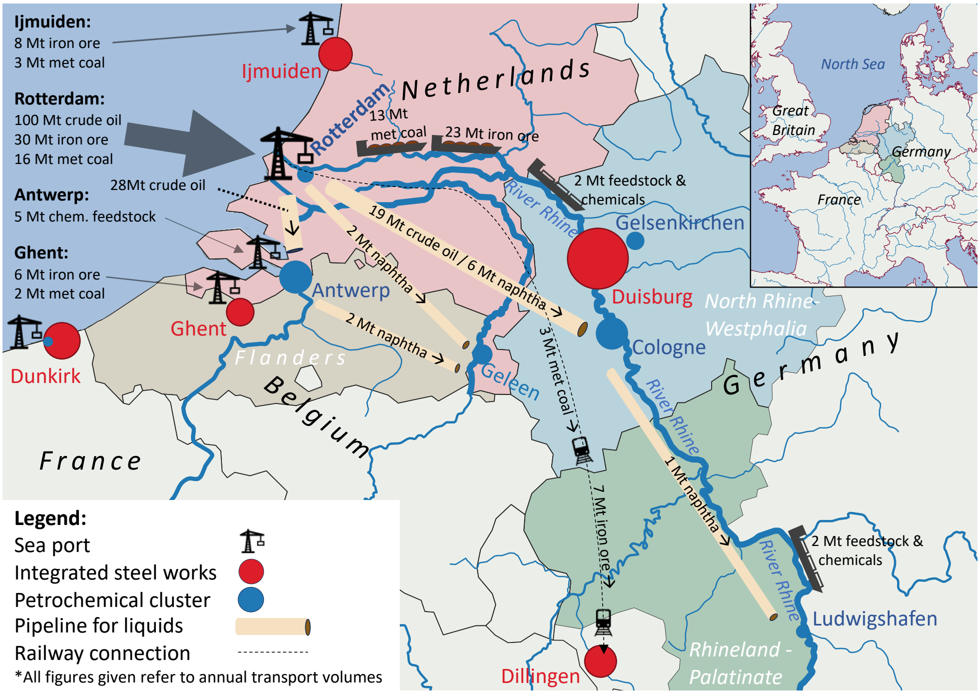

Figure 2: Raw material flows into and within the ARRRA associated with the steel and petrochemical industries. Source: own figure.

The map illustrates the crucial role of the Port of Rotterdam in feeding these two basic industries. It is by far the most important hub for the import of raw materials in the region, whether crude oil or metallurgical coal ("met coal") and iron ore, the two dry bulks processed in the iron and steel industry. At Rotterdam, half of the imported crude oil volume illustrated on the map is processed in five local refineries;

[5] If the two adjacent steel sites at Dunkirk in France and Dillingen in the German federal state of "Saarland" are included, the share increases to about one third of European primary steel capacity.

[6] Both % have been calculated based on production capacities within the region according to the Wuppertal Institute's database on production plants (see also section 4.2.1).

the other half is transferred via dedicated pipelines to refineries near Antwerp as well as to Cologne and Gelsenkirchen. Chemical naphtha and liquified petroleum gas (LPG) are the main refinery products used in the petrochemical industry as a feedstock. Naphtha is also transported in pipelines linking the refineries and the petrochemical sites, while the overall smaller volumes of LPG are transported by inland waterway vessels (Scholz et al. 2023). Iron ore and metallurgical coal are imported either directly to the coastal sites or from Rotterdam via vessels up the River Rhine to the port of Duisburg. Within the region, lignite and natural gas are the fossil fuels that are still extracted, but their direct relevance to the two industries considered in this thesis is limited. Due to the region's exceptionally high population density, renewable energy potential is limited (see Figure 4 below), although the physical potential for more onshore wind exists throughout the region. The Netherlands, with its long coastline, has significant potential for offshore wind development.

In the ARRRA, steel and polymers are important upstream industries in the value chain of the machinery and automotive producing industries. These downstream manufacturing industries typically require materials with very specific quality requirements, i.e., special grades of steel (Daehn, Cabrera Serrenho and Allwood 2017) or so-called engineering plastics (Plastics Europe 2022). Germany, the Netherlands and Belgium account for almost 50% of the total value added for these industries in the EU, while their share of total EU gross value added is only 29%. Machinery and transport equipment are much more important in terms of value added and employment than steel and chemicals[7] but, especially in Germany, steel and chemicals are seen as strategic parts of the value chain[8].

The focus on the ARRRA region is motivated not only by scientific interest and relevance. With its highly specialised knowledge and workforce, scientific institutions and their networks of policy makers (see also section 4.1), as well as existing infrastructure and other valuable assets, such a strategic region of global industrial importance will either be a laggard or a frontrunner in the transition. The aim is to contribute to the latter by asking whether this transition is possible and under what circumstances could it be realistic.

[7] See Eurostat's time series "nama_10_DBR", https://ec.europa.eu/eurostat/web/national-accounts/database.

[8] See the respective studies cited in the introduction, which were typically commissioned by industry stakeholders. During the energy crisis in 2022, a critical discussion arose among economists about the relevance of the basic industries for the German economy as a whole. A study by Bachmann et al. (2022) argued for a small effect, while Krebs (2022) argued for a large effect of gas shortages and high prices on the whole economy.

3 The disruptive potential of electrification

Electrification can be seen as a major systemic change for the two largest industrial fossil carbon users, the steel and the petrochemical industries. The possible technological change towards electrification described in section 3.1 is currently the most obvious, but we do not know how deep this transformation will be and what other mitigation options might be available in the future. After introducing the technological pathways, this chapter will describe the conceptual thinking that guided the scenario analysis around the locational effects presented in chapter 5.

3.1 Technological change in steel and petrochemicals

Figure 3 illustrates the technical production system in the two industries and the associated energy system. In both industries, a distinction can be made between the energy required to provide the raw materials shown as vertical flows and the heat required to process the raw materials shown as horizontal flows. The subsequent steps in the production chain are arranged vertically. The top half of the figure illustrates the current core production processes and their associated fossil energy flows. The lower half shows an electrified future, in which the steel industry replaces its blast furnace (BF) fleet (Vogl, Olsson and Nykvist 2021) – the core process in primary steel making where the iron ore is reduced to iron using coke and coal as reducing agents. Feasible technology to achieve this is the direct reduction (DR) process – an indirect electrification pathway via electrolytic hydrogen (Vogl, Åhman and Nilsson 2018). A second challenge is to change the energy source in the high-temperature step of hot rolling. Currently, steel gases, which are by-products of the blast furnace/basic oxygen furnace (BF/BOF) route, provide most of the energy used in this step: these gases will not be available in a DR-based future. Electricity, hydrogen or gasified biomass are possible substitutes. Increased circularity with higher shares of scrap and focused biomass use to supply the small remaining needs for carbon or to achieve net negative emissions via bioenergy use with carbon capture and storage (BECCS) are the necessary complements of an electrification strategy (e.g. Prognos, Öko-Institut and Wuppertal Institut 2021).

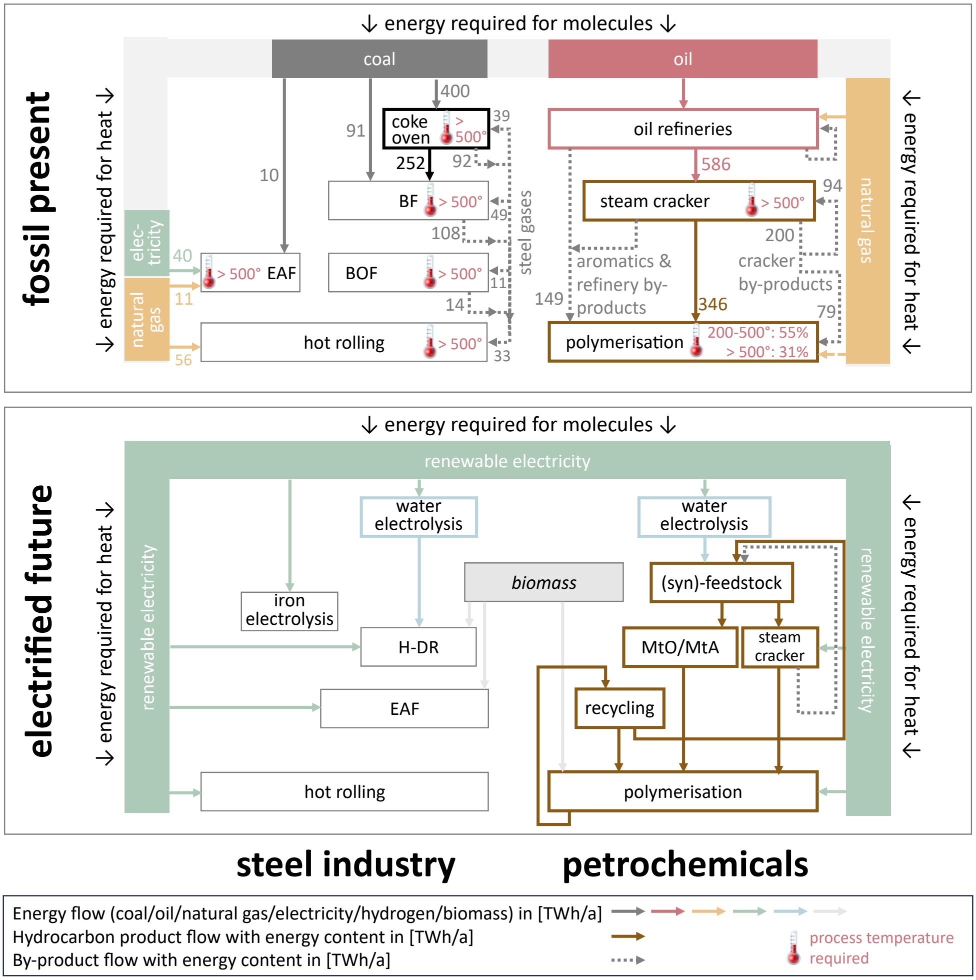

Figure 3: Challenges faced by technological defossilisation in the iron and steel and petrochemical industries in the EU. Source: Own figure; energy flow volumes based on own simulation calculations in the project "Breaking free from fossil gas" (see Table 1).

The petrochemical industry shows a similar kind of general energy flow. In this case, oil is currently the main energy source. The lighter cuts of the crude oil refining process are the feedstock for the steam cracking that delivers so-called high-value chemicals (HVC) for further processing into polymers (see a more detailed description of the production chain in section 3.3.2). The figure also shows a similar type of energy integration as the steel industry, as both the by-products of the BF/BOF route and the steam cracking are sufficient to meet the heat requirements of the core processes itself and the subsequent production steps. Both process routes even provide surplus energy, allowing for further energy integration and onsite electricity production. However, the nature of the heat demand is different in the petrochemical industry. The petrochemical industry requires not only temperatures above 500°C but also a lot of steam, i.e., temperature levels between 200° and 500°C as well as 100-200°C. In the future "post-petrochemical" industry, as shown in the lower right-hand corner of the figure, the energy to meet the demand for molecules will probably come partly from plastic waste and biomass, with a significant proportion from electricity (Material Economics 2019, Kätelhön et al. 2019, VCI and VDI 2023). In principle, all hydrocarbon by-products can be re-processed in such future systems to produce further feedstock and, therefore, build a carbon looping system that requires electricity (or hydrogen) as an energy carrier to provide the heat. In fact, the intensity of carbon looping will be a complex optimisation problem as storable chemical energy carriers (such as by-products) will also have a value in a future renewables-based energy system.

In summary, we see two general dimensions of energy demand for both industries where supply needs to change. The future demand for molecules can be met by water electrolysis, some biomass and increased use of secondary materials. Iron electrolysis and electrochemical processes could be even more disruptive in the more distant future. The future demand for heat, on the other hand, will no longer be met by by-products, but will require new sources. The types of sources used will depend largely on the local energy system.

In view of these technological challenges, the question arises whether a transformation will be possible by redesigning the existing system or whether it will necessitate the creation of a new system. Indeed, technologies related to electrification, such as iron electrolysis and electrochemical processes, could transform the entire production chain. Together with 3D printing and circularity, they could make the whole production system as we know it today obsolete, allowing for production that is much more decentralised. On the other hand, today's production facilities dedicated to continuous mass production have their merits in terms of economies of scale and energy-efficient production, which could lead to a transformation of the existing system rather than a disruption.

The steel and petrochemical industries have already undergone profound technological changes in their history, most recently in the steel industry with the introduction of the basic oxygen furnace in the 1950s (Cappel et al. 2022), which resulted in a spatial reorganisation of the supply chain.[9] However, industrial legacies from the period prior to that significant change are still in place. Many steel sites, especially rolling mills, are no longer optimally located in terms of energy and logistics costs; they are the legacy of previous integrated primary steel production, which often ceased decades ago. However, they remain in operation either because of the value of the plant, its associated infrastructure or the specialised workforce.

[9] For the USA, Giarratani, Madhavan and Gruver (2013) describe the very disruptive locational development associated with the introduction of the basic oxygen furnace and the subsequent diffusion of the EAF.

The literature of Science and Technology Studies (STS) observes that legacies clearly do matter in such technical systems. The framework of Large Technical Systems provides a concept to understand and analyse how technical systems evolve and consolidate (Hughes 1987), and how (and to what extent) they undergo transformation or are replaced (van der Vleuten 2006). This broad systems approach can be used to understand what major systemic changes mean in terms of changes to technology, economies, institutions or geographies. All are related to a change in power (whether political or economic) and are, consequently, relevant for society in general and for stakeholders in particular.

The InfraNeeds project, carried out in 2019[10], revealed a potential major systemic change. Figure 4 demonstrates that if the European production systems for steel, chemicals and cement undergo the technological changes outlined above, and the geographical structure of primary production in Europe remains untouched, the ARRRA will have to import massive amounts of green energy because local potentials are not sufficient. This is indicated by the intensity of the red colouring in the right-hand map of Figure 4. For the underlying analysis, the renewable electricity production potentials in the European NUTS-1 regions were compared with their future local electricity demand. The latter was derived from scenarios on the future electricity demand of the European transmission grid operators (TSO) that did not foresee a direct or indirect electrification of industry[11]. These were complemented with a site-specific bottom-up calculation of future direct and indirect electricity demand induced by an electrification strategy for the three basic industries, which are indicated by the magnitude of the dots in the left-hand map.

The challenge identified for the ARRRA affects a variety of stakeholders (see also section 4.1), who should be considered when researching such a transformation. The more specific research questions in this context are: (1) which steps of the value chain could be maintained in such a "renewables-poor" region; and (2) how and to what extent might the inner organisation of value chains within the ARRRA develop?

[10] See also Table 1.

[11] Location-specific scenarios with the electrification of the basic industries were not available in the electricity system forecasts by the European TSOs. However, other electrification strategies in the mobility and buildings sectors, such as electric cars and heat pumps, were reflected in their scenarios.

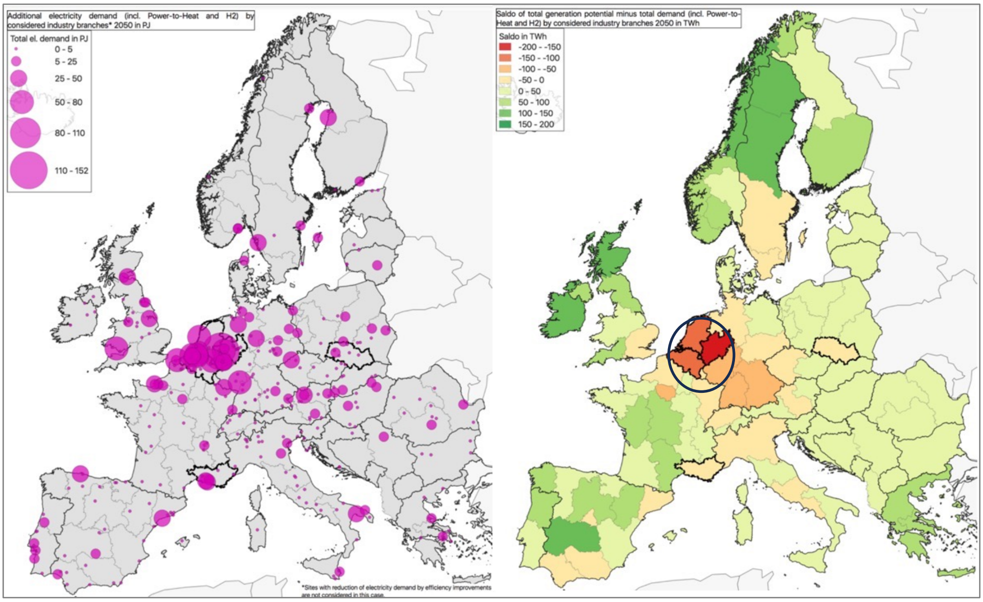

Figure 4: Electrification of existing heavy industry clusters and the resulting renewable electricity shortage and surpluses across Europe in a 2050 electrification scenario without locational change. Source: Merten et al. (2020).

3.2 Factors for the spatial organisation of value chains considered in the modelling and scenarios

This section illustrates and explains the portfolio of factors that were considered to understand and model how future value chains in the two focal industries might spatially develop, drawing on several concepts. In general, technical and economic variables that represent a "business logic" were used in the modelling, which is typical for bottom-up energy system models (see section 4.2.2). The storylines (see section 4.2.4), which are used to frame the scenarios, embed the modelling into important boundary conditions, including criteria usually analysed in social science.

3.2.1 Economic legacies and related persistence

A holistic explanation of industrial legacy and its associated technological and social legacy effects can be provided by the concept of large technical systems (LTS), a concept used in Science and Technology Studies (STS) to analyse the development and functions of large technical systems such as the electricity or gas supply systems. The steel and petrochemical production systems can also be framed as such systems but, according to van der Vleuten (2006), they can be considered as

2nd order LTS, which are based on 1st order systems such as the electricity grid, the gas grid or the transportation system. The LTS would be an adequate framework for analysis if our interest was limited to the interaction with these kinds of infrastructures and their legacies, i.e., the interaction between production and the energy system. However, in my view, the industrial production systems for the steel and petrochemical industries are much less opaque and much more challenged by international competition than the systems analysed in the classical LTS literature. The physical infrastructure and associated network effects are not as strong in the steel and petrochemical industries as in network-based energy supply industries. The applicability of the LTS framework for analysing spatial patterns in particular is, therefore, limited in this research context.

An established economic concept for capturing at least parts of industrial legacy and related persistence effects is "sunk costs" (Samuelson 1948). Once an investment is made, it may act as a barrier to market entry because the company can reduce the price of its products to the level of its variable costs (Baumol 1959). Many energy system models of the optimising kind do not account for such legacy as it requires a far more complex optimisation procedure. Bottom-up engineering models of the kind used during this PhD work (see section 4.2.2) typically try to account for this phenomenon and assess technical lifetimes of plants and retrofit costs for reinvestments that are typically less than 50% for a lifetime extension compared to a new investment (see e.g. for steel Eurofer 2013). Infrastructure is also a typical sunk-cost phenomenon, and this was considered in the modelling of the petrochemical system.

3.2.2 Energy and feedstock integration benefits of industrial clusters

The description of technological change above has already hinted at the potential energy and material efficiency benefits of the vertical integration of production at a site. This is only one aspect of the overall benefits of local clustering, which includes many more (Porter 1998). The industrial symbiosis literature as part of industrial ecology addresses these types of integration benefits when analysing inter-firm clustering benefits in chemical parks (Guo et al. 2016).[12] In their case study about an existing industrial symbiosis in a chemical park, Janipour et al. (2022) identified also specific clustering-related barriers for deep emission reduction.

3.2.3 Principles of modern supply chain management

Supply chain management is a tool of business economics that provides principles relating to how companies should organise their supply chains to best achieve their

[12] The firm level was not part of the analytical concept in the modelling during the PhD.

business objectives. It includes a spatial dimension as well as other dimensions. The portfolio of objectives includes profit maximisation alongside other possible objectives, such as meeting the SDGs. Supply chain management does not claim to be empirically valid in describing or predicting the actual development of supply chains. Instead, the empirical question in testing the validity of its principles would be whether companies that follow its principles perform better than other companies. As the principles of supply chain management are state-of-the-art and, therefore, used by many companies (Blanchard 2012), they provide a good insight into their rationale.

Guiding principles that are relevant to the geographical patterns of supply chains include the minimisation of transportation costs, short lead times, inventory management, risk management with regards to logistical chains, political instability and natural disasters, as well as flexibility and responsiveness (ibid). Their relevance for the steel and petrochemical industries will be discussed in section 3.3.

3.2.4 Green industrial policy and trade policy

Industrial policy instruments are often difficult to separate from climate policy. Green industrial policy typically has two main layers: (1) enabling existing strategic industries to transform in order to maintain employment and strategic independence; and (2) creating new industries capable of exporting green technologies or products. The differentiation is motivated by a country's perspective and objectives, rather than by the type of industry or product. Germany's major concern is downstream: it may be of strategic interest to preserve the value added in the steel industry within the country as it is needed for other strategic industries, such as the car and machinery industries. Sweden, on the other hand, may be interested in gaining more value added in the value chain attached to its major export commodity iron ore, with the new steel industry directly targeting a niche market of green steel. Consequently, both countries could aim to develop their domestic DRI capacity. Policy instruments to create markets could include, for example, "local content" provisions, such as those used in the US "Inflation Reduction Act". These policies interact with trade policy instruments, such as CBAM which aim to ensure that European producers are not disadvantaged by climate policies vis-à-vis companies outside Europe that do not meet European production standards in terms of carbon footprint (European Union 2023). A relatively new approach at the European level is that of critical raw material policies (European Commission 2023a), linked to the concept of de-risking supply. These are aimed at increasing political autonomy but can also be applied at company level. Such approaches seek to influence the spatial organisation of value chains, but industrial and trade policy considerations typically do not include a sub-national level, which is the main scope of the relocation analysis in this PhD. Nevertheless, industrial policy considerations are an important prerequisite for the scenario design work carried out in the thesis. The related assumption that the EU will try to maintain the production of basic materials at a level roughly equivalent to domestic demand allows us to focus on sub-EU and sub-national relocations.

3.2.5 Sub-national regional policies

In contrast to industrial policy, regional policy explicitly targets the sub-national level. It can include instruments, such as the design of public infrastructure, qualifications for the local workforce and direct subsidies from regional bodies, often as co-financing to attract targeted subsidies from national governments. The modelling work carried out during the PhD did not model such policies but was designed to inform and challenge them. The scenarios typically show developments without regional policy intervention (or with limited intervention) and attempt to assess the extent to which the economically-driven developments are robust, whether they could be influenced by regional policy or whether they might be too strong to be influenced. The core assumption is that regional policies can only have a limited impact on the transformation of the industries analysed, as they typically only address capital expenditure (capex) and transport costs, but not the dominant operational expenditure (opex). It could be argued that the permission process for renewable electricity generation could be an important exception to the opex problem, especially for onshore wind, where, for example, German states have discretion to pursue green siting policies. However, policies advocating the strong local expansion of renewable generation in densely populated regions, such as the ARRRA, have not been stable, with politicians often fearing public rejection.

3.2.6 R&D and innovation policies

Policies for both R&D and innovation often include a strong regional component as they may be part of a regional policy agenda; they may also be influenced by national or even supra-national policies that acknowledge the positive effects of clustering on innovation diffusion and the total economy (Porter 1998). In Germany, so called "Real-Labore" ("real laboratories", see e.g. Borner and Kraft (2018)) and, at EU level, "hydrogen valleys", have been introduced to establish local "eco-systems" for a hydrogen economy. If innovations create completely new solutions and start in niches (Schot and Geels 2007), the new sociotechnical systems may override the existing production system through diffusion. For this dissertation on the transformation of existing industrial clusters, these kinds of approaches focusing on completely new products have always been the most challenging as they question whether transformation will take place at all or whether the development will be completely disruptive. The neglect of the study of innovation processes at the product or consumption level in this thesis is a limitation that must be acknowledged when drawing conclusions.

3.3 Supply chain organisation in the steel and petrochemical industries

3.3.1 Steel industry

This section describes how the introduction of hydrogen-based direct reduced iron production will enable a spatial reorganisation of the current steel production chain, in particular the separation of the iron and steel production stages. The analysis begins with a description of the current rationale for companies' supply chain organisation and then argues for a new rationale.

To account for the special situation of steel production in the ARRRA, the focus of the following analysis is on the supply chain for steel coil produced for the automotive industry. Such coil is manufactured to order because it must meet the exact metallurgical and size requirements of the commissioning company. To achieve short lead times, the finished product should be produced close (in geographical terms) to the customer. In the ARRRA, only integrated BF/BOF mills are used to produce automotive coil.[13] Hot rolling mills located at the steel mills benefit from low-cost fuel supplies from off-gases and shorter lead times due to shorter transportation distances. On the other hand, the BF/BOF route requires continuous operation. The blast furnace runs most efficiently at full load, but it can also be stopped ("banking") or run at a certain level of partial load, e.g. during a crisis. The storage of solid iron is not efficient as the BOF needs the liquid phase coming out of the BF. The potential to respond to the market in terms of total steel output is, therefore, limited, but the plant can respond to a changing demand portfolio by shifting between grades and sizes of the finished products. A BF/BOF steelworks can, therefore, accept longer transportation times for raw material supplies, as these can be planned well in advance. The stockpiling of ore and coal at the steel plant is still necessary to manage risks in the long supply chain (Kawakami, Kobayashi, and Nakata 2021). To reduce revenue risks and optimise delivery capabilities, and to omit inefficient partial load operation, it is preferable to stock up on the raw materials rather than the iron, steel or finished product. In order to respond to the automotive industry as quickly as possible, all primary steel sites producing automotive coil in Germany (i.e., thyssenkrupp Duisburg, Salzgitter, ArcelorMittal Bremen, ArcelorMittal Eisenhüttenstadt), in Flanders (ArcelorMittal Ghent) and in the Netherlands (Tata Ijmuiden) have vertically integrated at least parts of the capacities in their supply chains at one site.

For other applications, product requirements are less specific. Reinforcing bars or wire rod used in construction are standardised products where stockpiling is

[13] In Italy and the USA, EAFs are also used to produce automotive coil, but in both countries high amounts of DRI and not only scrap are used in EAFs.

associated with lower revenue risks. In addition, the EAFs, usually operated with scrap as a feed and associated with this value chain, can be shut down completely. Figure 5 illustrates that in Germany EAF mills are operated with much greater flexibility than the BF/BOF operations. Unlike BOF operators, EAF operators can also afford a seasonal pattern, i.e., they shut down their plants during the holiday periods in summer and December.

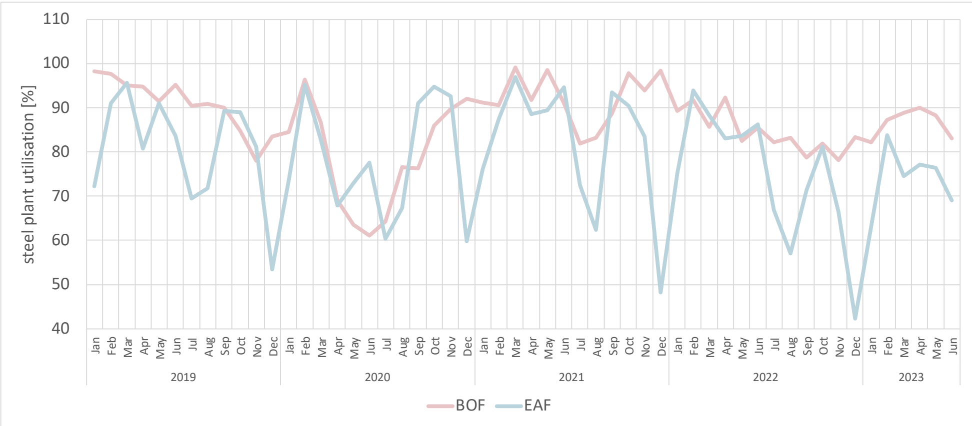

Figure 5: Monthly BOF and EAF steel plant utilisation in Germany from January 2019 to June 2023. Source: Own figure, production volumes based on the regular press releases from WV Stahl[14] and capacities on Eurofer (2019a).

The introduction of the DRI process into primary steel making is likely to impact supply chain organisation as it has four major impacts on the spatial organisation of supply chains:

1) The switch from coal to hydrogen as a reducing agent creates issues with transportation as hydrogen cannot be transported as efficiently as coal over long continental distances (Day 2022). Local renewable electricity potentials for the production of hydrogen are, therefore, key to achieving a competitive advantage.

2) Existing sintering and blast furnace facilities become stranded. The DRI-EAF route also makes the BOF obsolete. The sunk costs relating to the existing assets of the blast furnace may lead to a delaying strategy by incumbents, but as their business model for CO_2-intensive steel is already being challenged by the EU ETS, the sunk cost problem is reduced and entry into the market by competitors or the relocation of production is facilitated. At a later stage of the transition, hot rolling mills will have to be upgraded

[14] Data collected on the WV Stahl website: https://www.stahl-online.de/startseite/stahl-in-deutschland/konjunkturinformationen/ (accessed during August 2023).

and will require a climate neutral energy source, which will require partial retrofits and therefore decrease the value of these assets.

3) The DRI process does not require temperatures as high as iron reduction in a blast furnace. Consequently, the iron leaving a shaft furnace is solid, in contrast to the liquid iron produced by the BF. If it cools down for storage or transportation, less energy is lost than in the case of the BF/BOF route where the local integration of iron and steel making is key as the BOF requires liquid iron as infeed. The downstream energy integration benefit of the iron reduction step therefore decreases.

4) DRI production yields very few by-product gases which can be completely reused within the DRI process for preheating. In contrast to the BF/BOF route, there are no "excess" by-products that can be used downstream in hot rolling.

Effects (1) and (2) can be subsumed as the breaking of persistence effects and (3) and (4) as the breaking of clustering (energy integration) effects (see also Figure 3). Effects (3) and (4) together loosen the ties between the three main production steps of iron ore production, steel making and hot rolling. Technically, they allow more flexibility in terms of the spatial (and temporal) decoupling of production. Thus, for the introduction of the DRI route, a combination of low persistence effect and low supply chain clustering benefits implies that the DRI production step can be easily separated from the downstream steps and vice versa. On the other hand, the benefits of vertical integration and local production remain, particularly in terms of short lead times and inventory minimisation. A more specific product demands a shorter lead time and a lower inventory. Product specificity is very low at the DRI stage and can be very high at the level of an automotive steel slab – and it increases with each subsequent processing step. This type of supply chain management requirement would have to be weighed up against the limited energy cost benefits and the depreciation of existing rolling mill capacity if the entire supply chain were to be moved to a low energy cost region.

The hypothesis used in the steel production system modelling was that it is very likely that steel production will stay market-near in the future. This, and the respective assumptions in the modelling, were explained by the logics of supply chain management and industrial policy (see section 3.2.4). The PhD work on relocation in the steel industry presented below did not cover the full range of issues raised, but focused narrowly on relocation effects within a European region assuming uniform energy prices.

At the time of writing, most of the steel companies in Europe support the transformation pathway to DRI and have developed corresponding investment plans.[15] The process of electrification has begun, and empirical evidence is now available – an exciting area for further research.

3.3.2 Petrochemical industry

In the petrochemical industry, electrification would also be a strong force for relocation – but there are also strong persistence effects. Currently, the supply chain in the petrochemical industry faces different challenges to that in the primary steel industry. First, the beginning of the supply chain is far more diverse: most petrochemical producers in the ARRRA have formed a synergistic relationship with oil refineries as they rely on the by-products of crude oil refining. However, production sites at the coast within the ARRRA, as well as outside, also use imported feedstock like ethane (a by-product of shale gas extraction), which became available on the world market around 2010 (Cornot-Gandolphe 2013). In China, coal-based routes have also been established (Xu et al. 2017). In the main segment of the petrochemical industry, the supply of ethylene and propylene, there is strong worldwide competition between companies and production routes with volatile price spreads between the different kinds of feedstock (Kim and Oh 2020). As the petrochemical products at all stages of the production chain are homogenous, only production costs rather than product quality influence competition, which is a second significant difference to the steel industry value chain.[16] In the ARRRA, most producers are locked-in to their symbiotic relationship with the refineries and the use of light naphtha and LPG as feedstock for their steam crackers. Due to strong international competition, their profitability is also dependent on revenue from the smaller fractions in their total production yield, such as butadiene or aromatics, where naphtha offers better yields than ethane (Young et al. 2022).

Olefins and butadiene are the target products of naphtha steam cracking and are, therefore, referred to in the literature as high-value chemicals (HVC).[17] However, the naphtha steam cracking route also produces a wide range of hydrocarbon by-products, which are typically burned and used as heat for downstream operations where intermediates and polymers are produced (see Figure 3 above). In the ARRRA, production is not limited to standard commodity polymers; the more energy-intensive "engineering plastics" and polyurethane foams that require aromatics or butadiene as precursors are also produced (see paper IV). The

[15] See the "Green Steel Tracker" (https://www.industrytransition.org/green-steel-tracker/) provided by the Leadership Group for Industry Transition (LeadIT) or Agora Industry's "Global Steel Transformation Tracker" (https://www.agora-energiewende.de/en/service/global-steel-transformation-tracker/).

[16] Impacts on the SDGs associated with production, mainly circularity and carbon footprint, can however still matter as a quality feature.

[17] Benzene, toluene and xylenes (BTX) are other valuable products and are often included as HVCs.

production of these polymers, often with several intermediate steps, and the know-how to build and operate these plants is highly concentrated in a few locations around the world, and ARRRA producers can often realise high margins in these segments. Important customers for these special plastics include the automotive industry and the manufacturers of electrical equipment (Plastics Europe 2022). At least in the ARRRA, downstream petrochemical operations to produce intermediates and polymers are much more important in terms of energy use than their counterparts in the steel industry (i.e., hot rolling and finishing). Therefore, deeply integrated petrochemical parks also use natural gas to fire downstream operations (Scholz et al. 2023). Consequently, gas prices are an important location factor and the petrochemical industry is already under pressure to relocate.[18]

But what about the transformation of the petrochemical industry towards climate neutral production? The path is far from clear, which is another major difference to the steel industry. A roadmap published by the European Commission (2023b) in early 2023, based on work with industry stakeholders, emphasised the diversity of technology options rather than identifying clear 'no-regret' strategies. While this may help stakeholders, particularly at cluster level, to identify options, the surrounding system and the role of electrification in this industry at EU level remains unclear, leaving stakeholders with high uncertainty. This uncertainty hinders decision making.

However, some electrification options are discussed that could, together with the closure of crude oil refineries, create relocation effects in the petrochemical industry. The two main electrification dimensions in the petrochemical industry are feedstock (molecules) and heat supply (see Figure 3 above). In the steel industry, the electrification of basic material production (molecules) is the first priority, and the electrification of heat is the second. In the petrochemical industry, the situation is exactly the opposite. Due to a different temperature range distribution compared to steel, with a lot of steam required at temperatures between 200° and 500°C (see Figure 3 and Bazzanella and Ausfelder 2017), where direct electrification is a low-capex solution, hybrid steam supply can be economically very attractive if companies can switch to electric heating at very low electricity prices at times of high renewable feed-in (Bauer, T. et al. 2022).

For the most energy-intensive step of hydrocarbon feedstock supply there are various options, including increased circularity (waste and by-product upgrading) and biomass use. These potentials could be exploited before choosing electricity-based and CO_2-based synthetic feedstock (Prognos, Öko-Institut and Wuppertal Institut 2021), which are expensive options (see paper IV). In addition, not all

[18] In an empirical study of the US shale gas boom and its impact on energy-intensive manufacturing in the UK, Manderson and Kneller (2020) were able to statistically confirm a relocation effect due to increasing energy price differentials for UK manufacturing firms and found a stronger effect for multinationals.

companies have accepted full responsibility for their products' end-of-life-emissions (scope 3 emissions) in terms of climate neutral production. In their bottom-up analysis of company targets, Bauer, F. et al. (2022) conclude that the awareness of scope 3 emissions is still weak in several parts of the global petrochemical industry. Even if all European oil refineries were closed due to the electrification of the transport sector, the chemical industry could still choose to import fossil hydrocarbon feedstock from countries lagging behind in climate protection or from specialised "feedstock refineries", a picture sketched even in the IEA's (2021b) most ambitious "net zero emissions scenario". Such scenarios, however, neglect the enormous potential of the petrochemical industry to achieve further emissions reductions by binding CO_2 from the atmosphere in their products.

In terms of relocation, synthetic liquid hydrocarbon feedstock or methanol (see Figure 3) are likely to be produced in the world's renewable electricity sweet spots, as the associated transport costs are relatively low (Genge, Scheller and Müsgens 2023) – even using the existing tanker, port, storage and pipeline infrastructure. Olefins and butadiene, on the contrary, are gaseous, meaning their transport costs via tanker are relatively high, making a break-up of the value chain after the production step of HVC less likely. Finally, moving the entire production chain to a sweet spot is more plausible, as polymer granules are very easy to transport. In addition, supply chain management requirements for short lead times are less relevant for petrochemicals due to their homogeneity.[19] For each standard homogenous polymer the market volume is sufficiently large[20], making longer transportation distances and lead times less of a problem. However, the existing plants in Europe that produce intermediates and polymers with their specialised workforce are important assets, much more so than the downstream assets in the steel industry (like hot rolling). Under the assumption that the supply and demand portfolio for polymers does not change dramatically in favour of new polymers, and that the global demand for polymers continues to grow, the hypothesis that HVC and polymer production will still take place in Europe seems plausible. Within Europe, with its existing petrochemical overcapacity, and especially within the ARRRA, with its excellent infrastructure for exchanging products between sites, the question of internal relocation remains an interesting field of study for the PhD.

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[19] In contrast, intermediates such as isocyanates are not transported due to their reactivity and rapid degradation (US Department of health and human services 2018).

[20] According to Plastics Europe (2022), the global market volume of the standard polymer types polyethylene (HD-PE, LD-PE and LLD-PE), polypropylene (PP), polystyrene, PET, PVC, polycarbonate and PMMA is more than 20 Mt per year for each. Polyurethanes, polyamides and ABS are, however, not fully homogenous.

4 Methodological approach

The research questions discussed in chapters 1 and 2 have been raised in a specific project context, working both for and with stakeholders in consulting and transdisciplinary research projects. This context will be presented in the following section. Subsequently, section 4.2 will treat scenario analysis as the core methodical approach used throughout the thesis work and elaborate on the different steps that were taken to develop quantitative scenarios with bottom-up technology models, concluding with an overview of the different model approaches used.

4.1 Transdisciplinary setting

This section presents the stakeholder setting in the ARRRA region around the transformation of the steel and petrochemical industries and hints at the interrelationships between the stakeholders and the stream of projects in which the doctoral research was embedded. The series of publicly-funded research projects and contract-funded consultancy projects listed in Table 1 are part of the Wuppertal Institute's "transformative research agenda"[21], which aims to enable changes in the production systems for basic materials and a sustainable process of transformation towards climate neutral production.

The scope of the projects varied in terms of the industries and regions analysed, with the scope of analysis covering either single clusters or the sub-national, national and European levels. Most of the projects aimed to develop pathways or to outline a future vision. The main methods used were technology assessment and quantitative model-based scenario analysis. Industry pathways were sometimes analysed in the wider context of the whole energy system, and some were industry specific. In all the projects listed, electrification of the steel and/or chemical industries was at least part of the analysis and often the main focus.

[21] "Research at the Wuppertal Institute thus follows a transdisciplinary concept of knowledge: it does not only serve to generate "systems knowledge" (e.g. technological or resource-oriented systems analysis), but also integrates stakeholders in the process of generating "target knowledge" (visions and guiding principles) and "transformation knowledge" in concrete settings of urban or sectoral transitions to sustainability." (https://wupperinst.org/en/research/transformative-research, accessed 24 August 2023)

Table 1: Projects related to the PhD

	Project	Funding agency/client	PhD related topics	Type*)	Transdis-ciplinary	Project duration
1	REINVENT	EU Commission	Steel and petchem pathways	R	X	2016-2020
2	SCI4climate.NRW	NRW Ministry for Economic Affairs	Steel and petchem pathways in energy system context	R	X	2018-2022
3	Decarbonization Pathways for the Port of Rotterdam Region	PoR Authority	Paper II	C		2016
4	SteelLocations	Climate-KIC	Paper III	R	X	2018
5	GHG-neutral Flemish Industry	VLAIO	Initiatives for heavy industry decarbonisation	C		2020
6	GreenFeed	German Ministry for Economic Affairs	Pathways for petrochemical clusters in Germany and the ARA region	R	X	2022-2025
7	Climate Neutral Germany 2050/2045	Agora Energiewende, Stiftung Klima-neutralität	Pathways for the industry in the context of a climate neutral Germany	C		2020-2021
8	RLP-Flex	Ministry for Environment, Rhineland-Palatinate	Scenario for the industry in Rhineland-Palatine until 2050	C		2019-2020
9	H2 Emscher-Lippe	Mercator Foundation	Potential analysis for hydrogen in the industrial Emscher-Lippe region	R	X	2018-2020
10	INFRA-NEEDS	Climate-KIC	Spatially resolved scenarios of European industrial energy demand	R	X	2019
11	Climate Neutral Industry	Agora Energiewende	Technology assessment of steel and petrochemicals	C		2019
12	Breaking free from fossil gas	Agora Energiewende	Steel and petchem pathways in energy system context	C		2022-2023

*) R: Publicly-funded research project; C: Contract-funded consultancy

Source: own compilation.

Table 2 shows that interest in the transformation process goes beyond politics and individual actors: a range of institutional actors with decision making powers on the business side within the region are also involved. This differs from other heavy industry clusters in Europe, where in most cases the relevant company headquarters are not located in the region. These very specific conditions allowed for a transdisciplinary approach involving business actors to probably a greater extent than in other regions. Stakeholders from government, companies and state-dominated companies in the region regularly meet and companies have sufficient resources for lobbying, as well as technical and economic expertise. Apart from the actors listed in the table, local and national trade associations are also located within the region.[22] The opportunities for discussions with stakeholders are, therefore, optimal, and in all the projects listed (except projects 7, 8 and 12), stakeholder interactions were part of the research process. The intensity, however, differed. The transdisciplinary projects (those marked with an x in Table 1) included workshops where stakeholders could shape the scenarios or discuss possible conclusions for their business or for necessary policies. Government officials also make up part of the institutions with decision making power. They were involved, but are not listed individually in the table.

The paramount significance of the "petrochemical triangle" between Antwerp, Rotterdam and Cologne/Gelsenkirchen is mirrored in a cross-border public-private initiative called the "trilateral chemical region", where the Dutch, Flemish and North Rhine-Westphalian governments, companies and infrastructure providers collaborate to exchange knowledge and initiate projects of common interest. Table 3 also lists other selected initiatives where governments and companies work together to strengthen heavy industries. Other recent cross-border initiatives try to develop cross-national hydrogen infrastructure. In addition to the cross-border projects, every region has developed its own hydrogen strategy.

[22] Most German NGOs, however, are located in Berlin and thus outside the focal region.

Table 2: Relevant stakeholders in the steel and petrochemical industries located in the region and their involvement in the PhD-related research projects

Type	Stakeholder	Branch	Headquarters	Involved in project No.*
Companies	BASF	chemicals & polymers	Ludwigshafen	1, 2, 6, 10, 11
	Shell	oil & chemicals	*(The Hague)***	2, 3, 6
	BP Europa SE	oil & chemicals	Bochum***	2, 3
	Covestro	polymers	Leverkusen	2, 6, 11
	Lanxess	polymers	Cologne	2
	Evonik	polymers	Essen	2, 9
	LyondellBasell	chemicals & polymers	Rotterdam	10
	Brenntag	wholesale of chemicals	Essen	
	thyssenkrupp industrial solutions	engineering of chemical plants	Dortmund	2, 9
	thyssenkrupp steel	iron & steel	Duisburg	2, 4, 11
	ArcelorMittal	*iron & steel*	*(Luxembourg)*****	1, 10, 11
	Klöckner	wholesale of steel products	Duisburg	
	SMS	engineering of iron & steel plants	Düsseldorf	
State-owned or state-dominated companies or initiatives	Port of Rotterdam Authority	port operator	Rotterdam	1, 3, 10
	Port of Antwerp Authority	port operator	Antwerp	10
	TenneT	electricity TSO	Arnhem	
	Brightlands Chemical Campus	business development, R&D hub	Geleen	1, 10
Government agencies	Energy4climate.NRW	Green industry transformation and promotion	Gelsenkirchen	2, 6
	PBL	scientific advisor of the Dutch government in regard to environment and spatial planning	The Hague	1
	VLAIO	business promotion	Brussels	5

*) Project numeration according to Table 1; **) until 2021; ***) and Hamburg; ****outside ARRRA, but close.

Source: own compilation

In such exchange formats, companies are usually not allowed to share cost and/or capacity information with other stakeholders, e.g. due to relatively strict competition regulations. Many of the companies listed above have already been investigated by the German Monopolies Commission for illegal price-fixing and some of them have had to pay fines. On the other hand, government officials must assess the appropriate level of financial and regulatory support required by companies to start the transformation. This may explain why, throughout the thesis, the focus in the modelling was on economic criteria.

Table 3: Selected initiatives for heavy industry transformation in the ARRRA

Initiative	Targets	Involved stakeholders	Geographical coverage
trilateral chemical region	Strengthening the chemical "meta-cluster"	ministries, chemical companies, infrastructure providers	Netherlands, Flanders, NRW
VoltaChem	Developing electrochemical business cases for the Dutch industry	TNO, chemical companies	Netherlands
IN4climate.NRW	Strengthening NRW heavy industries on the way to climate neutrality	NRW ministry for Economic Affairs, companies, science	NRW

Source: own compilation.

4.2 Scenario analysis based on bottom-up technology models

In this section, the methodological toolbox developed during the PhD work is presented. Its subsections describe the four subsequent (and partially iterative) steps used to create one or several scenarios for the analysis of the techno-economic industrial production systems:

- System analysis
- Model building
- Use of scenario storylines
- Analysis and learning

4.2.1 System analysis of the production system

Technological transformation analysis requires an understanding of the current system, its stability, its reusability and its convertibility. Therefore, at the beginning of a quantitative scenario building process with engineering-type bottom-up technology models, a system analysis of the techno-economic production system is carried out. The four main steps are shown Figure 6 and are described in the following.

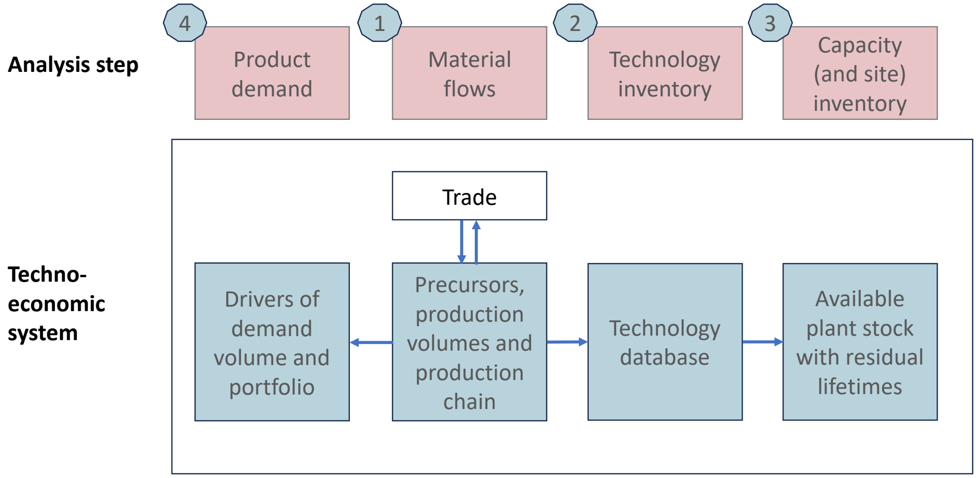

Figure 6: Steps in the system analysis of a techno-economic production system for basic materials. Source: own figure.

The boundaries of such a system usually follow statistical rules that assign the production of certain products to a particular industry. The first task within a material flow analysis (MFA) is to identify the inputs into the system in the form of raw materials or precursors. In the case of precursors, it is necessary to consider whether the industries producing them should be included in the system. In the case of steel and petrochemicals, the relevant upstream industries are coking and crude oil refining, neither of which are statistically part of the two focal industries. In practice, however, they are often part of a vertical integration within a company's production chain or in an industrial park that offers certain synergies. Therefore, depending on the research question, it may be justified to include them in the further system analysis. The next step of the MFA is to explore possible production chains within the industry (i.e., different ways of producing the same or a very similar product) to identify interdependencies between production steps. Once the steps in the production chain have been identified, an analysis of production and trade statistics should follow. The analysis of production is often not possible at national level due to statistical confidentiality, but such statistics are always available at EU level and are sometimes provided by trade associations at national level.

The second step is technology screening. This aims to identify the energy and emissions-intensive production steps with their specific product use (per tonne of target output), by-products, energy requirements and process-related emissions. This type of data is often listed in industry-specific system analysis studies or technology assessment studies. As an intermediate result, this produces a production and trade balance for a geographically-delimited system and along the industry's value chain, which can be used to explain the raw material input and the production quantities of intermediate and target products.

A deeper bottom-up analysis aiming to understand reinvestment cycles requires capacity and age screening as a third step. This analysis includes individual plant capacity and age (commissioning date and dates of major retrofits). If a multi-site model is the objective, it is also necessary to assign the plants to a specific location or local cluster. During the PhD and project work, a proprietary plant database evolved at the Wuppertal Institute, which started with the Rotterdam region, was extended to include several German heavy industries, and later to encompass steel in Northwestern Europe[23] and refinery and petrochemical plants at the European level[24]. The database is based on publicly available data, so there are no restrictions on publication.

These three steps may be followed by an analysis of the type of customers buying the final products. It may not be necessary to explain the industry's current energy use and emissions, but it may be interesting to understand drivers behind demand for a better-informed assessment of future product demand, which is typically an input parameter in the modelling. Customers may also demand different qualities of a product, which is particularly relevant for the steel industry where a particular feedstock or technological route may not be suitable for a distinct steel grade.

The system analysis can be completed by an analysis of the logistics system for raw materials, energy carriers and intermediates. This may include port terminals, pipelines or other infrastructure and is particularly relevant for the modelling of a multi-site production system.

System analysis is a prerequisite for modelling, which is described in the following section. However, these two steps are typically iterative, as hypothesis testing in modelling also validates the system analysis and often raises new research questions that require further and deeper system analysis. The building of a quantitative model, i.e., a representation of the system in the form of equations, starts with a representation of the initial observable technical system and can be seen as a permanent process of observation (data collection) and interpretation (ad hoc

[23] North-Western Europe here comprises France, Belgium, the Netherlands, Luxembourg and Germany.

[24] Europe means in this context the EU27-2020, plus the UK, Norway and Switzerland.

hypothesis building). The hypotheses are tested with redundant statistical data for one or several base years.

4.2.2 Model building

Several models were developed during the PhD work. These follow the tradition of energy system modelling, as the main objective is to investigate the type and amount of energy needed to ensure GHG mitigation over time and climate neutral production by mid-century. They can also be categorised as techno-economic 'engineering' type energy and production system models. This means that they follow a bottom-up philosophy (Herbst et al. 2012, Lund et al. 2017) with regards to the energy-consuming technologies and thus model, at the core, a technological production system with its energy use and GHG emissions consistent with framework conditions such as limited potentials or cost relationships between technologies and energy carriers. Figure 7 displays the modelling framework EDM[25] as it was developed within the PhD at the Wuppertal Institute.

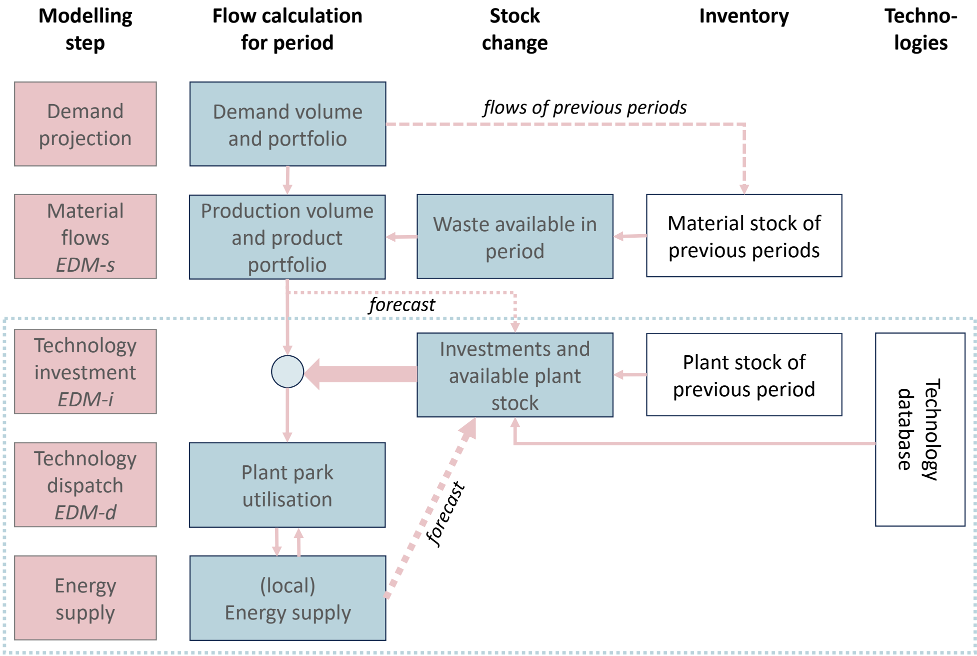

Figure 7: Bottom-up modelling framework of production systems for basic materials (EDM). Source: own figure.

[25] The acronym "EDM" stands for the Wuppertal Institute's modular Energy Demand Modelling platform. The framework presented represents the current states with its modules EDM-s, EDM-i and EDM-d.

The EDM has additional geographical layers (state, NUTS[26]-1 region and site), which are not displayed. They allow for the geographically-explicit modelling of production, energy use and GHG emissions. The core framework representing the production system in a narrow sense is displayed in the lower part of the illustration within the dotted box.

The smallest possible modelling scope is the calculation of technology dispatch with its associated energy consumption and emissions for a given production volume and plant park. To avoid using the term "model", I will refer to such an application as a balancing tool. This is required to validate the technology data in a base year using redundant statistical data on energy use, emissions or production volumes per technology and/or sub-region site. A balancing tool of this type can also be applied to a future system where production volumes and the technology portfolio have been determined ex-ante, as in the case of paper I (see section 5.1).

A next step would be to model the reinvestment cycle (step of "technology investment" in Figure 7), which drives systemic change over time and allows for the combination of the general scenario methods of backcasting and forecasting, and thus to understand a technological system transformation. If technologies are expected to have a certain lifetime, they must be replaced at the end of their lifetime. This is where economic thinking comes in, allowing for the implementation of certain rules to endogenise "decisions". In this respect, bottom-up models follow a "business economics" rather than a "macroeconomic" approach in their simulation (Herbst et al. 2012). Depending on the scenario and model type, the decision about the kind of future reinvestment can be achieved in two ways. This leads to a model differentiation called simulation versus optimisation (Lund et al. 2017, Herbst et al. 2012), or explanatory versus optimising (Börjeson et al. 2006). Due to the ambiguity of the word "simulation" in the modelling context, I will use the latter terminology, but both refer to the same kind of differentiation. In this thesis, both model types as well as mixed approaches were used, as explained in the following. Technology investment and dispatch can be modelled simultaneously as they are interrelated but, in reality, the rationale is different and this can be reflected in the modelling. Investment decisions are based on expected market volumes and associated expected revenues and costs. These decisions are made under high uncertainty. Technology dispatch, on the other hand, operates in the short term within the boundaries of a given plant portfolio (which is, in most cases, not optimal for a given market situation) and thus has to react to changing demand and changing price spreads for raw materials or energy, as well as unexpected external shocks. There are different ways to apply rules in the modelling and different ways of combining the different modelling principles.

[26] NUTS stands for the "Nomenclature of territorial units for statistics" of the EU and the UK.

A further broadening of the modelling scope (outside the dotted box in Figure 7) involves material flow analysis (MFA), which calculates stock inventories of the materials produced that become available as waste or secondary material over time. MFA is a helpful tool to account for a changing potential to use secondary materials over time, but also to better reflect future demand (and trade) volumes.

4.2.3 Applied modelling principles

Explanatory models

In an explanatory scenario exercise, which combines backcasting and forecasting, the modeller should check whether the technology corresponding to the desired target state at the end of the scenario horizon is available in time and to the required extent. To check this, the reinvestment cycle is modelled and checks are carried out to see whether a complete cycle can be run after the technology becomes available. For industrial plants, a 20-year economic lifetime can generally be assumed, but the technical lifetimes are significantly longer and can reach up to 50 years (Schlomann, Fleiter and Eichhammer 2013). The usual way to assess availability is the technology readiness level (TRL), a standardised way of assessing the market readiness of a technology. A TRL may be assessed for the status quo, and the necessary forecasting of the TRL requires specific technology assessment studies or expert judgement. By forecasting the reinvestments, it is possible to check whether the target state can be reached in time or to identify those conditions that should be met at a certain point in time to complete the reinvestment cycle in due time (e.g. acceleration of market readiness, subsidies, prohibition of certain other technologies etc.).

In addition to reinvesting in completely new production facilities, it is also necessary to adapt the energy supply of existing facilities during the transformation, which can often be achieved by minor retrofitting. Vad Mathiesen et al. (2023) provide an overview of the guiding principles that can be used to achieve a rule-based fuel switch.

The quantitative models may be verified in terms of correct operationalisation, but the actual validation (of the scenario) takes place in relation to the set of assumptions, as explanatory models require several assumptions based on expert judgements. One way of providing a framework for such assumptions is the use of scenario storylines (see section 4.2.4), which are also required if an optimising approach is used. However, in explanatory scenarios the need for assumptions is higher, and scenario storylines thus play a more important role.

Optimisation Models

Bottom-up sector models with optimisation are usually used to show a cost-efficient (optimal) development of the industry system, but they may also be used as a way of simulating functioning markets.[27] Börjeson et al. (2006) relate to this distinction by making a further differentiation between “normative preserving” and “explorative”.

In bottom-up energy systems, modellers use optimisation for two reasons: (1) to find a cost-efficient solution for a complex techno-economic intertemporal planning problem (efficiency paradigm of engineers); and (2) to simulate market behaviour. In the former, the model calculates the least cost by making best use of existing assets and accounting for the sunk costs (see section 3.2.1) combined, for example, with a specific production volume and a GHG emissions target as boundary conditions. Perfect foresight is used to derive an optimal pathway. To derive a more realistic result, a simulation[28] based on expectations rather than perfect foresight can be conducted, which is referred to as a myopic approach. The information about existing assets, cost structures etc. is assumed to be perfect. The model explores system behaviour under the assumption of functioning perfect markets under different circumstances, in particular external shocks. If used in such an explorative way, an optimisation model can be a powerful “learning tool” (Börjeson et al. 2006). The underlying core assumptions of functioning markets with perfect information and the homo-economicus paradigm indicate a proximity to neoclassical economic theory (Lund et al. 2017).

Mixed approaches

Optimisation principles were used in the PhD work, but always in mixed frameworks with explanatory principles. Such mixed approaches often use one approach for investment and another for calculating the 'dispatch' of a fleet. As investment is a very complex problem, it is sometimes optimised. In fact, optimisation techniques are better suited to solving dispatching problems because they do not require perfect foresight over a decade or more, which is a very strong assumption. Optimisation in dispatching is helpful to deal with complex production systems where a given portfolio of equipment can be used in multiple ways and the target range of products can be produced in multiple ways. Looking to the future, optimising plant dispatch may challenge an assumption about a particular strategic investment to assess its return. This is close to reality, where managing engineers also use such approaches for actual dispatching at site or company level and for investment planning.

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[27] It is because of this kind of simulation objective that the distinction between explanatory and optimising was preferred.

[28] The word “simulation” is used here in the context of an optimisation approach, and thus has a different meaning than when used in the literature to make the distinction between “simulation versus optimisation” (see above).

Industry system modelling as part of modular modelling projects

The industry system should be seen as part of other larger systems or in relation to other systems. The industry models developed in this thesis rely at their downstream edge on data on future demand for materials and at their upstream edge on the availability of raw materials and secondary materials as well as energy (particularly electricity and hydrogen). In the thesis work, the petrochemical model was coupled with a material flow analysis (see Figure 7) to calculate future demand and waste (see section 5.4). In other project work not included in the four PhD papers, the industry models were also coupled with electricity system models from the Wuppertal Institute, Prognos and Artelys (projects 2, 7 and 12[29]). The stand-alone operation of the models in the PhD thesis benefitted from the experience gained in these model coupling exercises.

4.2.4 Use of scenario storylines

Bottom-up modelling with its demand for many assumptions to be made for the future requires the use of scenario storylines. The consistency and plausibility check of the assumptions is the main stage in quantitative scenario modelling where different theoretical concepts can explicitly or implicitly come into play. A sound scenario storyline should involve the view of several disciplines put forward by scientists or stakeholders. It should describe the surrounding world that is not explicitly covered by the model and provide enough background to explain the numerical assumptions that need to be made to run the model. Based on learning gained from the PhD work, the storyline of a robust scenario can include the following elements from different scientific perspectives:

- Transitions should not overstress stakeholders, i.e., should not require extreme behavioural changes in a short period (social sciences) – or, if significant changes are assumed, they should be justified in the context of social science.
- The pathway should not overstress the capacity of the economy, i.e., should be cost-effective and not demand too much investment simultaneously (economics).
- The scenarios should omit possible fossil lock-in situations but consider beneficial ones (policy analysis).
- Value added in the regions should be retained, if possible, to foster the acceptance of the transformation (social sciences).

[29] Project numbers according to Table 1.

- It requires dialogue and thus takes time to create acceptable solutions for so-called “not-in-my-backyard” (NIMBY) problems (social sciences).

Storylines are not only used to describe the surrounding system; they can also describe strategic decisions in what-if scenarios.

4.2.5 Analysis and learning

The process of analysis and learning begins after the validation phase. During this process, the scenario is improved step by step. Interim results should be discussed within a scientific team including multiple disciplines or with stakeholders to test the validity of the scenario.

4.2.6 Overview of the model types applied in the four papers

Figure 8 provides an overview of how the different modelling challenges were addressed in the four PhD papers. Table entries in brackets indicate that the modelling step was not carried out, but the analysis was at least partly covered in other modelling steps or by alternative tools.

The table describes the journey in terms of modelling development, starting with a technology assessment and a balancing tool for Europe, developing an energy system model for the Rotterdam industrial cluster and a location-specific iron and steel plant investment model, to multi-stage modelling of the geography of the petrochemical production system in Europe, where the integration of individual sites into complex production networks can be analysed. The individual approaches are described in Chapter 5, where the methodological approach of each paper is explained in the context of the research questions and findings.

<table>
<tr><th>Modelling step</th><th>Paper I:
EU Industry</th><th>Paper II:
Rotterdam cluster</th><th>Paper III:
Steel industry in North-Western Europe</th><th>Paper IV:
EU and ARRRA petchem</th></tr>
<tr><td>Demand projection</td><td>-</td><td rowspan="2">(constant production volumes assumed, except for fuels)</td><td rowspan="2">(uncertainties covered by Monte Carlo analysis)</td><td>econometric</td></tr>
<tr><td>Material flows</td><td>(constant production volumes assumed)</td><td>MFA tool</td></tr>
<tr><td>Technology investment</td><td>exogenous
(only plant park in 2050)</td><td>exogenous</td><td>step-wise optimisation based on expectations</td><td rowspan="3">simultaneous optimisation with perfect foresight over a 20-years-period with EDM-I
(energy supply only partly considered)</td></tr>
<tr><td>Technology dispatch</td><td>energy and CO_2 balancing of production</td><td>rule-based & optimisation (refineries) with EDM-d</td><td>(expected opex regarded in invest)</td></tr>
<tr><td>Energy supply</td><td>-</td><td>rule-based:
power plants, CHP, steam, H_2</td><td>(only steel gas economically considered)</td></tr>
</table>

Figure 8: Classification of the chosen model approaches in the papers. Source: own figure.

5 Description of the research process and main findings

As mentioned in the introduction, the research process of this thesis addresses three overarching research questions:

1) How can European heavy industry become climate neutral by 2050 and what is the possible role of electrification in the climate neutral production systems of basic industries?
2) What sustainable strategies can steel and petrochemical companies in Europe and specific clusters adopt to adapt to climate neutral production and specifically to electrification, and how will these strategies interact with the energy system over time?
3) How strong will clustering benefits and possible relocation effects be due to electrification in the two industries and to what extent can the latter be addressed by policy?

Sections 5.1 to 5.5 describe the process of the PhD with a focus on the four core papers of this thesis. They represent major research efforts around the broad issue of the decarbonisation of major basic industries in Europe and its consequences for stakeholders and regions involved. It is a journey from the more general questions of how much electricity will be needed and whether it would be available, to more specific questions about the vertical and locational organisation of two major industrial sectors. At the same time, the research journey includes several scenario approaches, as well as different modelling approaches to analyse the research questions. Finally, I will complete the picture with key insights gained from the broader research that I have conducted in parallel in several research and consultancy projects at the Wuppertal Institute, which have resulted in a number of further publications on related topics. These projects also provided me with much of the data and technological and infrastructural information needed to construct the models used and to feed them with meaningful data from the actual industrial and energy system. Discussions with many stakeholders from industry, government, academia and civil society helped significantly to refine the questions and scenarios for analysis.

5.1 Electrification of the European heavy industry

Even after the 2015 Paris Agreement (which entered into force in 2016), there were few scenarios or visions that depicted the complete decarbonisation of heavy industries. Instead, most of the available studies or roadmaps claimed that even reduction targets of minus 80% would not be achievable with the available technology options, or only by using a huge volume of biomass and depending on carbon capture and storage as an end-of-the-pipe solution (Schneider et al. 2017) – despite the need to change more rapidly and become climate neutral by 2050.

Against this background of an almost complete lack of visions to fully decarbonise heavy industry, paper I undertook an experiment using a straightforward scenario and an engineering approach to clarify the question: “Would electrification be a techno-economically feasible strategy to decarbonise European heavy industry?”

The paper addresses the first research question in the doctoral work, which asks what possible role electrification might play in the climate neutral production systems of basic industries. My work within the paper addressed the core dimension of this question, the technical feasibility. It involved a broad literature analysis of available technologies for electrifying the core processes of basic materials industries and their performance with regards to energy use and GHG emissions, including own calculations based on the literature. The quantitative method used to derive overall energy demand was an energy and GHG balancing tool (see section 4.2.2), which included the main products and core processes of 11 major industries that currently account for more than two thirds of EU industrial GHG emissions. Available electrification routes were technically assessed for those products and a causal chain was implemented calculating energy demand and CO_2 emissions associated with the production activity using both current technology and future electrified processes. This approach can be subsumed as a deductive way of generating insights.

The analysis was carried out using a simple scenario that assumed constant production levels for all major products. This assumption was used: (1) because in recent years European production of basic materials, as well as consumption, has remained largely constant, making such a hypothesis both simple and not unrealistic; and (2) because this assumption enabled the focus to be on changes in production technology and energy supply rather than on changes in production volumes.

Results:

- Significant CO_2 emissions reductions of around 300 Mt per year would be possible in an electrification scenario (71% of scope 1 and 2 emissions in 2010), with a smaller share (85 Mt) remaining as process-related emissions from limestone use that would need CCS.

- Electrification would require an additional 1500 TWh of electricity in industry compared to current volumes, of which almost 1100 TWh in a conservative scenario (which does not assume greater circularity) would be for petrochemical feedstock.
- The additional electricity demand of 1500 TWh, in addition to the current demand of 1000 TWh, would be significant but within the available techno-economic potentials for renewable electricity production in Europe if direct electrification is prioritised over indirect solutions based on synthetic methane.

The analysis of the technical feasibility of industry electrification led to new research questions, which required a broader systemic approach:

- How could electrification progress in the different industrial sub-sectors given the existing technology stock and its investment cycles?
- Electrification will have an asymmetric impact on production costs, so what are the implications in terms of product substitution or changes in demand volumes?
- Electrification will require a massive expansion of renewable energy and electricity infrastructure: will this change location factors to the extent that relocation will occur?
- How will the direct (and indirect) electrification of heavy industry interact with the future evolution of the energy system (given that all other sectors will also follow an electrification path)?
- How can fossil-based industrial sites and clusters reconfigure themselves in the face of the challenges of decarbonisation and electrification of the whole energy system?

To provide useful insights, the more complex nature of these questions required a stronger focus in case studies, either on specific infrastructure, regions or on industry branches, which were followed up in the subsequent papers.

5.2 Reconfiguration of an industrial cluster in the face of decarbonisation and electrification

The subsequent question on the need for energy infrastructure for complete industrial decarbonisation based mainly on electrification was followed up in the context of a Climate-KIC-funded research project (see project 10 in Table 1); that resulted in a publication not included in this thesis[30]. However, the subsequent core research paper of the PhD focused on the decarbonisation of one of Europe's prime industrial clusters, the Port of Rotterdam. The paper is based on my modelling work in the context of a research project on behalf of the port authority.

Paper II represents a step forward in applying the vision of a largely electrified European heavy industry as sketched in paper I to the Port of Rotterdam's industrial cluster; it thereby addresses research questions 1 and 2. Research question 1, concerning the general role of electrification for heavy industries, is addressed not only in terms of technical feasibility, but involves two further dimensions. The first additional dimension assesses the role of electrification compared to biomass and CCS in the context of a local case study, and the second (temporal) dimension develops pathways describing the way to the future system. The Port of Rotterdam is one of the most important petrochemical clusters in Europe and thus also provided an excellent opportunity to address research question 2 by assessing strategic options and windows of opportunities for this industry in the context of the transformation of the local energy system.

The modelling approach used can be qualified as a bottom-up energy system model, with much higher technical and site-specific detail than the tool used in paper I to derive the European scenario. The work done here can be qualified as a Technology Assessment (TA), if this term is used in the wider sense according to Grunwald (2009). It is dedicated to a specific geographical situation, an existing energy supply structure and explores pathways towards different technological solutions that qualify a desired future state. Here, system analysis and scenario analysis come into play. The purpose of the work was to derive "strategic" scenarios (Börjeson et al. 2006) to test the possible impacts of certain core investments under different given external conditions; i.e., different climate policy ambitions. According to Börjeson et al. (2006), scenario building can be seen as a three-stage process aimed at "generation", "integration" and "consistency". In the generation stage, surveys and workshops were used to collect the relevant information. "Explanatory modelling" was then applied in the integration step and workshops were conducted again during the consistency phase. Boundary conditions for the modelling were the evolution of fuel demand in the cluster's market region, the reinvestment cycles for the cluster's core plants, the government's plan to phase out coal-fired power plants by 2030, and the availability of new technologies (TRL) over time and their possible pace of diffusion. The latter was investigated through a literature review and a subsequent survey of relevant companies in the port (power generation, crude oil refineries and chemical producers).

[30] I co-authored a paper by Merten et al. (2020), where I provided extrapolations of site-specific future electricity and hydrogen demands based on scenarios by Material Economics (2019) covering the European steel, chemical and cement industry as a whole.

The key performance indicators to calculate in the modelling were the primary energy demand of the cluster, the local GHG emissions and the timing of the core investments. Intentionally, only scope 1 emissions were calculated, but scope 2 and 3 emissions were regarded in so far as purchases (such as electricity) were assumed to be climate neutral and the products of the port cluster did phase out newly extracted fossil carbon by 2050, in order to ensure neutrality in their use phase.

A formal consistency check was not carried out, but the consistency of assumptions and results was discussed within the project team, with experts from the TU Delft and with stakeholders and the Port Authority when presenting preliminary scenario results in dedicated workshops.

Three of the four scenarios were developed with stakeholder interaction. By contrasting two different "Paris compatible" scenarios aiming for around a 95% reduction in emissions compared to the baseline situation, it was also possible to cross-check strong electrification combined with carbon circularity as a core strategy against a strategy that had a stronger focus on biomass and CCS.

Results:

- A climate neutral local industrial energy system can be achieved within usual investment cycles for key assets and with available technologies, but these must be scaled.
- Biomass and CCS use could be attractive when re-using existing plants, whereas electrification requires a huge overhaul of these production assets.
- The phasing out of local fossil generation of electricity and heat, combined with strong electrification, is turning the cluster from an electricity exporter to an importer.
- Electrification might, however, still be more attractive than biomass and CCS in terms of public acceptance and the long-term stability of the cluster.
- Plastics recycling might be a good complement to a defossilisation strategy for a petrochemical cluster.

New questions that emerged and that were partly addressed by project follow-ups:

- What is the future share and role of hydrogen and direct electrification in the heat supply of the industrial cluster?
- What are the respective infrastructure requirements, both locally at the electricity and gas distribution level, and at the transmission level?
- What are realistic future import options for the port, what kind of new hub functions could become business models (hydrogen, plastic waste, CO_2, DRI, etc.) in a "Paris compatible" scenario, and what kind of new port hinterland relationships could develop?

5.3 The locational structure of future hydrogen-based steel making in Northwestern Europe

Having analysed potential futures of one of the prime petrochemical clusters, the doctoral work focused on the industry with the highest scope 1 and 2 GHG emissions: the steel industry. The analysis included here emanated from several studies on a climate neutral European and German industry where I was responsible for modelling the steel sector, and which had already shown that for the steel industry the conversion of primary production from the coal-based BF/BOF route to hydrogen-based DRI, in combination with electrified steel making, would probably be the most attractive route to full decarbonisation.[31] The question, already identified in paper I, of how such decarbonisation would affect the configuration of an industry in terms of where it locates its production steps and routes became more and more interesting. The third paper thus addresses research question 3, which concerns how strong the clustering benefits and possible relocation effects due to electrification might be and sheds light on the following sub-questions: (1) how might supply chains be re-organised in an electrified future steel production system and what might be the effect on the associated port-hinterland relationships; and (2) whether possible locational disadvantages might be compensated by company or policy measures.

A new modelling approach was developed for paper III, which can be qualified as an investment simulation. The greater complexity of the system analysed was driven by the main research question, which necessitated a multi-site and multi-product model. This model had to account for a geographical dimension and a multitude of process steps and target products (of hot rolled steel). The analysis also included secondary steel making in electric arc furnaces (EAF) and a likely increasing market share of secondary steel making over time. A linear cost-optimisation procedure was implemented to reach a higher degree of model endogenisation in order to cope with the increased complexity.

In the underlying system analysis, key production steps and their respective production capacities at concrete sites were identified. In the model building, theoretical concepts of neo-classical economics are explicitly integrated into the functionalities of the model, with perfect information about the present and rational behaviour (homo-economicus paradigm), but without perfect foresight. The relative simplicity of neoclassical theory makes it easy to operationalise in an optimisation model. The regional scope of the study was delimited to Northwestern Europe (France, BENELUX and Germany), which was identified as a possible front running region in a lead market for green steel. The model minimised total cost of ownership, a common indicator in investment planning, to rate the economic viability of an

[31] See projects 1, 2, 7 and 11 in Table 1 and section 5.5.

investment. In addition to the capex of key processes, the opex and specific transport costs of raw materials, intermediates and products were taken into account for all sites. Its special feature, developed to address the research question and completely new to energy system modelling of industrial sectors, was its ability to account for the vertical integration of production at sites, which typically offers both logistical and energy integration benefits. The Climate-KIC project funding[32] provided not only financial support, but also better access to industry stakeholders to validate the assumptions and, more importantly, to challenge the modelling approach.

The analysis finally produced a scenario showing a complete shift in primary steel production to hydrogen-based DRI production (H-DR) by 2040 and contrasted it with a business-as-usual scenario to identify possible differences to existing trends in relocation. Drawing on the hypothesis that business cycles or structural crises in the demand for certain steel products might be highly relevant drivers of relocation if coinciding with electrification, a variety of sensitivity tests were carried out: these were in the form of a Monte-Carlo analysis with a random-based variation of parameter values, such as the demand for different steel products over time, the interest rate or scrap availability. As future investments were modelled using a myopic approach, i.e., based on expected futures instead of perfect foresight, the model also accounted for possible capital misallocations due to imperfect information about the future.

Results:

- Inland steel sites, i.e., the hinterland of the ports, could successfully invest in hydrogen-based steel making if the hydrogen price was equal throughout the region. This would require relevant infrastructure, in particular hydrogen pipelines, as a crucial enabler.
- The presence of the steel industry does not guarantee that the demand for hydrogen in the port hinterland will reach a critical mass that will make the relevant infrastructure economically viable; there are risks of underutilisation due to business cycles or market crises (as well as DRI imports, although these were not explicitly analysed).

Further research questions arising from the analysis and additional project work:

- What kind of relocations of iron or steel making within Europe could occur?
- What difference could potential DRI imports to Europe from sweet spots with very low renewable energy generation costs make in terms of the necessary DRI capacities at European sites?

[32] See project 4 in Table 1.

- What are the possible interconnections between electrification and a circular economy; will or should electrification foster secondary production?
- How flexible could future European production be in terms of make-or-buy (e.g. of DRI) and also product storage, and what would this mean for hydrogen demand, hydrogen infrastructure capacity and the required DRI capacity, as well as for competitiveness?

5.4 Impacts of defossilisation on petrochemical production networks

The analysis of the potential effects of decarbonisation on the vertical and locational organisation of the steel industry produced very interesting results and also addressed pressing location-related questions in the second focus industry of the PhD, the petrochemical industry. However, the industry is far more complex than steel making with many production routes producing many products from a smaller number of raw materials. These routes are closely interlinked, closely interact with each other and have many substitution options and several production steps from the raw materials to the final product. A detailed model of the petrochemical sector, modelling the different production steps and the supply chains, as well as the interactions between them, goes far beyond other existing industry models and should also deliver more differentiated answers to research questions 1 and 2, which concern technical feasibility and strategic options for companies. Chapter 2.2 also illustrated that the ARRRA "meta-cluster" has huge stakes in this industry, representing about half of the European petrochemical production. To address research question 3 more specifically and to consider the future competitiveness of the ARRRA, a spatial focus limited to Northwestern Europe would not be sufficient. A more powerful model than the one devised to model the steel sector (described above) was required to analyse the interrelationships between plastics demand in Europe as a whole and the production system, with its production networks and local clusters. While I had developed the steel investment model as a stand-alone PhD project and coded it myself in R, the petrochemical model was developed using a new software platform, coded in Python, which allowed for modularity, better intersubjective understandability and better evolvability. It included a more powerful solver to tackle the more complex optimisation problems, as well as synergies with other model projects at the Wuppertal Institute. I conceptualised the new model and carried out most of the data research required for parameterisation and model validation, but the coding was done by one of the co-authors of paper IV.

Whereas the steel production system model developed in paper III can be rated as an investment simulation approach, the procedures developed for the analysis of the petrochemical sector's transformation as analysed in paper IV use perfect foresight as a feature and can thus be qualified formally as a "normative preserving" approach according to Börjeson et al. (2006), see section 4.2.3.2. The model covers the petrochemical system in Europe, starting with the refineries and port terminals as the sector's offspring, to steam crackers and downstream production facilities that produce intermediates, and ultimately to polymers. The existing assets are attributed to sites, and the sites are partly interlinked by infrastructure (pipelines, shipping routes) that allow for low costs when exchanging goods or intermediates between these sites. In contrast to steel, the petrochemical industry scenarios envisage different energy costs according to the region. This approach is explained by the larger area covered (EU27+UK+Norway+Switzerland, as opposed to Northwestern Europe), and the fact that, in addition to hydrogen (which can be transported relatively easily via pipelines within Europe), electricity is likely to play a much more important role in the chemical industry, especially in the future provision of heat. In the case of electricity, the procurement costs for companies already vary considerably from region to region. The model developed (EDM-i[33]) optimises the European petrochemical production network by minimising the total discounted system costs, while ensuring that the required portfolio of different polymers is produced in each modelling period.[34]

Stakeholders were involved in different steps of the model and scenario building. The modelling concept and scenario storylines, as well as a concept for the analysis of the results, were validated in two workshops under Chatham House Rules with several company and trade association experts. Results from the model have already been used in various projects and were discussed with representatives of companies, the trade association and scientific partners in a joint online workshop.[35]

In paper IV, one main scenario was developed which was complemented by various sensitivities, which are essentially stress tests that show the possible utilisation rates of plants in situations where market imbalances occur.

[33] The acronym "EDM-i" stands for the "invest module" of Wuppertal Institute's modular Energy Demand Modelling platform (see section 4.2.2).

[34] To calculate scenarios for the future demand of different plastic types and the future availability of plastic waste, I developed a material flow analysis (MFA) tool in Excel. The EDM-i is further refined for the petrochemical industry in the GreenFeed project (see project 6 in Table 1) and will also be adapted to simulate the evolution of the European steel production system in a subsequent research project.

[35] The model was used in projects 1, 2, 6 and 7 listed in Table 1. The validation work with stakeholders was carried out in project 2.

Results:

- In terms of research question 1, the scenario developed demonstrates the technical feasibility of a defossilised European plastics production system in 2050. It is not the first scenario of its kind, but it is much more differentiated than other scenarios in the literature (Bazzanella and Ausfelder 2017, VCI and VDI 2023, Kätelhön et al. 2019), as it is simultaneously specific about feedstock requirements due to a target portfolio of polymers and about geography (Europe and its production sites).
- The scenario developed also addresses research question 2 by presenting a pathway and the specific challenges that occur over time, including investment requirements and a marginal cost analysis. It shows that different polymers will experience significantly different price increases (from a doubling to a tenfold increase), which is a strong indication of future substitution effects between polymers towards those with lower price increases.
- Finally, the paper also provides insights into possible future relocations connected to the defossilisation of the petrochemical industry (research question 3). This indicates that the ARRRA meta-cluster could lose competitiveness compared to other European regions if it does not succeed in lowering electricity prices for industry; e.g. by increased supply and/or flexible demand.
- The deep horizontal integration of the ARRRA could still be a stabilising factor, but this horizontal integration would probably be challenged by product substitution, as the production costs of some of the specialty polymers in which the ARRRA plays a dominant production role could become prohibitively high.

Further research questions:

- The scenario analysis identified several techno-economic challenges to overcome, particularly for sites in the ARRRA meta-cluster. These include the development of a more carbon-efficient system with efficient monomer recycling routes and by-product upgrading to reduce the need for expensive electricity-derived feedstocks and associated production costs.
- An even more important issue was identified: the efficient electrification and flexibilisation of heat supply in the petrochemical industry could rapidly decrease natural gas demand and lead to deep GHG emissions reductions. This is because the electricity available during periods of high renewable infeed could be efficiently used in hybrid steam supply systems combining heat pumps and electrode boilers with back-up solutions using

storable chemical energy carriers such as chemical by-products, natural gas and increasing amounts of hydrogen – a research issue addressed in project 12[36].

5.5 Additional key insights from the project work

In addition to the insights gained from working on the papers, I would like to highlight three key insights that were gained from working on other research and consultancy projects. These insights became very important for the work on the papers.

- INFRA-NEEDS (project 10[37]): The project demonstrated a bad fit of local renewable electricity potentials and the energy needs of heavy industry hot spots (see Figure 4 above), which could cause relocation (see chapter 3). On the other hand, there is a good fit of existing gas transmission infrastructure with local potential hydrogen requirements of heavy industries, which offers the repurposing of gas transmission pipelines to become a "hydrogen backbone".
- Climate Neutral Germany 2050/2045 (project 7): The steel and chemical industries could become possible frontrunners to achieve the sector and overall GHG mitigation 2030 targets in Germany (and Europe). This could be possible due to the rapid electrification of these industries, which requires only a limited infrastructure extension for hydrogen and electricity transmission lines. The time-consuming strengthening of the distribution grid is not necessary in the short term. Together with the first insight above, this encouraged the assumption in papers III and IV of the rapid introduction of a hydrogen backbone linking the steel and petrochemical industries with electrolysers, port terminals and geological storage sites. The two focal industries could, therefore, compensate for the assumed slow action in the building and transport sectors, as well as in the minerals industry.
- Climate neutral industry: (project 11): The project showed that the CCU narrative in the steel industry was largely a myth, as the same amount of GHG mitigation can be reached with H-DR and lower associated costs. In addition, CCU with fossil carbon will not be attractive for the chemical industry. This insight encouraged the approach in paper III to assume a complete transformation of primary steel industry to DRI-based steel making.

[36] Project numbers according to Table 1.

[37] Project numbers according to Table 1.

5.6 Methodological reflections

The scenario technique, with its three steps of system analysis, modelling and analysis/learning (see section 4.2), is suitable for application at several stages of transformative research. The Wuppertal Institute's research agenda specifies four stages for its transformative research concept:

- Problem analysis
- Vision development
- Experiments
- Diffusion & learning

Table 4: Scenario types and related modelling approaches applied in the four PhD papers

Paper	Research questions	Transformative research contribution	Scenario type	Model type
Paper I (2016)	How much electricity will it take to electrify? Which technologies are available?	Problem analysis & vision development	Normative/ transforming	Balancing tool
Paper II (2019)	How can the industry cluster adapt to the Paris ambition of climate policy? Which are the technology/investment pathways?	Problem analysis & vision development	Explorative/ external & strategic	Bottom-up technology model
Paper III (2022)	How could steel sites evolve in the context of electrification? What is the impact of electrification on the competitiveness of sites?	Experiment	Explorative/ external	Investment simulation with optimisation (based on expectations, no perfect foresight), stress tests
Paper IV (forthcoming)	What might efficient production networks for polymers look like in the future? Can the ARRRA cluster remain competitive?	Problem analysis, vision development & experiment	Normative/ preserving and explorative/ external	Total system optimisation with perfect foresight and stress test simulation

Source: own compilation, scenario classification according to Börjeson et al. (2006).

Illustrated by Table 4, the PhD work can be seen as a journey along three of the four stages, with a focus on the second and third stages. The fourth step is still to be taken in a transformative research project such as GreenFeed (project 6 in Table 1).

Roadmaps have become a common tool for industry stakeholders to demonstrate that their existing business and assets can be made sustainable. They are a means of providing a vision, not only of the destination but also of the journey. Roadmaps are used in public relations, financing, approval processes and in research and development fundraising. The official industry roadmaps are usually produced by the trade associations themselves or by consultancies, such as Boston Consulting Group, Accenture or Deloitte (Eurofer 2013, Cefic 2013, Accenture 2017, Eurofer 2019b, VCI and VDI 2023) and tend not to go beyond what has already been discussed in the public discourse. Bottom-up models (including the optimisation type) used in interdisciplinary and transdisciplinary research projects can add considerable insight beyond existing knowledge. Their use requires multi-step iterative scenario building that considers whether the original assumptions taken are still valid or whether the model results indicate that they should be challenged. From a modeller's point of view, this kind of iterative approach may be seen as "clumsy", but it offers enormous learning potential, especially when the challenge to the original assumptions is discussed in a multidisciplinary group or with stakeholders. The use of bottom-up technology models throughout the PhD work often revealed limitations in the existing technology assessment literature and in the usual technology databases on which the models are based. For this reason, it was often necessary to draw analogies when analysing the possible transformation of an existing industry. Examples include the reuse of existing gasification units or steam crackers, the use of biochar in electric iron smelters, the use of bio-syngas as a reducing agent for DRI, or climate neutral benzene production. System analysis and modelling identified the need for solutions in these cases, but they had not yet been identified by technical research as relevant parts of future business models or parts of a technical vision. Therefore, scientific roadmaps developed with bottom-up models, as described in papers I, II and IV, are an important complement to industry roadmaps and the engineering literature, as they can make new links to relevant systems (e.g. by introducing "electrification" as a new link between industry and the electricity system), add additional stakeholder positions (e.g. governments, workers, civil society) and thus better offer new solutions and challenge the overall sustainability of future production and business models proposed by the industries in their roadmaps.

The experimental stage of transformative research is difficult to address in the case of the transformation of heavy industry, as billions of euros of investment are at stake from the outset.[38] Simulations such as those carried out in papers III and IV can help to gather knowledge about how a system change can occur and what kind

[38] Eurofer reports that total investment of €31 billion is needed by 2030 to kick-start the steel transformation in Europe (https://www.eurofer.eu/issues/climate-and-energy/maps-of-key-low-carbon-steel-projects/, accessed at 21 August 2023). Individual plants have already received state funding approvals of up to €2 billion (https://ec.europa.eu/commission/presscorner/detail/en/ip_23_3928, accessed at 21 August 2023).

of impacts it can have, e.g. locational effects. However, learning from paper III highlighted that exploratory discussions about uncertainty, instability or cycles are difficult topics for most stakeholders. Engineers in both industries are used to running their plants at full capacity and one political claim often made is the need for "investment security". Government officials in the area of energy and industrial policy were also not used to discussing economic cycles or instabilities. However, following the Russian military campaign against Ukraine that started in early 2022, stakeholders became more interested in issues such as geopolitical instability. A mix of quantitative scenarios and qualitative workshops could be a good way of addressing these needs. If having steel and chemical production capacity in the country is seen as a public good, a model-based stress test together with industry stakeholders might be a good way for political stakeholders to better understand the real impact of a disruption such as electrification in the context of instable markets or trade relations. It could also help politicians better understand how to define and operationalise the actual public good.

The use of an optimisation model (paper IV) facilitated an informed discussion with stakeholders on the critical issue of possible relocation in a Chatham House format. The basic industry stakeholder arena is dominated by senior engineers. This group is used to cost-optimisation as a key performance indicator in their internal strategic supply chain management. As they perceive cost-optimality as their main driving force, they are likely to accept a theoretical concept in a model that assumes this – as was the case with the petrochemical production system model. Having accepted the theoretical concept behind the model as an appropriate rationale, stakeholders had to react to the results presented without criticising the core methodology, thereby revealing additional information about their motivations and the value of their assets. On the other hand, when civil society stakeholders participated in workshops, in most cases these were dedicated, exclusive formats for exchange. The main motivation was the experience of asymmetric information between industry and NGOs, where industry stakeholders tend to dominate the discussion in joint formats. Therefore, in the workshops with industry – which took up most of the time in the stakeholder exchange – the scientific side also had to represent the interests of civil society.

5.7 Summary of main findings

Electrification is a feasible strategy for defossilising heavy industry in Europe and offers reasonable efficiency gains and good acceptability compared to other strategies, such as extensive biomass use and/or CCS. It will require huge amounts of additional renewable electricity and its implementation needs to be studied at high spatial and temporal resolution and requires local case studies. Electrification will require huge investment in the plant fleet of heavy industries. In the steel industry, these investments need to be implemented within the relatively short timeframe of 20 years. However, the related investment required in the overall energy system is much higher: significant investment will be needed for renewable power generation, electrolysers, transmission lines and pipelines. However, there are excellent early opportunities for direct electrification, particularly in the chemical industry, that are flexible enough to support the expansion of renewables and offer good business models. The ARRRA, in particular, requires cheap renewable electricity and a market design that rewards flexible demand to kick-start electrification.

In terms of hydrogen infrastructure, there is a good match between existing gas infrastructure and industrial sites. It is, therefore, relatively straightforward to establish a hydrogen infrastructure exclusively for the steel and petrochemical industrial clusters by repurposing existing pipelines. However, its use and the corresponding return on the required investment in electrolysers is not guaranteed, as there are many ways in which a future production system could develop.

Electrification, whether direct or indirect, will change the way plants are operated and is also likely to change the spatial organisation of supply chains. In the PhD work, some new relocation drivers and some existing retention drivers were analysed. According to the model-based scenarios, electrification will increase existing relocation forces, and the occurrence of strong business cycles or geopolitical crises affecting the two focal industries would most likely accelerate such a development – but not only in an electrification scenario. However, the actual scope of future relocation and the point at which supply chains may break up is not clear and depends also on other factors that were not explicitly analysed in the thesis.

Directionality and possible future path dependencies can be identified for the steel industry, which has committed itself to hydrogen-based steel production as its main pillar. Scenario work and technology assessment have shown that the alternative of CCU in the steel industry and a possible future synergy between the steel and petrochemical industries is largely a myth: it would be very expensive and unattractive for the chemical industry to absorb the fossil carbon discarded by the steel industry. The petrochemical industry, on the other hand, still lacks such a direction. In addition to its hope for a prolonged fossil future, there are the two main defossilisation paths already outlined in the study for the Port of Rotterdam. The first is based on the continued import of hydrocarbon carriers, such as synthetic feedstock or biomass, while the second could be described as a lean carbon strategy, relying more on secondary materials and more efficient carbon conversion into products. Both strategies have advantages for a port operator such as the Port of Rotterdam Authority, but the actual future mix is not yet clear. For the operators of the ARRRA petrochemical plants, recovery of well-sorted waste streams and recycling of monomers are likely to be crucial to be competitive with fossil production and avoid heavy product substitution. The extent of carbon looping and the respective local need for hydrogen versus hydrocarbon feedstock imports is far from clear and may also depend on the local production portfolio and energy system. However, by around 2030, large scale reinvestments will be required at many locations, leading to certain path dependencies with respect to CCS, hydrogen use and direct electrification.

In terms of the methodological findings, the use of explanatory (assumption-based) bottom-up models in transdisciplinary road mapping processes were shown to be valuable. In such settings, they can be combined with optimisation tools that visualise the possible impact of certain investments on plant dispatch or in different market situations. Models that also optimise investments can still be useful, but they should be seen as an auxiliary tool in an exploratory research process, as a possible stimulus for discussion with and between stakeholders, and as a learning tool. According to the experiences gained in the project work, they may be useful in situations where there is an asymmetric distribution of information between different stakeholder groups, and where the 'privileged' stakeholder group (i.e., usually industry) wishes to prevent an informed discussion, typically to obtain more state aid or their preferred regulations. In such situations, the presentation of a cost-optimised scenario may encourage industry stakeholders to reveal their interests and motivations by confronting them with a scenario based on their claimed rationale of cost-optimisation. This may allow for a more informed discussion and result in a refined scenario, either assumption-based or cost-optimised, but with strong exogenous constraints. Several iterations may be necessary to cope with the bias introduced by the original neoclassically-inspired cost-optimisation framework.

6 Conclusions from the research process and recommendations for future research

At the end of a PhD journey with transdisciplinary ambitions, the question arises as to what transformative science might have achieved or perhaps even 'solved' during the doctoral research period. To start with the good news: although none of the large DRI plants announced by the major European primary steel producers has yet come on stream, the expectations of steelmakers and governments in Europe have been successfully anchored in a future DRI-based production system. Companies are also carefully considering the increased use of scrap, and there is a growing expectation that a carbon neutral and more circular system can be achieved by 2050 – or perhaps even earlier.

In particular, the pathway study described in paper II helped the Port of Rotterdam to create a strategy and take a proactive role in the transformation of the industrial production system in the port region and the port hinterland. The Paris-compatible scenarios developed in this work were used as inspiration, or even as a quantitative basis, to start infrastructure planning processes and strategic thinking about new business models and value chains in the port cluster and about new hub functions of the port for climate neutral products. The Port Authority's decision to be proactive, rather than to adopt a delaying strategy aimed at preserving established business models, allows incumbents in the port hinterland to confidently seek early solutions in the global market and promises access to the North Sea energy region, helping to accelerate change across the region.

I am also confident that research into industrial decarbonisation, including my own work, has deepened our understanding of the production networks and value chains affected by electrification. It has become clear that the production costs for some specific high-value products in the petrochemical industry would increase significantly. From the industry's perspective, further research is needed to counter this increase and the related possible substitution effects. On the other hand, the SCI4climate.NRW project initiated a discussion on possible relocations of industrial production (Samadi et al. 2021), which is being discussed more specifically for steel, also under the heading of "green iron trade" (Agora Industry and Wuppertal

Institut 2023). This discussion also emphasises the associated opportunities for reducing the cost of climate neutral products and increasing competitiveness.

However, in the petrochemical industry, there are few clear shared visions regarding future development in the context of climate neutrality. The EU chemical roadmaps are far too open to lock in expectations. The openness of its future feedstock supply in terms of biomass availability, the intensity of circularity, the availability of fossil and synthetic feedstocks, together with uncertainty about future market volumes and product portfolios, prevents the chemical industry from developing a clearer direction (in contrast to the steel industry). Probably the most important issue to address regarding the future development of the petrochemical industry is to make clear that the defossilisation of its feedstock is a necessary part of climate neutrality and could be operationalised, for example, through a tax on the use of fossil resources to complement the existing EU ETS. There is still a need for further research into carbon loops: firstly into the intensity of carbon looping and by-product upgrading within the petrochemical industry, and secondly into the systemic assessment of CCU projects, e.g. related to waste incineration, where many local investments in waste incinerators are at stake. There is no general lack of road mapping work in the chemical industry, at least at national level in Germany (Geres et al. 2019, VCI and VDI 2023), the Netherlands (Stork et al. 2018) and Flanders (Deloitte et al. 2020). However, concrete visions or plans are still lacking at the company and cluster level, a shortfall explicitly identified by Janipour et al. (2022) in their study on the Dutch Chemelot cluster. It could thus be helpful to initiate cluster-specific vision creation and road mapping embedded in broader system analysis and scenarios.

Encouraging efforts are being made at European, Dutch and German level to install "hydrogen backbones", i.e., transmission pipelines. Such hydrogen infrastructure has the character of a public good, maintaining a diversified heavy industry structure in the region to enable new production routes and hydrogen-based business models. However, the German government has recently abandoned its ambition to establish a national grid operator to treat this investment as a public good, regarding the issue as a private initiative for the gas transmission grid operators. The steel industry is often cited as an enabler for a business model around such a grid. It is argued that it could secure high volume demand, thereby offering robust revenues for early developments in grid operation and hydrogen production. This view is perhaps overly optimistic and overlooks two aspects: (1) the steel industry is very cyclical; and (2) it is likely to operate much more flexibly in the future than it does today – which in turn has the potential to mitigate business cycles that are mainly driven by today’s inflexible production assets. DRI could indeed revolutionise not only the technical process of steel making, but – due to the flexible way it can be operated in volatile markets – also business models and the organisation of the supply chain. This thesis could only hint at these challenges and opportunities, but future research should explicitly address plant operation in a volatile environment (economic and political). Such research would require more collaboration between industry and electricity system modelling but could build on the concept of stress testing presented in the thesis and on the vast experiences with electricity market modelling in a high temporal resolution. Even if not fully used by the steel industry, a hydrogen infrastructure could be of value in the energy system. In the 2030s, "excess" hydrogen capacity – if it exists – could be used to decarbonise the chemical industry's steam supply. In hybrid steam supply systems with electrode boilers, as well as heat pumps and a combustion-based back-up, hydrogen could be used instead of natural gas in the back-up section during periods of low renewable electricity infeed. In the long term, hydrogen will inevitably be required to back up the electricity system.

This thesis analysed the possible relocation effects of electrification – especially within Europe, which is an important limitation. At the end of the journey, it is still not possible to quantify the possible effects. In addition to electrification with a strong relocation force (especially in the context of strong business cycles or crises) and other factors already discussed, there are additional factors that are probably equally important – including individual company performance and a skilled workforce, to name but a few.

A dedicated steel industry value retention strategy for the ARRRA region, if politically accepted, should probably focus on steel making rather than on green iron production via DRI. The planned and publicly funded DRI plants, with their limited capacity, may act as insurance for the incumbents against supply chain risks in a future DRI market (global or European), but the more important strategy to implement in the ARRRA region is investment in electric arc furnaces or iron smelters to create possible lock-ins to retain steel production in the region. A frontrunner strategy, which creates sunk costs and an associated competitive advantage, may work for the steel production stage, but not for DRI production, which is much more opex-dominated. This possible ARRRA mid-term priority contrasts with the global steel industry, where the move to DRI is the most pressing issue. For the ARRRA, this means a strong focus on direct electrification with a corresponding need for large amounts of cheap electricity. In the chemical industry, the situation is similar: energy-intensive downstream equipment, such as the polymerisation of engineering plastics, requires large amounts of steam, which can be efficiently provided by electricity. A massive supply of renewable electricity in the region and strong transmission grids are, therefore, far more important than an extensive hydrogen network and should be given clear priority in grid planning and financing.

However, the relevance of an industrial policy to retain production steps in the region is linked to other transformation processes. A successful transformation of the automotive industry in Western Europe is probably an important prerequisite to support the business model for future green primary steel production in the ARRRA, and for the petrochemical industry it may at least be a relevant driver.

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Interaction between defossilisation of basic industries and relocation

Author Clemens Schneider.

The cross-border heavy industry cluster around Antwerp, Rotterdam and the Rhine-Ruhr area is the industrial heart of Europe. The production sites for primary steel and petrochemicals have historically grown up around the coal deposits and the infrastructure for processing crude oil. This dissertation asks how the production of basic materials can become fossil-free in this region, which is still locked into fossils. Yet many people in the region are thinking about electrification as a way to defossilise production, whether they are business leaders, workers, politicians or researchers. Can they use their existing production facilities, infrastructure and skilled workforce to become a driver of defossilisation?

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